
IDAES Documentation

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IDAES team

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CHAPTER 1

Project Goals

The Institute for the Design of Advanced Energy Systems (IDAES) will be the world's premier resource for the development and analysis of innovative advanced energy systems through the use of process systems engineering tools and approaches. IDAES and its capabilities will be applicable to the development of the full range of advanced fossil energy systems, including chemical looping and other transformational CO₂ capture technologies, as well as integration with other new technologies such as supercritical CO₂.

CHAPTER 2

Collaborating institutions

The IDAES team is comprised of collaborators from the following institutions:

- National Energy Technology Laboratory (Lead)
- Sandia National Laboratory
- Lawrence Berkeley National Laboratory
- Carnegie-Mellon University (subcontract to LBNL)
- West Virginia University (subcontract to LBNL)
- University of Notre Dame (subcontract to LBNL)

CHAPTER 3

Contact, contributions and more information

General, background and overview information is available at the [IDAES main website](#). Framework development happens at our [GitHub repo](#) where you can [report issues/bugs](#) or [make contributions](#). For further enquiries, send an email to: [<idaes-support@idaes.org>](mailto:idaes-support@idaes.org)

4.1 Installation

To install the IDAES PSE framework, follow the set of instructions below that are appropriate for your needs and operating system. If you get stuck, please contact idaes-support@idaes.org.

The OS specific instructions provide information about optionally installing Miniconda. If you already have a Python installation you prefer, you can skip the Miniconda install section.

Note: IDAES supports Python 3.6 and above.

System	Section
Linux	<i>Linux</i>
Windows	<i>Windows</i>
Mac OSX	<i>Mac/OSX</i>
Generic	<i>Generic install</i>

Warning: If you are using Python for other complex projects, you may want to consider using environments of some sort to avoid conflicting dependencies. There are several good options including conda environments if you use Anaconda.

4.1.1 Windows

Install Miniconda (optional)

1. Download: https://repo.anaconda.com/miniconda/Miniconda3-latest-Windows-x86_64.exe
2. Install anaconda from the downloaded file in (1).

3. Open the Anaconda Prompt (Start -> “Anaconda Prompt”).
4. In the Anaconda Prompt, follow the *Generic install* instructions.

4.1.2 Linux

Install Miniconda (optional)

1. Download: https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
2. Open a terminal window
3. Run the script you downloaded in (1).

Install Dependencies

1. The IPOPT solver depends on the GNU FORTRAN, GOMP, Blas, and Lapack libraries, If these libraries are not already installed on your Linux system, you or your system administrator can use the sample commands below to install them. If you have a Linux distribution that is not listed, IPOPT should still work, but you the commands to install the required libraries may differ. If these libraries are already installed, you can skip this and proceed with the next step.

Note: Depending on your distribution, you may need to prepend `sudo` to these commands or switch to the “root” user.

apt-get (Current Ubuntu based distributions):

```
sudo apt-get install libgfortran4 libgomp1 liblapack3 libblas3
```

yum (Current RedHat based distributions, including CentOS):

```
yum install lapack blas libgfortran libgomp
```

Complete Generic Install

Follow the *Generic install* instructions.

4.1.3 Mac/OSX

Install Miniconda (optional)

1. Download: https://repo.anaconda.com/miniconda/Miniconda3-latest-MacOSX-x86_64.sh
2. For the next steps, open a terminal window
3. Run the script you downloaded in (1).

Complete Generic Install

Follow the *Generic install* instructions.

4.1.4 Generic install

The remaining steps performed in either the Linux or OSX Terminal or Powershell. If you installed Miniconda on Windows use the Anaconda Prompt or Anaconda Powershell Prompt. Regardless of OS and shell, the following steps are the same.

Install IDAES

1. Install IDAES with pip:

```
pip install idaes-pse
```

2. Run the *idaes get-extensions command* to install the compiled binaries:

```
idaes get-extensions
```

Warning: The IDAES binary extensions are not yet supported on Mac/OSX

Note: If you are installing on Linux, you can specify a specific platform. While most Linux builds are interchangeable, specifying a build can make managing dependencies considerably easier. By default Linux will use the CentOS 7 build. To specify a build use the command `idaes get-extensions --platform <platform>`. Supported Linux platforms are: `rhel6`, `rhel7`, `rhel8`, `centos6`, `centos7`, `centos8`, `ubuntu1804`, `ubuntu1910`, and `ubuntu2004`. If you are not using a supported platform, everything should still work, just choose the platform that best matches your Linux distribution. You can also use the `idaes get-extensions-platforms` command to see a list of supported platforms.

3. Run the *idaes get-examples command* to download and install the example files:

```
idaes get-examples
```

By default this will install in a folder “examples” in the current directory. The command has many options, but an important one is `-dir`, which specifies the folder in which to install.

for Mac and Linux users this would look like:

```
idaes get-examples --dir ~/idaes/examples
```

or, for Windows users, it would look like:

```
idaes get-examples --dir C:\Users\MyName\IDAES\Examples
```

Refer to the full *idaes get-examples command documentation* for more information.

4. Run tests:

```
pytest --pyargs idaes -W ignore
```

5. You should see the tests run and all should pass to ensure the installation worked. You may see some “Error” level log messages, but they are okay, and produced by tests for error handling. The number of tests that failed and succeeded is reported at the end of the pytest output. You can report problems on the [Github issues page](#) (Please try to be specific about the command and the offending output.)

4.2 Examples

The IDAES PSE software includes a number of example scripts and Jupyter Notebooks. They are maintained the repository <https://github.com/IDAES/examples-pse> on Github, and the online documentation can be found at <https://examples-pse.readthedocs.io/>. This documentation includes browsable versions of the Jupyter Notebooks.

You can install the examples from within an IDAES installation by running `idaes get-examples` in a command-line shell. This requires that you have installed the IDAES PSE toolkit. See the installation instructions for details.

4.3 IDAES Modeling Standards

Contents

- *IDAES Modeling Standards*
 - *Model Formatting and General Standards*
 - * *Headers and Meta-data*
 - * *Coding Standard*
 - * *Model Organization*
 - * *Commenting*
 - *Units of Measurement and Reference States*
 - *Standard Variable Names*
 - * *Standard Naming Format*
 - * *Constants*
 - * *Thermophysical and Transport Properties*
 - * *Reaction Properties*
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4.3.1 Model Formatting and General Standards

The section describes the recommended formatting used within the IDAES framework. Users are strongly encouraged to follow these standards in developing their models in order to improve readability of their code.

Headers and Meta-data

Model developers are encouraged to include some documentation in the header of their model files which provides a brief description of the purpose of the model and how it was developed. Some suggested information to include is:

- Model name,
- Model publication date,
- Model author
- Any necessary licensing and disclaimer information (see below).
- Any additional information the modeler feels should be included.

Coding Standard

All code developed as part of IDAES should conform to the PEP-8 standard.

Model Organization

Whilst the overall IDAES modeling framework enforces a hierarchical structure on models, model developers are still encouraged to arrange their models in a logical fashion to aid other users in understanding the model. Model constraints should be grouped with similar constraints, and each grouping of constraints should be clearly commented.

For property packages, it is recommended that all the equations necessary for calculating a given property be grouped together, clearly separated and identified by using comments.

Additionally, model developers are encouraged to consider breaking their model up into a number of smaller methods where this makes sense. This can facilitate modification of the code by allowing future users to inherit from the base model and selectively overload sub-methods where desired.

Commenting

To help other modelers and users understand the how a model works, model builders are strongly encouraged to comment their code. It is suggested that every constraint should be commented with a description of the purpose of the constraint, and if possible/necessary a reference to a source or more detailed explanation. Any deviations from standard units or formatting should be clearly identified here. Any initialization procedures, or other procedures required to get the model to converge should be clearly commented and explained where they appear in the code. Additionally, modelers are strongly encouraged to add additional comments explaining how their model works to aid others in understanding the model.

4.3.2 Units of Measurement and Reference States

Due to the flexibility provided by the IDAES modeling framework, there is no standard set of units of measurement or standard reference state that should be used in models. This places the onus on the user to understand the units of measurement being used within their models and to ensure that they are consistent.

The IDAES developers have generally used SI units without prefixes (i.e. Pa, not kPa) within models developed by the institute, with a default thermodynamic reference state of 298.15 K and 101325 Pa. Supercritical fluids have been consider to be part of the liquid phase, as they will be handled via pumps rather than compressors.

4.3.3 Standard Variable Names

In order for different models to communicate information effectively, it is necessary to have a standard naming convention for any variable that may need to be shared between different models. Within the IDAES modeling framework, this occurs most frequently with information regarding the state and properties of the material within the system, which is calculated in specialized property blocks, and then used in others parts of the model. This section of the documentation discusses the standard naming conventions used within the IDAES modeling framework.

Standard Naming Format

There are a wide range of different variables which may be of interest to modelers, and a number of different ways in which these quantities can be expressed. In order to facilitate communication between different parts of models, a naming convention has been established to standardize the naming of variables across models. Variable names within IDAES follow to the format below:

```
{property_name}_{basis}_{state}_{condition}
```

Here, property_name is the name of the quantity in question, and should be drawn from the list of standard variable names given later in this document. If a particular quantity is not included in the list of standard names, users are encouraged to contact the IDAES developers so that it can be included in a future release. This is followed by a

number of qualifiers which further indicate the specific conditions under which the quantity is being calculated. These qualifiers are described below, and some examples are given at the end of this document.

Basis Qualifier

Many properties of interest to modelers are most conveniently represented on an intensive basis, that is quantity per unit amount of material. There are a number of different bases that can be used when expressing intensive quantities, and a list of standard basis qualifiers are given below.

Basis	Standard Name
Mass Basis	mass
Molar Basis	mol
Volume Basis	vol

State Qualifier

Many quantities can be calculated either for the whole or a part of a mixture. In these cases, a qualifier is added to the quantity to indicate which part of the mixture the quantity applies to. In these cases, quantities may also be indexed by a Pyomo Set.

Basis	Standard Name	Comments
Component	comp	Indexed by component list
Phase	phase	Indexed by phase list
Phase & Component	phase_comp	Indexed by phase and component list
Total Mixture		No state qualifier

Phase	Standard Name
Supercritical Fluid	liq
Ionic Species	ion
Liquid Phase	liq
Solid Phase	sol
Vapor Phase	vap
Multiple Phases	e.g. liq1

Condition Qualifier

There are also cases where a modeler may want to calculate a quantity at some state other than the actual state of the system (e.g. at the critical point, or at equilibrium).

Basis	Standard Name
Critical Point	crit
Equilibrium State	equil
Ideal Gas	ideal
Reduced Properties	red
Reference State	ref

Constants

IDAES contains a library of common physical constants of use in process systems engineering models, which can be imported from `idaes.core.util.constants`. Below is a list of these constants with their standard names and values (SI units).

Constant	Standard Name	Value	Units
Acceleration due to Gravity	<code>acceleration_gravity</code>	9.80665	ms^{-2}
Avogadro's Number	<code>avogadro_number</code>	6.02214076e23	mol^{-1}
Boltzmann Constant	<code>boltzmann_constant</code>	1.38064900e-23	JK^{-1}
Elementary Charge	<code>elementary_charge</code>	1.602176634e-19	C
Faraday's Constant	<code>faraday_constant</code>	96485.33212	$Cmol^{-1}$
Gas Constant	<code>gas_constant</code>	8.314462618	$Jmol^{-1}K^{-1}$
Newtonian Constant of Gravitation	<code>gravitational_constant</code>	6.67430e-11	$m^3kg^{-1}s^{-2}$
Mass of an Electron	<code>mass_electron</code>	9.1093837015e-31	kg
Pi (Archimedes' Constant)	<code>pi</code>	3.141592 [1]	
Planck Constant	<code>planck_constant</code>	6.62607015e-34	Js
Stefan-Boltzmann Constant	<code>stefan_constant</code>	5.67037442e-8	$Wm^{-2}K^{-4}$
Speed of Light in a Vacuum	<code>speed_light</code>	299792458	ms^{-1}

[1] pi imported from the Python *math* library and is available to machine precision.

Values for fundamental constants and derived constants are drawn from the definitions of SI units (<https://www.bipm.org/utils/common/pdf/si-brochure/SI-Brochure-9.pdf>) and are generally defined to 9 significant figures.

Acceleration due to gravity, gravitational constant and electron mass are sourced from NIST (<https://physics.nist.gov>) and used the significant figures reported there.

Thermophysical and Transport Properties

Below is a list of all the thermophysical properties which currently have a standard name associated with them in the IDAES framework.

Variable	Standard Name
Activity	<code>act</code>
Activity Coefficient	<code>act_coeff</code>
Bubble Pressure	<code>pressure_bubble</code>
Bubble Temperature	<code>temperature_bubble</code>
Compressibility Factor	<code>compress_fact</code>
Concentration	<code>conc</code>
Density	<code>dens</code>
Dew Pressure	<code>pressure_dew</code>
Dew Temperature	<code>temperature_dew</code>
Diffusivity	<code>diffus</code>
Diffusion Coefficient (binary)	<code>diffus_binary</code>
Enthalpy	<code>enth</code>
Entropy	<code>entr</code>
Fugacity	<code>fug</code>
Fugacity Coefficient	<code>fug_coeff</code>
Gibbs Energy	<code>energy_gibbs</code>
Heat Capacity (const. P)	<code>cp</code>

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Variable	Standard Name
Heat Capacity (const. V)	cv
Heat Capacity Ratio	heat_capacity_ratio
Helmholtz Energy	energy_helmholtz
Henry's Constant	henry
Internal Energy	energy_internal
Mass Fraction	mass_frac
Material Flow	flow
Molecular Weight	mw
Mole Fraction	mole_frac
pH	pH
Pressure	pressure
Speed of Sound	speed_sound
Surface Tension	surf_tens
Temperature	temperature
Thermal Conductivity	therm_cond
Vapor Pressure	pressure_sat
Viscosity (dynamic)	visc_d
Viscosity (kinematic)	visc_k
Vapor Fraction	vap_frac
Volume Fraction	vol_frac

Reaction Properties

Below is a list of all the reaction properties which currently have a standard name associated with them in the IDAES framework.

Variable	Standard Name
Activation Energy	energy_activation
Arrhenius Coefficient	arrhenius
Heat of Reaction	dh_rxn
Entropy of Reaction	ds_rxn
Equilibrium Constant	k_eq
Reaction Rate	reaction_rate
Rate constant	k_rxn
Solubility Constant	k_sol

Solid Properties

Below is a list of all the properties of solid materials which currently have a standard name associated with them in the IDAES framework.

Variable	Standard Name
Min. Fluidization Velocity	velocity_mf
Min. Fluidization Voidage	voidage_mf
Particle Size	particle_dia
Pore Size	pore_dia
Porosity	particle_porosity
Specific Surface Area	area_{basis}
Sphericity	sphericity
Tortuosity	tort
Voidage	bulk_voidage

Naming Examples

Below are some examples of the IDAES naming convention in use.

Variable Name	Meaning
enth	Specific enthalpy of the entire mixture (across all phases)
flow_comp["H2O"]	Total flow of H2O (across all phases)
entr_phase["liq"]	Specific entropy of the liquid phase mixture
conc_phase_comp["liq", "H2O"]	Concentration of H2O in the liquid phase
temperature_red	Reduced temperature
pressure_crit	Critical pressure

4.4 Configuration

Some behavior of IDAES, especially logging, is configurable through configuration files. IDAES's configuration is obtained by first setting everything to internal defaults; then loading a global config file, if it exists; then loading a config file from the current working directory, if it exists.

Configuration file are in **JSON format**. The default configuration is shown below and can be used as a template to create new configuration files. This is the configuration used by IDAES if nothing else is provided.

```
{
  "use_idaes_solvers":true,
  "logger_capture_solver":true,
  "logger_tags":[
    "framework",
    "model",
    "flowsheet",
    "unit",
    "control_volume",
    "properties",
    "reactions"
  ],
  "valid_logger_tags":[
    "framework",
    "model",
    "flowsheet",
    "unit",
    "control_volume",
    "properties",
```

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```

    "reactions"
  ],
  "logging": {
    "version": 1,
    "disable_existing_loggers": false,
    "formatters": {
      "default_format": {
        "format": "%(asctime)s [%(levelname)s] %(name)s: %(message)s",
        "datefmt": "%Y-%m-%d %H:%M:%S"
      }
    },
    "handlers": {
      "console": {
        "class": "logging.StreamHandler",
        "formatter": "default_format",
        "stream": "ext://sys.stdout"
      }
    },
    "loggers": {
      "idaes": {
        "level": "INFO",
        "propagate": true,
        "handlers": ["console"]
      },
      "idaes.solve": {
        "propagate": false,
        "level": "INFO",
        "handlers": ["console"]
      },
      "idaes.init": {
        "propagate": false,
        "level": "INFO",
        "handlers": ["console"]
      },
      "idaes.model": {
        "propagate": false,
        "level": "INFO",
        "handlers": ["console"]
      }
    }
  }
}

```

4.4.1 Global Configuration

IDAES configuration files are named `idaes.conf`. The easiest way to find where the global configuration file should be placed is to run the command `idaes data-directory`. A global configuration file won't exist unless a user creates one. The default configuration above can be used as a start.

Windows

On Windows the global configuration file is located at `%LOCALAPPDATA%\idaes\idaes.conf`.

UNIX-Like

On Unix-like systems the global configuration files is located at `$HOME/.idaes/idaes.conf`.

Other

On systems that have neither an `%LOCALAPPDATA%` or `$HOME` environment variable, global config files are not currently supported.

4.4.2 Important Configuration Entries

The configuration file has several fields, but they are not all important to end-users. This section lists the commonly used entries.

logging

This section of the file configures IDAES loggers. Once the configuration is read, Python's standard `logging.config.dictConfig()` is used to set the logger configuration. See Python's logging documentation for more information.

IDAES has four main loggers defined in the standard configuration, although additional loggers can be added if desired. The standard loggers are:

1. `idaes`, this is the root logger of most IDAES logging, unless otherwise noted.
2. `idaes.init`, this is the root of IDAES initialization loggers.
3. `idaes.solve`, this is the root of IDAES solver loggers and solver information.
4. `idaes.model`, this is the root of model loggers. Model loggers are usually used by models written using the IDAES framework, but not part of the `idaes` package.

use_idaes_solvers

This option can be set to `false` to direct the IDAES framework not to use solvers obtained with the `idaes get-extensions` command. This can be used if a user would prefer to use solver versions they have installed apart from IDAES.

logger_capture_solver

If a solver call is done from inside a solver logging context, this setting will send the solver output to the logger if `true`, and not capture the solver output for the logger if `false`. If solver output is not captured it will be sent to the screen, and not be logged.

logger_tags

Loggers created with the `idaes.logging` module can be assigned tags. Output from these loggers is recorded if the loggers tag is in the `logger_tags` set. The default behavior can be configured in a configuration file. The tag set can also be modified at any time via functions in the `idaes.logging` module.

valid_log_tags

When setting logger tags for `idaes.logging` loggers they are compared against a list of valid tags. This is done to guard against spelling errors. If the default set of defined tags is not sufficient tags can be added here, or later through functions in the `idaes.logging` module.

4.5 Logging

IDAES provides some logging extensions to provide finer control over information logging and to allow solver output to be logged.

4.5.1 Getting Loggers

There are four main roots of IDAES loggers (`idaes`, `idaes.model`, `idaes.init`, `idaes.solve`). All of these loggers are standard Python loggers, and can be used as such. The main differences between using the IDAES logging functions to get the loggers and plain Python methods are that the IDAES functions make it a little easier to get loggers that fit into IDAES's standard logging hierarchy, and the IDAES loggers have a few additional named logging levels, which allow for finer control over the information displayed. Logging levels are described in detail later.

A tag can also be specified and used to filter logging records. By default the tag is `None` and log records won't be filtered. Valid tags are in the set `{None, "framework", "model", "flowsheet", "unit", "control_volume", "properties", "reactions"}`. Users may add to the set of valid names. To see how to control which logging tags are logged, see section “Tags” below. To avoid filtering out import warning and error messages, records logged at the `WARNING` level and above are not filtered out regardless of tag.

idaes Logger

Loggers descending from `idaes` (other than `idaes.init`, `idaes.model`, or `idaes.solve`) are used for general IDAES framework logging. Typically the module name `__name__` is used for the logger name. Modules in the `idaes` package already start with `idaes`, but if an IDAES logger is requested for a module outside of the `idaes` package `idaes.` is prepended to the name.

`idaes.logger.getLogger` (*name*, *level=None*, *tag=None*)

Return an `idaes` logger.

Parameters

- **name** – usually `__name__`
- **level** – standard IDAES logging level (default use IDAES config)
- **tag** – logger tag for filtering, see `valid_log_tags()`

Returns logger

Example

```
import idaes.logger as idaeslog

_log = idaeslog.getLogger(__name__, tag="framework")
```

idaes.init Logger

The init logger will always descend from “idaes.init”. This logger is used in IDAES model initialization methods, and can be used in user models as well. Initialization methods are usually attached to a Pyomo Block. Blocks have a `name` attribute. So the logger name is usually given as the block name, and the `getInitLogger()` function prepends `idaes.init..` The advantage of using the block name over the module name is that users can see exactly which model instance the initialization log messages are coming from.

`idaes.logger.getInitLogger(name, level=None, tag=None)`
Get a model initialization logger

Parameters

- **name** – Object name (usually Pyomo Component name)
- **level** – Log level
- **tag** – logger tag for filtering, see `valid_log_tags()`

Returns logger

Example

```
import idaes.logger as idaeslog

class DummyBlock(object):
    """A dummy block for demonstration purposes"""
    def __init__(name):
        self.name = name

    def initialize(outlvl=idaeslog.INFO):
        init_log = idaeslog.getInitLogger(self.name, level=outlvl, tag="unit")
```

idaes.model Logger

The model logger is used to provide a standard way to produce log messages from user models that are not part of the `idaes` package. The logger name has `idaes.model` prepended to the name provided by the user. This is convenient because it provides a way to use a standard configuration system for user model loggers. The user can choose any name they like for these loggers.

`idaes.logger.getModelLogger(name, level=None, tag=None)`
Get a logger for an IDAES model. This function helps users keep their loggers in a standard location and use the IDAES logging config.

Parameters

- **name** – Name (usually `__name__`). Any starting ‘idaes.’ is stripped off, so if a model is part of the `idaes` package, ‘idaes’ won’t be repeated.
- **level** – Standard Python logging level (default use IDAES config)
- **tag** – logger tag for filtering, see `valid_log_tags()`

Returns logger

Example

```
import idaes.logger as idaeslog

_log = idaeslog.getModelLogger("my_model", level=idaeslog.DEBUG, tag="model")
```

idaes.solve Logger

The solve logger will always descend from “idaes.solve”. This logger is used to log solver output. Since solvers may produce a lot of output, it can be useful to specify different handlers for the solve logger to direct it to a separate file.

`idaes.logger.getSolveLogger(name, level=None, tag=None)`

Get a solver logger

Parameters

- **name** – logger name is “idaes.solve.” + name (if name starts with “idaes.” it is removed before creating the logger name)
- **level** – Log level
- **tag** – logger tag for filtering, see `valid_log_tags()`

Returns logger

4.5.2 Tags

Logger tags are provided to allow control over what types of log records to display. The logger tag is just a string that gets attached to a logger, which specifies that a logger generates records of a certain type. You can then specify what tags you want to see information from. A filter removes any tags that are not in the list of tags to display at levels below WARNING.

The set of tags to display information from is a global setting in the `idaes.logger` module. When getting a logger, you can set its tag by providing the `tag` argument, see “Getting Loggers” above.

The following functions can be used to specify which logging tags to display:

`idaes.logger.log_tags()`

Returns a set of logging tags to be logged.

Returns (set) tags to be logged

`idaes.logger.set_log_tags(tags)`

Specify a set of tags to be logged

Parameters **tags** (*iterable of str*) – Tags to log

Returns None

`idaes.logger.add_log_tag(tag)`

Add a tag to the list of tags to log.

Parameters **tag** (*str*) – Tag to log

Returns None

`idaes.logger.remove_log_tag(tag)`

Remove a tag from the list of tags to log.

Parameters **tag** (*str*) – Tag to no longer log

Returns None

The tags are validated against a list of valid tags to provide error checking for typos and to enforce some standard tag names. To provide more flexibility, users can add to the list of valid tag names, but cannot remove names.

`idaes.logger.valid_log_tags()`

Returns a set of valid logging tag names.

Returns (set) valid tag names


```
idaes.logger.add_valid_log_tag(tag)
```

Add a tag name to the list of valid names.

Parameters `tag` (*str*) – A tag name

Returns None

4.5.3 Levels

Several logging level constants are defined in the `idaes.logger` module. These include the standard Python Levels. The following levels are provided for IDAES loggers. The additional levels of info provide finer control over the amount of logging information produced by IDAES loggers.

Constant Name	Value	Name	Log Method
CRITICAL	50	CRITICAL	<code>critical()</code>
ERROR	40	ERROR	<code>error(), exception()</code>
WARNING	30	WARNING	<code>warning()</code>
INFO_LOW	21	INFO	<code>unit_low()</code>
INFO	20	INFO	<code>info()</code>
INFO_HIGH	19	INFO	<code>unit_high()</code>
DEBUG	10	DEBUG	<code>debug()</code>
NOTSET	0	NOTSET	–

4.5.4 Utility Functions

There are some additional utility functions to perform logging tasks that are common in the IDAES framework.

```
idaes.logger.condition(res)
```

Get the solver termination condition to log. This isn't a specific value that you can really depend on, just a message to pass on from the solver for the user's benefit. Sometimes the solve is in a try-except, so we'll handle None and str for those cases, where you don't have a real result.

4.5.5 Logging Solver Output

The solver output can be captured and directed to a logger using the `idaes.logger.solver_log(logger, level)` context manager, which uses `pyutilib.misc.capture_output()` to temporarily redirect `sys.stdout` and `sys.stderr` to a string buffer. The `logger` argument is the logger to log to, and the `level` argument is the level at which records are sent to the logger. The output is logged by a separate logging thread, so output can be logged as it is produced instead of after the solve completes. If the `solver_log()` context manager is used, it can be turned on and off by using the `idaes.logger.solver_capture_on()` and `idaes.logger.solver_capture_off()` functions. If the capture is off solver output won't be logged and it will go to standard output as usual.

The `solver_log` context yields an object with `tee` and `thread` attributes. `thread` is the logging thread, which is not needed for most uses. The `tee` attribute should be passed to the `tee` argument of the `solve` method. Tee tells the Pyomo solver to display solver output. The solver log context can provide this argument by determining if the solver output would be logged at the given level.

Example

```
import idaes.logger as idaeslog
import pyomo.environ as pyo
```

(continues on next page)

(continued from previous page)

```
solver = pyo.SolverFactory("ipopt")

model = pyo.ConcreteModel()
model.x = pyo.Var()
model.y = pyo.Var()
model.x.fix(3)
model.c = pyo.Constraint(expr=model.y==model.x**2)

log = idaeslog.getSolveLogger("solver.demo")
log.setLevel(idaeslog.DEBUG)

with idaeslog.solver_log(log, idaeslog.DEBUG) as slc:
    res = solver.solve(model, tee=slc.tee)
```

4.6 Command-line interface

The IDAES PSE Toolkit includes a command-line tool that can be invoked by typing *idaes* in a UNIX or Mac OSX shell, or Windows Powershell, that is in an installed IDAES environment. For the most part, this means that wherever you installed IDAES will have this command available.

This section of the documentation describes the capabilities of this command-line program.

4.6.1 idaes command

The base *idaes* command does not do anything by itself, besides set some shared configuration values. All the real work is done by one of the sub-commands, each of which is described on a separate page below.

idaes bin-directory: Show IDAES executable file directory

This page lists the options for the *idaes* “bin-directory” bin-directory. This is invoked like:

```
idaes [general options] bin-directory [bin-directory options]
```

general options

The following general options from the *idaes* base command affect the bin-directory bin-directory. They should be placed *before* the “bin-directory” bin-directory, on the command-line.

- *-v*/*--verbose*
- *-q*/*--quiet*

See the *idaes command* for details.

idaes bin-directory

This subcommand shows the IDAES executable file directory.

options

--help

Show the help message and exit.

--exists

Show if the directory exists.

--create

Create the directory.

idaes copyright: Show IDAES copyright information

This page lists the options for the *idaes* “copyright” subcommand. This is invoked like:

```
idaes [general options] copyright [subcommand options]
```

general options

The following general options from the *idaes* base command affect the copyright subcommand. They should be placed *before* the “copyright” subcommand, on the command-line.

- -v/--verbose
- -q/--quiet

See the *idaes command* for details.

idaes copyright

This subcommand prints the IDAES copyright notice to standard output.

options

--help

Show the help message and exit.

idaes data-directory: Show IDAES data directory

This page lists the options for the *idaes* “data-directory” subcommand. This is invoked like:

```
idaes [general options] data-directory [subcommand options]
```

general options

The following general options from the *idaes* base command affect the data-directory subcommand. They should be placed *before* the “data-directory” subcommand, on the command-line.

- -v/--verbose
- -q/--quiet

See the *idaes command* for details.

idaes data-directory

This subcommand shows the IDAES data directory.

options

- help**
Show the help message and exit.
- exists**
Show if the directory exists.
- create**
Create the directory.

idaes get-examples: Fetch example scripts and Jupyter Notebooks

This page lists the options for the *idaes* “get-examples” subcommand. This is invoked like:

```
idaes [general options] get-examples [subcommand options]
```

general options

The following general options from the *idaes* base command affect the *get-examples* subcommand. They should be placed *before* the “get-examples” subcommand, on the command-line.

- **-v/--verbose**
- **-q/--quiet**

See the *idaes command* for details.

idaes get-examples

This subcommand fetches example scripts and Jupyter Notebooks from a given release in [Github](#), and puts them in a directory of the users’ choosing. If the user does not specify a directory, the default is *examples*.

options

- help**
Show the help message and exit.
- d, --dir** TEXT

Select the installation target directory. See *example usage* for several examples of this option.

- I, --no-install**

Do *not* install examples into ‘idaes_examples’ package. Examples are installed by default so they can be imported directly from Python. Not installing them might cause some tests, which import the examples, to fail.

-l, --list-releases

List all available released versions, and stop. This lets people browse the releases and select one. By default, the release that matches the version of the currently installed “idaes” package is used. See also the *--unstable* option.

-N, --no-download

Do not download anything. If the *--no-install* option is also given, this means the command will essentially do nothing. Or, looked at another way, this option means that only action will be the installation of the “idaes_examples” package from the selected directory.

-U, --unstable

Allow and list unstable/pre-release versions. This applies to both download and the *--list-releases* option. Unstable releases are marked with “rcN” or similar suffixes.

-V, --version TEXT

Version of examples to download. The default version, which is shown for the *--help* option, is the same as the version of the IDAES PSE toolkit for which the *idaes* command is installed. If the version to install is unstable (ends with “rcN”) then you will need to add the *--unstable* option to avoid errors.

example usage

idaes get-examples Download examples from release matching release for the *idaes* command, install them in the *examples* subdirectory of this directory, and install the modules found under *examples/src* as a package named *idaes_examples*. The *examples* directory must not exist, i.e. the program will refuse to overwrite the contents of an existing directory.

idaes get-examples -d /tmp/examples Same as above, but put downloaded code in */tmp/examples* instead.

idaes get-examples -d /tmp/examples -I Download to */tmp/examples*, but do not install.

idaes get-examples -d /tmp/examples -N Install the examples found under */tmp/examples*.

idaes get-examples --version 1.4.2-pre Download examples from release *1.4.2-pre*, install them in the *examples* subdirectory of this directory, and install the modules found under *examples/src* as a package named *idaes_examples*.

idaes get-examples --list-releases List available releases of the examples in Github repository, *idaes/examples-pse*. Do not attempt to download or install anything.

idaes get-examples --list-releases --unstable Same as above, but include non-stable releases.

idaes get-extensions: Get solvers and libraries

This page lists the options for the *idaes* “get-extensions” subcommand. This is invoked like:

```
idaes [general options] get-extensions [subcommand options]
```

general options

The following general options from the *idaes* base command affect the get-extensions subcommand. They should be placed *before* the “get-extensions” subcommand, on the command-line.

- -v/--verbose
- -q/--quiet

See *idaes command* for details.

idaes get-extensions

This subcommand gets the compiled solvers and libraries from a remote repository, and installs them locally.

options

--help

Show the help message and exit.

--url

URL from which to download the solvers/libraries.

idaes lib-directory: Show IDAES library file directory

This page lists the options for the *idaes* “lib-directory” subcommand. This is invoked like:

```
idaes [general options] lib-directory [subcommand options]
```

general options

The following general options from the *idaes* base command affect the lib-directory subcommand. They should be placed *before* the “lib-directory” subcommand, on the command-line.

- -v/--verbose
- -q/--quiet

See the *idaes command* for details.

idaes lib-directory

This subcommand shows the IDAES library file directory.

options

--help

Show the help message and exit.

--exists

Show if the directory exists.

--create

Create the directory.

shared configuration

-v

--verbose

Increase verbosity. Show warnings if given once, then info, and then debugging messages.

-q

--quiet

Increase quietness. If given once, only show critical messages. If given twice, show no messages.

4.7 Core Library

4.7.1 Core Contents

Process Blocks

Example

ProcessBlock is used to simplify inheritance of Pyomo's Block. The code below provides an example of how a new ProcessBlock class can be implemented. The new ProcessBlock class has a ConfigBlock that allows each element of the block to be passed configuration options that affect how a block is built. ProcessBlocks have a rule set by default that calls the build method of the contained ProcessBlockData class.

```
from pyomo.environ import *
from pyomo.common.config import ConfigValue
from idaes.core import ProcessBlockData, declare_process_block_class

@declare_process_block_class("MyBlock")
class MyBlockData(ProcessBlockData):
    CONFIG = ProcessBlockData.CONFIG()
    CONFIG.declare("xinit", ConfigValue(default=1001, domain=float))
    CONFIG.declare("yinit", ConfigValue(default=1002, domain=float))
    def build(self):
        super(MyBlockData, self).build()
        self.x = Var(initialize=self.config.xinit)
        self.y = Var(initialize=self.config.yinit)
```

The following example demonstrates creating a scalar instance of the new class. The `default` key word argument is used to pass information on the the MyBlockData ConfigBlock.

```
m = ConcreteModel()
m.b = MyBlock(default={"xinit":1, "yinit":2})
```

The next example creates an indexed MyBlock instance. In this case, each block is configured the same, using the `default` argument.

```
m = ConcreteModel()
m.b = MyBlock([0,1,2,3,4], default={"xinit":1, "yinit":2})
```

The next example uses the `initialize` argument to override the configuration of the first block. Initialize is a dictionary of dictionaries where the key of the top level dictionary is the block index and the second level dictionary is arguments for the config block.

```
m = ConcreteModel()
m.b = MyBlock([0,1,2,3,4], default={"xinit":1, "yinit":2},
              initialize={0:{"xinit":1, "yinit":2}})
```

The next example shows a more complicated configuration where there are three configurations, one for the first block, one for the last block, and one for the interior blocks. This is accomplished by providing the `idx_map` argument to `MyBlock`, which is a function that maps a block index to a index in the initialize dictionary. In this case 0 is mapped to 0, 4 is mapped to 4, and all elements between 0 and 4 are mapped to 1. A lambda function is used to convert the block index to the correct index in initialize.

```
m = ConcreteModel()
m.b = MyBlock(
    [0,1,2,3,4],
    idx_map = lambda i: 1 if i > 0 and i < 4 else i,
    initialize={0:{"xinit":2001, "yinit":2002},
               1:{"xinit":5001, "yinit":5002},
               4:{"xinit":7001, "yinit":7002}})
```

The build method

The core part of any IDAES Block is the build method, which contains the instructions on how to construct the variables, constraints and other components that make up the model. The build method serves as the default rule for constructing an instance of an IDAES Block, and is triggered automatically whenever an instance of an IDAES Block is created unless a custom rule is provided by the user.

ProcessBlock Class

```
idaes.core.process_block.declare_process_block_class(name,      block_class=<class
                                                         'idaes.core.process_block.ProcessBlock'>,
                                                         doc="")
```

Declare a new `ProcessBlock` subclass.

This is a decorator function for a class definition, where the class is derived from Pyomo's `_BlockData`. It creates a `ProcessBlock` subclass to contain the decorated class. The only requirement is that the subclass of `_BlockData` contain a `build()` method. The purpose of this decorator is to simplify subclassing Pyomo's block class.

Parameters

- **name** – name of class to create
- **block_class** – `ProcessBlock` or a subclass of `ProcessBlock`, this allows you to use a subclass of `ProcessBlock` if needed. The typical use case for Subclassing `ProcessBlock` is to impliment methods that operate on elements of an indexed block.
- **doc** – Documentation for the class. This should play nice with sphinx.

Returns Decorator function

```
class idaes.core.process_block.ProcessBlock(*args, **kwargs)
```

`ProcessBlock` is a Pyomo Block that is part of a system to make Pyomo Block easier to subclass. The main difference between a Pyomo Block and `ProcessBlock` from the user perspective is that a `ProcessBlock` has a rule assigned by default that calls the `build()` method for the contained `ProcessBlockData` objects. The default rule can be overridden, but the new rule should always call `build()` for the `ProcessBlockData` object.

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls `build()`.

- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config
- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (ProcessBlock) New instance

classmethod base_class_module ()

Return module of the associated ProcessBase class.

Returns (str) Module of the class.

Raises *AttributeError*, if no base class module was set, e.g. this class – was not wrapped by the *declare_process_block_class* decorator.

classmethod base_class_name ()

Name given by the user to the ProcessBase class.

Returns (str) Name of the class.

Raises *AttributeError*, if no base class name was set, e.g. this class – was not wrapped by the *declare_process_block_class* decorator.

class `idaes.core.process_base.ProcessBlockData` (*component*)

Base class for most IDAES process models and classes.

The primary purpose of this class is to create the local config block to handle arguments provided by the user when constructing an object and to ensure that these arguments are stored in the config block.

Additionally, this class contains a number of methods common to all IDAES classes.

build ()

The build method is called by the default ProcessBlock rule. If a rule is sepecified other than the default it is important to call ProcessBlockData’s build method to put information from the “default” and “initialize” arguments to a ProcessBlock derived class into the BlockData object’s ConfigBlock.

The the build method should usually be overloaded in a subclass derived from ProcessBlockData. This method would generally add Pyomo components such as variables, expressions, and constraints to the object. It is important for build() methods implimented in derived classes to call build() from the super class.

Parameters **None** –

Returns **None**

fix_initial_conditions (*state='steady-state'*)

This method fixes the initial conditions for dynamic models.

Parameters **state** – initial state to use for simulation (default = ‘steady-state’)

Returns : **None**

flowsheet ()

This method returns the components parent flowsheet object, i.e. the flowsheet component to which the model is attached. If the component has no parent flowsheet, the method returns **None**.

Parameters None –

Returns Flowsheet object or None

`unfix_initial_conditions()`

This method unfixed the initial conditions for dynamic models.

Parameters None –

Returns : None

IDAES Modeling Concepts

Contents

- *IDAES Modeling Concepts*
 - *Introduction*
 - *Time Domain*
 - *Flowsheets*
 - *Unit Models*
 - *Component References*
 - *What Belongs in Each Type of Block?*

Introduction

The purpose of this section of the documentation is to explain the different parts of the IDAES modeling framework, and what components belong in each part for the hierarchy. Each component is described in greater detail later in the documentation, however this section provides a general introduction to different types of components.

Time Domain

Before starting on the different types of models present in the IDAES framework, it is important to discuss how time is handled by the framework. When a user first declares a Flowsheet model a time domain is created, the form of which depends on whether the Flowsheet is declared to be dynamic or steady-state (see FlowsheetBlock documentation). In situations where the user makes use of nested flowsheets, each sub-flowsheet refers to its parent flowsheet for the time domain.

Different models may handle the time domain differently, but in general all IDAES models refer to the time domain of their parent flowsheet. The only exception to this are blocks associated with Property calculations. PropertyBlocks represent the state of the material at a single point in space and time, and thus do not contain the time domain. Instead, PropertyBlocks are indexed by time (and space where applicable) - i.e. there is a separate PropertyBlock for each point in time. The user should keep this in mind when working with IDAES models, as it is important for understanding where the time index appears within a model.

In order to facilitate referencing of the time domain, all Flowsheet objects have a *time* configuration argument which is a reference to the time domain for that flowsheet. All IDAES models contain a *flowsheet* method which returns the parent flowsheet object, thus a reference to the time domain can always be found using the following code: *flowsheet().config.time*.

Another important thing to note is that steady-state models do contain a time domain, however this is generally a single point at time = 0.0. However, models still contain a reference to the time domain, and any components are still indexed by time even in a steady-state model (e.g. PropertyBlocks).

Flowsheets

The top level of the IDAES modeling framework is the Flowsheet model. Flowsheet models represent traditional process flowsheets, containing a number of Unit models representing process unit operations connected together into a flow network. Flowsheets generally contain three types of components:

1. Unit models, representing unit operations,
2. Arcs, representing connections between Unit models, and,
3. Property Parameter blocks, representing the parameters associated with different materials present within the flowsheet.

Flowsheet models may also contain additional constraints relating to how different Unit models behave and interact, such as control and operational constraints. Generally speaking, if a Constraint is purely internal to a single unit, and does not depend on information from other units in the flowsheet, then the Constraint should be placed inside the relevant Unit model. Otherwise, the Constraint should be placed at the Flowsheet level.

Unit Models

Unit models generally represent individual pieces of equipment present within a process which perform a specific task. Unit models in turn are generally composed of two main types of components:

1. Control Volume Blocks, which represent volume of material over which we wish to perform material, energy and/or momentum balances, and,
2. StateBlocks and ReactionBlocks, which represent the thermophysical, transport and reaction properties of the material at a specific point in space and time.
3. Inlets and Outlets, which allow Unit models to connect to other Unit models.

Unit models will also contain Constraints describing the performance of the unit, which will relate terms in the balance equations to different phenomena.

Control Volumes

A key feature of the IDAES modeling framework is the use of Control Volume Blocks. As mentioned above, Control Volumes represent a volume of material over which material, energy and/or momentum balances can be performed. Control Volume Blocks contain methods to automate the task of writing common forms of these balance equations. Control Volume Blocks can also automate the creation of StateBlocks and ReactionBlocks associated with the control volume.

Property Blocks

Property blocks represent the state of a material at a given point in space and time within the process flowsheet, and contain the state variables, thermophysical, transport and reaction properties of a material (which are functions solely of the local state of the material). Within the IDAES process modeling framework, properties are divided into two types:

- Physical properties (StateBlocks), including thermophysical and transport properties, and

- Reaction properties (ReactionBlocks), which include all properties associated with chemical reactions.

Additionally, StateBlocks contain information on the extensive flow of material at that point in space and time, which is a departure from how engineers generally think about properties. This is required to facilitate the flexible formulation of the IDAES Framework by allowing the property package to dictate what form the balance equations will take, which requires the StateBlock to know the extensive flow information.

The calculations involved in property blocks of both types generally require a set of parameters which are constant across all instances of that type of property block. Rather than each property block containing its own copy of each of these parameters (thus duplicating parameters between blocks), each type of property block is associated with a Property Parameter Block (PhysicalParameterBlock or ReactionParameterBlock). Property Parameter Blocks serve as a centralized location for the constant parameters involved in property calculations, and all property blocks of the associated type link to the parameters contained in the parameter block.

Component References

There are many situations in the IDAES modeling framework where a developer may want to make use of a modeling component (e.g. a variable or parameter) from one Block in another Block. The time domain is a good example of this - almost all Blocks within an IDAES model need to make use of the time domain, however the time domain exists only at the top level of the flowsheet structure. In order to make use of the time domain in other parts of the framework, references to the time domain are used instead. By convention, all references within the IDAES modeling framework are indicated by the suffix “_ref” attached to the name of the reference. E.g. all references to the time domain within the framework are called “time_ref”.

What Belongs in Each Type of Block?

A common question with the hierarchical structure of the IDAES framework is where does a specific variable or constraint belong (or conversely, where can I find a specific variable or constraint). In general, variables and constraints are divided based on the following guidelines:

1. Property Parameter Blocks - any parameter or quantity that is consistent across all instances of a Property Block belongs in the Property Parameter Block. This includes:
 - component lists,
 - lists of valid phases,
 - universal constants (e.g. R , π),
 - constants used in calculating properties (e.g. coefficients for calculating c_p),
 - reference states (e.g. P_{ref} and T_{ref}),
 - lists of reaction identifiers,
 - reaction stoichiometry.
2. Property Blocks - all state variables (including extensive flow information) and any quantity that is a function only of state variables plus the constraints required to calculate these. These include:
 - flow rates (can be of different forms, e.g. mass or molar flow, on a total or component basis),
 - temperature,
 - pressure,
 - intensive and extensive state functions (e.g. enthalpy); both variables and constraints.
3. Control Volume Blocks - material, energy and momentum balances and the associated terms. These include:

- balance equations,
 - holdup volume,
 - material and energy holdups; both variables and constraints,
 - material and energy accumulation terms (Pyomo.dae handles the creation of the associated derivative constraints),
 - material generation terms (kinetic reactions, chemical and phase equilibrium, mass transfer),
 - extent of reaction terms and constraints relating these to the equivalent generation terms,
 - phase fraction within the holdup volume and constrain on the sum of phase fractions,
 - heat and work transfer terms,
 - pressure change term
 - diffusion and conduction terms (where applicable) and associated constraints,
 - Mixer and Splitter blocks for handling multiple inlets/outlets.
4. Unit Model - any unit performance constraints and associated variables, such as:
- constraints relating balance terms to physical phenomena or properties (e.g. relating extent of reaction to reaction rate and volume),
 - constraints describing flow of material into or out of unit (e.g. pressure driven flow constraints),
 - unit level efficiency constraints (e.g. relating mechanical work to fluid work).
5. Flowsheet Model - any constraints related to interaction of unit models and associated variables. Examples include:
- control constraints relating behavior between different units (e.g. a constraint on valve opening based on the level in another unit).

Flowsheet Model Class

Contents

- *Flowsheet Model Class*
 - *Default Property Packages*
 - *Flowsheet Configuration Arguments*
 - *Flowsheet Classes*

Flowsheet models make up the top level of the IDAES modeling framework, and represent the flow of material and energy through a process. Flowsheets will generally contain a number of UnitModels to represent unit operations within the process, and will contain one or more Property Packages which represent the thermophysical and transport properties of material within the process.

Flowsheet models are responsible for establishing and maintaining the time domain of the model, including declaring whether the process model will be dynamic or steady-state. This time domain is passed on to all models attached to the flowsheet (such as Unit Models and sub-Flowsheets). The Flowsheet model also serves as a centralized location for organizing property packages, and can set one property package to use as a default throughout the flowsheet.

Flowsheet Blocks may contain other Flowsheet Blocks in order to create nested flowsheets and to better organize large, complex process configurations. In these cases, the top-level Flowsheet Block creates the time domain, and each sub-flowsheet creates a reference this time domain. Sub-flowsheets may make use of any property package declared at a higher level, or declare new property package for use within itself - any of these may be set as the default property package for a sub-Flowsheet.

Default Property Packages

Flowsheet Blocks may assign a property package to use as a default for all UnitModels within the Flowsheet. If a specific property package is not provided as an argument when constructing a UnitModel, the UnitModel will search up the model tree until it finds a default property package declared. The UnitModel will use the first default property package it finds during the search, and will return an error if no default is found.

Flowsheet Configuration Arguments

Flowsheet blocks have three configuration arguments which are stored within a Config block (flowsheet.config). These arguments can be set by passing arguments when instantiating the class, and are described below:

- **dynamic** - indicates whether the flowsheet should be dynamic or steady-state. If `dynamic = True`, the flowsheet is declared to be a dynamic flowsheet, and the time domain will be a Pyomo ContinuousSet. If `dynamic = False`, the flowsheet is declared to be steady-state, and the time domain will be an ordered Pyomo Set. For top level Flowsheets, `dynamic` defaults to `False` if not provided. For lower level Flowsheets, the `dynamic` will take the same value as that of the parent model if not provided. It is possible to declare steady-state sub-Flowsheets as part of dynamic Flowsheets if desired, however the reverse is not true (cannot have dynamic Flowsheets within steady-state Flowsheets).
- **time** - a reference to the time domain for the flowsheet. During flowsheet creation, users may provide a Set or ContinuousSet that the flowsheet should use as the time domain. If not provided, then the flowsheet will look for a parent flowsheet and set this equal to the parent's time domain, otherwise a new time domain will be created and assigned here.
- **time_set** - used to initialize the time domain in top-level Flowsheets. When constructing the time domain in top-level Flowsheets, `time_set` is used to initialize the ContinuousSet or Set created. This can be used to set start and end times, and to establish points of interest in time (e.g. times when disturbances will occur). If `dynamic = True`, `time_set` defaults to `[0.0, 1.0]` if not provided, if `dynamic = False` `time_set` defaults to `[0.0]`. `time_set` is not used in sub-Flowsheets and will be ignored.
- **default_property_package** - can be used to assign the default property package for a Flowsheet. Defaults to `None` if not provided.

Flowsheet Classes

class `idaes.core.flowsheet_model.FlowsheetBlockData` (*component*)

The FlowsheetBlockData Class forms the base class for all IDAES process flowsheet models. The main purpose of this class is to automate the tasks common to all flowsheet models and ensure that the necessary attributes of a flowsheet model are present.

The most significant role of the FlowsheetBlockData class is to automatically create the time domain for the flowsheet.

build()

General build method for FlowsheetBlockData. This method calls a number of sub-methods which automate the construction of expected attributes of flowsheets.

Inheriting models should call *super().build*.

Parameters None –

Returns None

is_flowsheet ()

Method which returns True to indicate that this component is a flowsheet.

Parameters None –

Returns True

model_check ()

This method runs model checks on all unit models in a flowsheet.

This method searches for objects which inherit from UnitModelBlockData and executes the model_check method if it exists.

Parameters None –

Returns None

serialize (*file_base_name*, *overwrite=False*)

Serializes the flowsheet and saves it to a file that can be read by the idaes-model-vis jupyter lab extension.

Parameters

- **file_base_name** – The file prefix to the .idaes.vis file produced. The file is created/saved in the directory that you ran from Jupyter Lab.
- **overwrite** – Boolean to overwrite an existing file_base_name.idaes.vis. If True, the existing file with the same file_base_name will be overwritten. This will cause you to lose any saved layout. If False and there is an existing file with that file_base_name, you will get an error message stating that you cannot save a file to the file_base_name (and therefore overwriting the saved layout). If there is not an existing file with that file_base_name then it saves as normal. Defaults to False.

Returns None

stream_table (*true_state=False*, *time_point=0*, *orient='columns'*)

Method to generate a stream table by iterating over all Arcs in the flowsheet.

Parameters

- **true_state** – whether the state variables (True) or display variables (False, default) from the StateBlocks should be used in the stream table.
- **time_point** – point in the time domain at which to create stream table (default = 0)
- **orient** – whether stream should be shown by columns (“columns”) or rows (“index”)

Returns A pandas dataframe containing stream table information

class idaes.core.flowsheet_model.**FlowsheetBlock** (*args, **kwargs)

FlowsheetBlock is a specialized Pyomo block for IDAES flowsheet models, and contains instances of FlowsheetBlockData.

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic, **default** - useDefault. **Valid values:** { **useDefault** - get flag from parent or False, **True** - set as a dynamic model, **False** - set as a steady-state model. }

time Pointer to the time domain for the flowsheet. Users may provide an existing time domain from another flowsheet, otherwise the flowsheet will search for a parent with a time domain or create a new time domain and reference it here.

time_set Set of points for initializing time domain. This should be a list of floating point numbers, **default** - [0].

default_property_package Indicates the default property package to be used by models within this flowsheet if not otherwise specified, **default** - None. **Valid values:** { **None** - no default property package, a **ParameterBlock** object. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (FlowsheetBlock) New instance

Property Packages

Physical Property Package Classes

Contents

- *Physical Property Package Classes*
 - *Physical Parameter Blocks*
 - *State Blocks*

Physical property packages represent a collection of calculations necessary to determine the state properties of a given material. Property calculations form a critical part of any process model, and thus property packages form the core of the IDAES modeling framework.

Physical property packages consist of two parts:

- PhysicalParameterBlocks, which contain a set of parameters associated with the specific material(s) being modeled, and
- StateBlocks, which contain the actual calculations of the state variables and functions.

Physical Parameter Blocks

Physical Parameter blocks serve as a central location for linking to a property package, and contain all the parameters and indexing sets used by a given property package.

PhysicalParameterBlock Class

The role of the `PhysicalParameterBlock` class is to set up the references required by the rest of the IDAES framework for constructing instances of `StateBlocks` and attaching these to the `PhysicalParameter` block for ease of use. This allows other models to be pointed to the `PhysicalParameter` block in order to collect the necessary information and to construct the necessary `StateBlocks` without the need for the user to do this manually.

Physical property packages form the core of any process model in the IDAES modeling framework, and are used by all of the other modeling components to inform them of what needs to be constructed. In order to do this, the IDAES modeling framework looks for a number of attributes in the `PhysicalParameter` block which are used to inform the construction of other components.

- `state_block_class` - a pointer to the associated class that should be called when constructing `StateBlocks`.
- `phase_list` - a Pyomo Set object defining the valid phases of the mixture of interest.
- `component_list` - a Pyomo Set defining the names of the chemical species present in the mixture.
- `element_list` - (optional) a Pyomo Set defining the names of the chemical elements that make up the species within the mixture. This is used when doing elemental material balances.
- `element_comp` - (optional) a dict-like object which defines the elemental composition of each species in `component_list`. Form: `component: {element_1: value, element_2: value, ...}`.
- `supported_properties_metadata` - a list of supported physical properties that the property package supports, along with instruction to the framework on how to construct the associated variables and constraints, and the units of measurement used for the property. This information is set using the `add_properties` attribute of the `define_metadata` class method.

Physical Parameter Configuration Arguments

Physical Parameter blocks have one standard configuration argument:

- `default_arguments` - this allows the user to provide a set of default values for construction arguments in associated `StateBlocks`, which will be passed to all `StateBlocks` when they are constructed.

class `idaes.core.property_base.PhysicalParameterBlock` (*component*)

This is the base class for thermophysical parameter blocks. These are blocks that contain a set of parameters associated with a specific thermophysical property package, and are linked to by all instances of that property package.

build()

General build method for `PropertyParameterBlocks`. Inheriting models should call `super().build`.

Parameters None –

Returns None

get_phase_component_set()

Method to get phase-component set for property package. If a phase- component set has not been constructed yet, this method will construct one.

Parameters None –

Returns Phase-component Set object

State Blocks

State Blocks are used within all IDAES Unit models (generally within ControlVolume Blocks) in order to calculate physical properties given the state of the material. State Blocks are notably different to other types of Blocks within IDAES as they are always indexed by time (and possibly space as well). There are two base Classes associated with State Blocks:

- `StateBlockData` forms the base class for all `StateBlockData` objects, which contain the instructions on how to construct each instance of a State Block.
- `StateBlock` is used for building classes which contain methods to be applied to sets of Indexed State Blocks (or to a subset of these). See the documentation on `declare_process_block_class` and the IDAES tutorials and examples for more information.

State Block Construction Arguments

State Blocks have the following construction arguments:

- `parameters` - a reference to the associated Physical Parameter block which will be used to make references to all necessary parameters.
- `defined_state` - this argument indicates whether the State Block should expect the material state to be fully defined by another part of the flowsheet (such as by an upstream unit operation). This argument is used to determine whether constraints such as sums of mole fractions should be enforced.
- `has_phase_equilibrium` - indicates whether the associated Control Volume or Unit model expects phase equilibrium to be enforced (if applicable).

StateBlockData Class

`StateBlockData` contains the code necessary for implementing the as needed construction of variables and constraints.

class `idaes.core.property_base.StateBlockData` (*component*)

This is the base class for state block data objects. These are blocks that contain the Pyomo components associated with calculating a set of thermophysical and transport properties for a given material.

build()

General build method for `StateBlockData`s.

Parameters None –

Returns None

calculate_bubble_point_pressure (**args, **kwargs*)

Method which computes the bubble point pressure for a multi- component mixture given a temperature and mole fraction.

calculate_bubble_point_temperature (**args, **kwargs*)

Method which computes the bubble point temperature for a multi- component mixture given a pressure and mole fraction.

calculate_dew_point_pressure (**args, **kwargs*)

Method which computes the dew point pressure for a multi- component mixture given a temperature and mole fraction.

calculate_dew_point_temperature (*args, **kwargs)

Method which computes the dew point temperature for a multi- component mixture given a pressure and mole fraction.

define_display_vars ()

Method used to specify components to use to generate stream tables and other outputs. Defaults to define_state_vars, and developers should overload as required.

define_port_members ()

Method used to specify components to populate Ports with. Defaults to define_state_vars, and developers should overload as required.

define_state_vars ()

Method that returns a dictionary of state variables used in property package. Implement a placeholder method which returns an Exception to force users to overload this.

get_energy_density_terms (*args, **kwargs)

Method which returns a valid expression for enthalpy density to use in the energy balances.

get_energy_diffusion_terms (*args, **kwargs)

Method which returns a valid expression for energy diffusion to use in the energy balances.

get_enthalpy_flow_terms (*args, **kwargs)

Method which returns a valid expression for enthalpy flow to use in the energy balances.

get_material_density_terms (*args, **kwargs)

Method which returns a valid expression for material density to use in the material balances .

get_material_diffusion_terms (*args, **kwargs)

Method which returns a valid expression for material diffusion to use in the material balances.

get_material_flow_basis (*args, **kwargs)

Method which returns an Enum indicating the basis of the material flow term.

get_material_flow_terms (*args, **kwargs)

Method which returns a valid expression for material flow to use in the material balances.

StateBlock Class

class `idaes.core.property_base.StateBlock` (*args, **kwargs)

This is the base class for state block objects. These are used when constructing the SimpleBlock or IndexedBlock which will contain the PropertyData objects, and contains methods that can be applied to multiple StateBlock-Data objects simultaneously.

initialize (*args, **kwargs)

This is a default initialization routine for StateBlocks to ensure that a routine is present. All StateBlockData classes should overload this method with one suited to the particular property package

Parameters None –

Returns None

report (index=0, true_state=False, dof=False, ostream=None, prefix=’')

Default report method for StateBlocks. Returns a Block report populated with either the display or state variables defined in the StateBlockData class.

Parameters

- **index** – tuple of Block indices indicating which point in time (and space if applicable) to report state at.

- **true_state** – whether to report the display variables (False default) or the actual state variables (True)
- **dof** – whether to show local degrees of freedom in the report (default=False)
- **ostream** – output stream to write report to
- **prefix** – string to append to the beginning of all output lines

Returns Printed output to ostream

Reaction Property Package Classes

Contents

- *Reaction Property Package Classes*
 - *Reaction Parameter Blocks*
 - *Reaction Blocks*

Reaction property packages represent a collection of calculations necessary to determine the reaction behavior of a mixture at a given state. Reaction properties depend upon the state and physical properties of the material, and thus must be linked to a StateBlock which provides the necessary state and physical property information.

Reaction property packages consist of two parts:

- ReactionParameterBlocks, which contain a set of parameters associated with the specific reaction(s) being modeled, and
- ReactionBlocks, which contain the actual calculations of the reaction behavior.

Reaction Parameter Blocks

Reaction Parameter blocks serve as a central location for linking to a reaction property package, and contain all the parameters and indexing sets used by a given reaction package.

ReactionParameterBlock Class

The role of the ReactionParameterBlock class is to set up the references required by the rest of the IDAES framework for constructing instances of ReactionBlocks and attaching these to the ReactionParameter block for ease of use. This allows other models to be pointed to the ReactionParameter block in order to collect the necessary information and to construct the necessary ReactionBlocks without the need for the user to do this manually.

Reaction property packages are used by all of the other modeling components to inform them of what needs to be constructed when dealing with chemical reactions. In order to do this, the IDAES modeling framework looks for a number of attributes in the ReactionParameter block which are used to inform the construction of other components.

- **reaction_block_class** - a pointer to the associated class that should be called when constructing ReactionBlocks.
- **phase_list** - a Pyomo Set object defining the valid phases of the mixture of interest.
- **component_list** - a Pyomo Set defining the names of the chemical species present in the mixture.
- **rate_reaction_idx** - a Pyomo Set defining a list of names for the kinetically controlled reactions of interest.

- `rate_reaction_stoichiometry` - a dict-like object defining the stoichiometry of the kinetically controlled reactions. Keys should be tuples of (`rate_reaction_idx`, `phase_list`, `component_list`) and values equal to the stoichiometric coefficient for that index.
- `equilibrium_reaction_idx` - a Pyomo Set defining a list of names for the equilibrium controlled reactions of interest.
- `equilibrium_reaction_stoichiometry` - a dict-like object defining the stoichiometry of the equilibrium controlled reactions. Keys should be tuples of (`equilibrium_reaction_idx`, `phase_list`, `component_list`) and values equal to the stoichiometric coefficient for that index.
- `supported_properties_metadata` - a list of supported reaction properties that the property package supports, along with instruction to the framework on how to construct the associated variables and constraints, and the units of measurement used for the property. This information is set using the `add_properties` attribute of the `define_metadata` class method.
- `required_properties_metadata` - a list of physical properties that the reaction property calculations depend upon, and must be supported by the associated StateBlock. This information is set using the `add_required_properties` attribute of the `define_metadata` class method.

Reaction Parameter Configuration Arguments

Reaction Parameter blocks have two standard configuration arguments:

- `property_package` - a pointer to a `PhysicalParameterBlock` which will be used to construct the StateBlocks to which associated ReactionBlocks will be linked. Reaction property packages must be tied to a single Physical property package, and this is used to validate the connections made later when constructing ReactionBlocks.
- `default_arguments` - this allows the user to provide a set of default values for construction arguments in associated ReactionBlocks, which will be passed to all ReactionBlocks when they are constructed.

class `idaes.core.reaction_base.ReactionParameterBlock` (*component*)

This is the base class for reaction parameter blocks. These are blocks that contain a set of parameters associated with a specific reaction package, and are linked to by all instances of that reaction package.

build ()

General build method for ReactionParameterBlocks. Inheriting models should call `super().build`.

Parameters None –

Returns None

Reaction Blocks

Reaction Blocks are used within IDAES Unit models (generally within ControlVolume Blocks) in order to calculate reaction properties given the state of the material (provided by an associated StateBlock). Reaction Blocks are notably different to other types of Blocks within IDAES as they are always indexed by time (and possibly space as well), and are also not fully self contained (in that they depend upon the associated state block for certain variables). There are two bases Classes associated with Reaction Blocks:

- `ReactionBlockDataBase` forms the base class for all `ReactionBlockData` objects, which contain the instructions on how to construct each instance of a Reaction Block.
- `ReactionBlockBase` is used for building classes which contain methods to be applied to sets of Indexed Reaction Blocks (or to a subset of these). See the documentation on `declare_process_block_class` and the IDAES tutorials and examples for more information.

Reaction Block Construction Arguments

Reaction Blocks have the following construction arguments:

- `parameters` - a reference to the associated Reaction Parameter block which will be used to make references to all necessary parameters.
- `state_block` - a reference to the associated StateBlock which will provide the necessary state and physical property information.
- `has_equilibrium` - indicates whether the associated Control Volume or Unit model expects chemical equilibrium to be enforced (if applicable).

ReactionBlockDataBase Class

ReactionBlockDataBase contains the code necessary for implementing the as needed construction of variables and constraints.

class `idaes.core.reaction_base.ReactionBlockDataBase` (*component*)

This is the base class for reaction block data objects. These are blocks that contain the Pyomo components associated with calculating a set of reaction properties for a given material.

build ()

General build method for PropertyBlockDatas. Inheriting models should call `super().build`.

Parameters None –

Returns None

get_reaction_rate_basis ()

Method which returns an Enum indicating the basis of the reaction rate term.

ReactionBlockBase Class

class `idaes.core.reaction_base.ReactionBlockBase` (**args, **kwargs*)

This is the base class for reaction block objects. These are used when constructing the SimpleBlock or IndexedBlock which will contain the PropertyData objects, and contains methods that can be applied to multiple ReactionBlockData objects simultaneously.

initialize (**args*)

This is a default initialization routine for ReactionBlocks to ensure that a routine is present. All Reaction-BlockData classes should overload this method with one suited to the particular reaction package

Parameters None –

Returns None

IDAES Property Packages

The IDAES process modeling framework divides property calculations into two parts;

- physical and transport properties
- chemical reaction properties

Defining the calculations to be used when calculating properties is done via “property packages”, which contain a set of related calculations for a number of properties of interest. Property packages may be general in purpose, such as ideal gas equations, or specific to a certain application.

As Needed Properties

Process flow sheets often require a large number of properties to be calculate, but not all of these are required in every unit operation. Calculating additional properties that are not required is undesirable, as it leads to larger problem sizes and unnecessary complexity of the resulting model.

To address this, the IDAES modeling framework supports “as needed” construction of properties, where the variables and constraints required to calculate a given quantity are not added to a model unless the model calls for this quantity. To designate a property as an “as needed” quantity, a method can be declared in the associated property BlockData class (StateBlockData or ReactionBlockData) which contains the instructions for constructing the variables and constraints associated with the quantity (rather than declaring these within the BlockData’s build method). The name of this method can then be associated with the property via the `add_properties` metadata in the property packages ParameterBlock, which indicates to the framework that when this property is called for, the associated method should be run.

The `add_properties` metadata can also indicate that a property should always be present (i.e. constructed in the BlockData’s build method) by setting the method to `None`, or that it is not supported by setting the method to `False`.

Unit Model Class

The UnitModelBlock class is designed to form the basis of all IDAES Unit Models, and contains a number of methods which are common to all Unit Models.

UnitModelBlock Construction Arguments

The UnitModelBlock class by default has only one construction argument, which is listed below. However, most models inheriting from UnitModelBlock should declare their own set of configuration arguments which contain more information on how the model should be constructed.

- `dynamic` - indicates whether the Unit model should be dynamic or steady-state, and if `dynamic = True`, the unit is declared to be a dynamic model. `dynamic` defaults to `useDefault` if not provided when instantiating the Unit model (see below for more details). It is possible to declare steady-state Unit models as part of dynamic Flowsheets if desired, however the reverse is not true (cannot have dynamic Unit models within steady-state Flowsheets).

Collecting Time Domain

The next task of the UnitModelBlock class is to establish the time domain for the unit by collecting the necessary information from the parent Flowsheet model. If the dynamic construction argument is set to `useDefault` then the Unit model looks to its parent model for the dynamic argument, otherwise the value provided at construction is used.

Finally, if the Unit model has a construction argument named “`has_holdup`” (not part of the base class), then this is checked to ensure that if `dynamic = True` then `has_holdup` is also `True`. If this check fails then a `ConfigurationError` exception will be thrown.

Modeling Support Methods

The UnitModelBlock class also contains a number of methods designed to facilitate the construction of common components of a model, and these are described below.

Build Inlets Method

All (or almost all) Unit Models will have inlets and outlets which allow material to flow in and out of the unit being modeled. In order to save the model developer from having to write the code for each inlet themselves, UnitModelBlock contains a method named *build_inlet_port* which can automatically create an inlet to a specified ControlVolume block (or linked to a specified StateBlock). The *build_inlet_port* method is described in more detail in the documentation below.

Build Outlets Method

Similar to *build_inlet_port*, UnitModelBlock also has a method named *build_outlet_port* for constructing outlets from Unit models. The *build_outlet_port* method is described in more detail in the documentation below.

Model Check Method

In order to support the IDAES Model Check tools, UnitModelBlock contains a simple *model_check* method which assumes a single Holdup block and calls the *model_check* method on this block. Model developers are encouraged to create their own *model_check* methods for their particular applications.

Initialization Routine

All Unit Models need to have an initialization routine, which should be customized for each Unit model. In order to ensure that all Unit models have at least a basic initialization routine, UnitModelBlock contains a generic initialization procedure which may be sufficient for simple models with only one Holdup Block. Model developers are strongly encouraged to write their own initialization routines rather than relying on the default method.

UnitModelBlock Classes

class `idaes.core.unit_model.UnitModelBlockData` (*component*)

This is the class for process unit operations models. These are models that would generally appear in a process flowsheet or superstructure.

add_inlet_port (*name=None, block=None, doc=None*)

This is a method to build inlet Port objects in a unit model and connect these to a specified control volume or state block.

The name and block arguments are optional, but must be used together. i.e. either both arguments are provided or neither.

Keyword Arguments

- **name** – name to use for Port object (default = “inlet”).
- **block** – an instance of a ControlVolume or StateBlock to use as the source to populate the Port object. If a ControlVolume is provided, the method will use the inlet state block as defined by the ControlVolume. If not provided, method will attempt to default to an object named *control_volume*.
- **doc** – doc string for Port object (default = “Inlet Port”)

Returns A Pyomo Port object and associated components.

add_outlet_port (*name=None, block=None, doc=None*)

This is a method to build outlet Port objects in a unit model and connect these to a specified control volume or state block.

The name and block arguments are optional, but must be used together. i.e. either both arguments are provided or neither.

Keyword Arguments

- **name** – name to use for Port object (default = “outlet”).
- **block** – an instance of a ControlVolume or StateBlock to use as the source to populate the Port object. If a ControlVolume is provided, the method will use the outlet state block as defined by the ControlVolume. If not provided, method will attempt to default to an object named control_volume.
- **doc** – doc string for Port object (default = “Outlet Port”)

Returns A Pyomo Port object and associated components.

add_port (*name=None, block=None, doc=None*)

This is a method to build Port objects in a unit model and connect these to a specified StateBlock.

Keyword Arguments

- **name** – name to use for Port object.
- **block** – an instance of a StateBlock to use as the source to populate the Port object
- **doc** – doc string for Port object

Returns A Pyomo Port object and associated components.

add_state_material_balances (*balance_type, state_1, state_2*)

Method to add material balances linking two State Blocks in a Unit Model. This method is not intended to replace Control Volumes, but to automate writing material balances linking isolated State Blocks in those models where this is required.

Parameters

- – **a MaterialBalanceType Enum indicating the type**
(*balance_type*) – of material balances to write
- – **first State Block to be linked by balances** (*state_1*) –
- – **second State Block to be linked by balances** (*state_2*) –

Returns None

build ()

General build method for UnitModelBlockData. This method calls a number of sub-methods which automate the construction of expected attributes of unit models.

Inheriting models should call *super().build*.

Parameters None –

Returns None

initialize (*state_args=None, outlvl=0, solver='ipopt', optarg={'tol': 1e-06}*)

This is a general purpose initialization routine for simple unit models. This method assumes a single ControlVolume block called controlVolume, and first initializes this and then attempts to solve the entire unit.

More complex models should overload this method with their own initialization routines,

Keyword Arguments

- **state_args** – a dict of arguments to be passed to the property package(s) to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={ ‘tol’: 1e-6})
- **solver** – str indicating which solver to use during initialization (default = ‘ipopt’)

Returns None

model_check()

This is a general purpose initialization routine for simple unit models. This method assumes a single ControlVolume block called controlVolume and tries to call the model_check method of the controlVolume block. If an AttributeError is raised, the check is passed.

More complex models should overload this method with a model_check suited to the particular application, especially if there are multiple ControlVolume blocks present.

Parameters None –

Returns None

```
class idaes.core.unit_model.UnitModelBlock(*args, **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.

Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (UnitModelBlock) New instance

Control Volume Classes**0D Control Volume Class**

Contents

- *0D Control Volume Class*
 - *ControlVolume0DBlock Equations*

The ControlVolume0DBlock block is the most commonly used Control Volume class, and is used for systems where there is a well-mixed volume of fluid, or where variations in spatial domains are considered to be negligible. ControlVolume0DBlock blocks generally contain two *StateBlocks* - one for the incoming material and one for the material within and leaving the volume - and one *StateBlocks*.

class `idaes.core.control_volume0d.ControlVolume0DBlock(*args, **kwargs)`

ControlVolume0DBlock is a specialized Pyomo block for IDAES non-discretized control volume blocks, and contains instances of ControlVolume0DBlockData.

ControlVolume0DBlock should be used for any control volume with a defined volume and distinct inlets and outlets which does not require spatial discretization. This encompasses most basic unit models used in process modeling.

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic, **default** - useDefault. **Valid values:** { **useDefault** - get flag from parent, **True** - set as a dynamic model, **False** - set as a steady-state model }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **True** - construct holdup terms, **False** - do not construct holdup terms }

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

reaction_package Reaction parameter object used to define reaction calculations, **default** - None. **Valid values:** { **None** - no reaction package, **ReactionParameterBlock** - a ReactionParameterBlock object. }

reaction_package_args A ConfigBlock with arguments to be passed to a reaction block(s) and used when constructing these, **default** - None. **Valid values:** { see reaction package for documentation. }

auto_construct If set to True, this argument will trigger the auto_construct method which will attempt to construct a set of material, energy and momentum balance equations based on the parent unit’s config block. The parent unit must have a config block which derives from CONFIG_Base, **default** - False. **Valid values:** { **True** - use automatic construction, **False** - do not use automatic construction. }

- **initialize**(*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map**(*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (ControlVolume0DBlock) New instance

class `idaes.core.control_volume0d.ControlVolume0DBlockData` (*component*)
0-Dimensional (Non-Discretised) ControlVolume Class

This class forms the core of all non-discretized IDAES models. It provides methods to build property and reaction blocks, and add mass, energy and momentum balances. The form of the terms used in these constraints is specified in the chosen property package.

add_geometry ()

Method to create volume Var in ControlVolume.

Parameters None –

Returns None

add_phase_component_balances (*has_rate_reactions=False, has_equilibrium_reactions=False, has_phase_equilibrium=False, has_mass_transfer=False, custom_molar_term=None, custom_mass_term=None*)

This method constructs a set of 0D material balances indexed by time, phase and component.

Parameters

- **has_rate_reactions** – whether default generation terms for rate reactions should be included in material balances
- **has_equilibrium_reactions** – whether generation terms should for chemical equilibrium reactions should be included in material balances
- **has_phase_equilibrium** – whether generation terms should for phase equilibrium behaviour should be included in material balances
- **has_mass_transfer** – whether generic mass transfer terms should be included in material balances
- **custom_molar_term** – a Pyomo Expression representing custom terms to be included in material balances on a molar basis. Expression must be indexed by time, phase list and component list
- **custom_mass_term** – a Pyomo Expression representing custom terms to be included in material balances on a mass basis. Expression must be indexed by time, phase list and component list

Returns Constraint object representing material balances

add_phase_energy_balances (**args, **kwargs*)

Method for adding energy balances (including kinetic energy) indexed by phase to the control volume.

See specific control volume documentation for details.

add_phase_enthalpy_balances (**args, **kwargs*)

Method for adding enthalpy balances indexed by phase to the control volume.

See specific control volume documentation for details.

add_phase_momentum_balances (**args, **kwargs*)

Method for adding momentum balances indexed by phase to the control volume.

See specific control volume documentation for details.

add_phase_pressure_balances (*args, **kwargs)

Method for adding pressure balances indexed by phase to the control volume.

See specific control volume documentation for details.

add_reaction_blocks (has_equilibrium=None)

This method constructs the reaction block for the control volume.

Parameters

- **has_equilibrium** – indicates whether equilibrium calculations will be required in reaction block
- **package_arguments** – dict-like object of arguments to be passed to reaction block as construction arguments

Returns None

add_state_blocks (information_flow=<FlowDirection.forward: 1>, has_phase_equilibrium=None)

This method constructs the inlet and outlet state blocks for the control volume.

Parameters

- **information_flow** – a FlowDirection Enum indicating whether information flows from inlet-to-outlet or outlet-to-inlet
- **has_phase_equilibrium** – indicates whether equilibrium calculations will be required in state blocks
- **package_arguments** – dict-like object of arguments to be passed to state blocks as construction arguments

Returns None

add_total_component_balances (has_rate_reactions=False, has_equilibrium_reactions=False, has_phase_equilibrium=False, has_mass_transfer=False, custom_molar_term=None, custom_mass_term=None)

This method constructs a set of 0D material balances indexed by time and component.

Parameters

- **whether default generation terms for rate** (has_rate_reactions) – reactions should be included in material balances
- **whether generation terms should for** (has_equilibrium_reactions) – chemical equilibrium reactions should be included in material balances
- **whether generation terms should for phase** (has_phase_equilibrium) – equilibrium behaviour should be included in material balances
- **whether generic mass transfer terms should be** (has_mass_transfer) – included in material balances
- **a Pyomo Expression representing custom terms to** (custom_molar_term) – be included in material balances on a molar basis. Expression must be indexed by time, phase list and component list
- **a Pyomo Expression representing custom terms to** – be included in material balances on a mass basis. Expression must be indexed by time, phase list and component list

Returns Constraint object representing material balances

add_total_element_balances (*has_rate_reactions=False, has_equilibrium_reactions=False,*
has_phase_equilibrium=False, has_mass_transfer=False,
custom_elemental_term=None)

This method constructs a set of 0D element balances indexed by time.

Parameters

- **whether default generation terms for rate**
(*has_rate_reactions*) – reactions should be included in material balances
- **whether generation terms should for** (*has_equilibrium_reactions*)
– chemical equilibrium reactions should be included in material balances
- **whether generation terms should for phase**
(*has_phase_equilibrium*) – equilibrium behaviour should be included in material balances
- **whether generic mass transfer terms should be**
(*has_mass_transfer*) – included in material balances
- **a Pyomo Expression representing custom**
(*custom_elemental_term*) – terms to be included in material balances on a molar elemental basis. Expression must be indexed by time and element list

Returns Constraint object representing material balances

add_total_energy_balances (**args, **kwargs*)

Method for adding a total energy balance (including kinetic energy) to the control volume.

See specific control volume documentation for details.

add_total_enthalpy_balances (*has_heat_of_reaction=False, has_heat_transfer=False,*
has_work_transfer=False, custom_term=None)

This method constructs a set of 0D enthalpy balances indexed by time and phase.

Parameters

- **whether terms for heat of reaction should**
(*has_heat_of_reaction*) – be included in enthalpy balance
- **whether terms for heat transfer should be**
(*has_heat_transfer*) – included in enthalpy balances
- **whether terms for work transfer should be**
(*has_work_transfer*) – included in enthalpy balances
- **a Pyomo Expression representing custom terms to**
(*custom_term*) – be included in enthalpy balances. Expression must be indexed by time and phase list

Returns Constraint object representing enthalpy balances

add_total_material_balances (**args, **kwargs*)

Method for adding a total material balance to the control volume.

See specific control volume documentation for details.

add_total_momentum_balances (**args, **kwargs*)

Method for adding a total momentum balance to the control volume.

See specific control volume documentation for details.

add_total_pressure_balances (*has_pressure_change=False, custom_term=None*)

This method constructs a set of 0D pressure balances indexed by time.

Parameters

- **whether terms for pressure change should be** (*has_pressure_change*) – included in enthalpy balances
- **a Pyomo Expression representing custom terms to** (*custom_term*) – be included in pressure balances. Expression must be indexed by time

Returns Constraint object representing pressure balances

build()

Build method for ControlVolume0DBlock blocks.

Returns None

initialize (*state_args=None, outlvl=0, optarg=None, solver='ipopt', hold_state=True*)

Initialization routine for 0D control volume (default solver ipopt)

Keyword Arguments

- **state_args** – a dict of arguments to be passed to the property package(s) to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output log level of initialization routine
- **optarg** – solver options dictionary object (default=None)
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')
- **hold_state** – flag indicating whether the initialization routine should unfix any state variables fixed during initialization, **default** - True. **Valid values:** **True** - states variables are not unfixed, and a dict of returned containing flags for which states were fixed during initialization, **False** - state variables are unfixed after initialization by calling the `release_state` method.

Returns If `hold_states` is True, returns a dict containing flags for which states were fixed during initialization.

model_check()

This method executes the `model_check` methods on the associated state blocks (if they exist). This method is generally called by a unit model as part of the unit's `model_check` method.

Parameters None –

Returns None

release_state (*flags, outlvl=0*)

Method to release state variables fixed during initialization.

Keyword Arguments

- **flags** – dict containing information of which state variables were fixed during initialization, and should now be unfixed. This dict is returned by `initialize` if `hold_state = True`.
- **outlvl** – sets output level of logging

Returns None

ControlVolume0DBlock Equations

This section documents the variables and constraints created by each of the methods provided by the ControlVolume0DBlock class.

- t indicates time index
- p indicates phase index
- j indicates component index
- e indicates element index
- r indicates reaction name index

add_geometry

The add_geometry method creates a single variable within the control volume named *volume* indexed by time (allowing for varying volume over time). A number of other methods depend on this variable being present, thus this method should generally be called first.

Variables

Variable Name	Symbol	Indices	Conditions
volume	V_t	t	None

Constraints

No additional constraints

add_phase_component_balances

Material balances are written for each component in each phase (e.g. separate balances for liquid water and steam). Physical property packages may include information to indicate that certain species do not appear in all phases, and material balances will not be written in these cases (if *has_holdup* is True holdup terms will still appear for these species, however these will be set to 0).

Variables

Variable Name	Symbol	Indices	Conditions
material_holdup	$M_{t,p,j}$	t, p, j	has_holdup = True
phase_fraction	$\phi_{t,p}$	t, p	has_holdup = True
material_accumulation	$\frac{\partial M_{t,p,j}}{\partial t}$	t, p, j	dynamic = True
rate_reaction_generation	$N_{kinetic,t,p,j}$	t, p, j	has_rate_reactions = True
rate_reaction_extent	$X_{kinetic,t,r}$	t, r	has_rate_reactions = True
equilibrium_reaction_generation	$N_{equilibrium,t,p,j}$	t, p, j	has_equilibrium_reactions = True
equilibrium_reaction_extent	$X_{equilibrium,t,r}$	t, r	has_equilibrium_reactions = True
phase_equilibrium_generation	$N_{pe,t,p,j}$	t, p, j	has_phase_equilibrium = True
mass_transfer_term	$N_{transfer,t,p,j}$	t, p, j	has_mass_transfer = True

Constraints

material_balances(t, p, j):

$$\frac{\partial M_{t,p,j}}{\partial t} = F_{in,t,p,j} - F_{out,t,p,j} + N_{kinetic,t,p,j} + N_{equilibrium,t,p,j} + N_{pe,t,p,j} + N_{transfer,t,p,j} + N_{custom,t,p,j}$$

The $N_{custom,t,p,j}$ term allows the user to provide custom terms (variables or expressions) in both mass and molar basis which will be added into the material balances, which will be converted as necessary to the same basis as the material balance (by multiplying or dividing by the component molecular weight). The basis of the material balance is determined by the physical property package, and if undefined (or not mass or mole basis), an Exception will be returned.

If *has_holdup* is True, *material_holdup_calculation*(*t*, *p*, *j*):

$$M_{t,p,j} = \rho_{t,p,j} \times V_t \times \phi_{t,p}$$

where $\rho_{t,p,j}$ is the density of component *j* in phase *p* at time *t*

If *dynamic* is True:

Numerical discretization of the derivative terms, $\frac{\partial M_{t,p,j}}{\partial t}$, will be performed by Pyomo.DAE.

If *has_rate_reactions* is True, *rate_reaction_stoichiometry_constraint*(*t*, *p*, *j*):

$$N_{kinetic,t,p,j} = \alpha_{r,p,j} \times X_{kinetic,t,r}$$

where $\alpha_{r,p,j}$ is the stoichiometric coefficient of component *j* in phase *p* for reaction *r* (as defined in the PhysicalParameterBlock).

If *has_equilibrium_reactions* argument is True, *equilibrium_reaction_stoichiometry_constraint*(*t*, *p*, *j*):

$$N_{equilibrium,t,p,j} = \alpha_{r,p,j} \times X_{equilibrium,t,r}$$

where $\alpha_{r,p,j}$ is the stoichiometric coefficient of component *j* in phase *p* for reaction *r* (as defined in the PhysicalParameterBlock).

add_total_component_balances

Material balances are written for each component across all phases (e.g. one balance for both liquid water and steam). Most terms in the balance equations are still indexed by both phase and component however. Physical property packages may include information to indicate that certain species do not appear in all phases, and material balances will not be written in these cases (if *has_holdup* is True holdup terms will still appear for these species, however these will be set to 0).

Variables

Variable Name	Symbol	Indices	Conditions
material_holdup	$M_{t,p,j}$	t, p, j	has_holdup = True
phase_fraction	$\phi_{t,p}$	t, p	has_holdup = True
material_accumulation	$\frac{\partial M_{t,p,j}}{\partial t}$	t, p, j	dynamic = True
rate_reaction_generation	$N_{kinetic,t,p,j}$	t, p, j	has_rate_reactions = True
rate_reaction_extent	$X_{kinetic,t,r}$	t, r	has_rate_reactions = True
equilibrium_reaction_generation	$N_{equilibrium,t,p,j}$	t, p, j	has_equilibrium_reactions = True
equilibrium_reaction_extent	$X_{equilibrium,t,r}$	t, r	has_equilibrium_reactions = True
mass_transfer_term	$N_{transfer,t,p,j}$	t, p, j	has_mass_transfer = True

Constraints

material_balances(*t*, *j*):

$$\sum_p \frac{\partial M_{t,p,j}}{\partial t} = \sum_p F_{in,t,p,j} - \sum_p F_{out,t,p,j} + \sum_p N_{kinetic,t,p,j} + \sum_p N_{equilibrium,t,p,j} + \sum_p N_{pe,t,p,j} + \sum_p N_{transfer,t,p,j} + N_{cust}$$

The $N_{custom,t,j}$ term allows the user to provide custom terms (variables or expressions) in both mass and molar basis which will be added into the material balances, which will be converted as necessary to the same basis as the material balance (by multiplying or dividing by the component molecular weight). The basis of the material balance is determined by the physical property package, and if undefined (or not mass or mole basis), an Exception will be returned.

If *has_holdup* is True, *material_holdup_calculation*(*t*, *p*, *j*):

$$M_{t,p,j} = \rho_{t,p,j} \times V_t \times \phi_{t,p}$$

where $\rho_{t,p,j}$ is the density of component *j* in phase *p* at time *t*

If *dynamic* is True:

Numerical discretization of the derivative terms, $\frac{\partial M_{t,p,j}}{\partial t}$, will be performed by Pyomo.DAE.

If *has_rate_reactions* is True, *rate_reaction_stoichiometry_constraint*(*t*, *p*, *j*):

$$N_{kinetic,t,p,j} = \alpha_{r,p,j} \times X_{kinetic,t,r}$$

where $\alpha_{r,p,j}$ is the stoichiometric coefficient of component *j* in phase *p* for reaction *r* (as defined in the PhysicalParameterBlock).

If *has_equilibrium_reactions* argument is True, *equilibrium_reaction_stoichiometry_constraint*(*t*, *p*, *j*):

$$N_{equilibrium,t,p,j} = \alpha_{r,p,j} \times X_{equilibrium,t,r}$$

where $\alpha_{r,p,j}$ is the stoichiometric coefficient of component *j* in phase *p* for reaction *r* (as defined in the PhysicalParameterBlock).

add_total_element_balances

Material balances are written for each element in the mixture.

Variables

Variable Name	Symbol	Indices	Conditions
element_holdup	$M_{t,e}$	t, e	has_holdup = True
phase_fraction	$\phi_{t,p}$	t, p	has_holdup = True
element_accumulation	$\frac{\partial M_{t,e}}{\partial t}$	t, e	dynamic = True
elemental_mass_transfer_term	$N_{transfer,t,e}$	t, e	has_mass_transfer = True

Expressions

elemental_flow_in(*t*, *p*, *e*):

$$F_{in,t,p,e} = \sum_j F_{in,t,p,j} \times n_{j,e}$$

elemental_flow_out(*t*, *p*, *e*):

$$F_{out,t,p,e} = \sum_j F_{out,t,p,j} \times n_{j,e}$$

where $n_{j,e}$ is the number of moles of element *e* in component *j*.

Constraints

element_balances(t, e):

$$\frac{\partial M_{t,e}}{\partial t} = \sum_p F_{in,t,p,e} - \sum_p F_{out,t,p,e} + \sum_p N_{transfer,t,e} + N_{custom,t,e}$$

The $N_{custom,t,e}$ term allows the user to provide custom terms (variables or expressions) which will be added into the material balances.

If *has_holdup* is True, *elemental_holdup_calculation(t, e):*

$$M_{t,e} = V_t \times \sum_{p,j} \phi_{t,p} \times \rho_{t,p,j} \times n_{j,e}$$

where $\rho_{t,p,j}$ is the density of component j in phase p at time t

If *dynamic* is True:

Numerical discretization of the derivative terms, $\frac{\partial M_{t,e}}{\partial t}$, will be performed by Pyomo.DAE.

add_total_enthalpy_balances

A single enthalpy balance is written for the entire mixture.

Variables

Variable Name	Symbol	Indices	Conditions
enthalpy_holdup	$E_{t,p}$	t, p	has_holdup = True
phase_fraction	$\phi_{t,p}$	t, p	has_holdup = True
enthalpy_accumulation	$\frac{\partial E_{t,p}}{\partial t}$	t, p	dynamic = True
heat	Q_t	t	has_heat_transfer = True
work	W_t	t	has_work_transfer = True

Expressions

heat_of_reaction(t):

$$Q_{rxn,t} = \text{sum}_r X_{kinetic,t,r} \times \Delta H_{rxn,r} + \text{sum}_r X_{equilibrium,t,r} \times \Delta H_{rxn,r}$$

where $Q_{rxn,t}$ is the total enthalpy released by both kinetic and equilibrium reactions, and $\Delta H_{rxn,r}$ is the specific heat of reaction for reaction r .

Parameters

Parameter Name	Symbol	Default Value
scaling_factor_energy	s_{energy}	1E-6

Constraints

enthalpy_balance(t):

$$s_{energy} \times \sum_p \frac{\partial E_{t,p}}{\partial t} = s_{energy} \times \sum_p H_{in,t,p} - s_{energy} \times \sum_p H_{out,t,p} + s_{energy} \times Q_t + s_{energy} \times W_t + s_{energy} \times Q_{rxn,t} + s_{energy} \times E_{custom,t}$$

The $E_{custom,t}$ term allows the user to provide custom terms which will be added into the energy balance.

If *has_holdup* is True, *enthalpy_holdup_calculation(t, p):*

$$E_{t,p} = h_{t,p} \times V_t \times \phi_{t,p}$$

where $h_{t,p}$ is the enthalpy density (specific enthalpy) of phase p at time t

If *dynamic* is True:

Numerical discretization of the derivative terms, $\frac{\partial E_{t,p}}{\partial t}$, will be performed by Pyomo.DAE.

add_total_pressure_balances

A single pressure balance is written for the entire mixture.

Variables

Variable Name	Symbol	Indices	Conditions
deltaP	ΔP_t	t	has_pressure_change = True

Parameters

Parameter Name	Symbol	Default Value
scaling_factor_pressure	$s_{pressure}$	1E-4

Constraints

pressure_balance(t):

$$0 = s_{pressure} \times P_{in,t} - s_{pressure} \times P_{out,t} + s_{pressure} \times \Delta P_t + s_{pressure} \times \Delta P_{custom,t}$$

The $\Delta P_{custom,t}$ term allows the user to provide custom terms which will be added into the pressure balance.

1D Control Volume Class

Contents

- *1D Control Volume Class*
 - *ControlVolume1DBlock Equations*

The ControlVolume1DBlock block is used for systems with one spatial dimension where material flows parallel to the spatial domain. Examples of these types of unit operations include plug flow reactors and pipes. ControlVolume1DBlock blocks are discretized along the length domain and contain one StateBlock and one ReactionBlock (if applicable) at each point in the domain (including the inlet and outlet).

class `idaes.core.control_volume1d.ControlVolume1DBlock` (*args, **kwargs)

ControlVolume1DBlock is a specialized Pyomo block for IDAES control volume blocks discretized in one spatial direction, and contains instances of ControlVolume1DBlockData.

ControlVolume1DBlock should be used for any control volume with a defined volume and distinct inlets and outlets where there is a single spatial domain parallel to the material flow direction. This encompasses unit operations such as plug flow reactors and pipes.

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.

- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic, **default** - useDefault. **Valid values:** { **useDefault** - get flag from parent, **True** - set as a dynamic model, **False** - set as a steady-state model }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **True** - construct holdup terms, **False** - do not construct holdup terms }

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

reaction_package Reaction parameter object used to define reaction calculations, **default** - None. **Valid values:** { **None** - no reaction package, **ReactionParameterBlock** - a ReactionParameterBlock object. }

reaction_package_args A ConfigBlock with arguments to be passed to a reaction block(s) and used when constructing these, **default** - None. **Valid values:** { see reaction package for documentation. }

auto_construct If set to True, this argument will trigger the auto_construct method which will attempt to construct a set of material, energy and momentum balance equations based on the parent unit’s config block. The parent unit must have a config block which derives from CONFIG_Base, **default** - False. **Valid values:** { **True** - use automatic construction, **False** - do not use automatic construction. }

area_definition Argument defining whether area variable should be spatially variant or not. **default** - DistributedVars.uniform. **Valid values:** { DistributedVars.uniform - area does not vary across spatial domain, DistributedVars.variant - area can vary over the domain and is indexed by time and space. }

transformation_method Method to use to transform domain. Must be a method recognised by the Pyomo TransformationFactory.

transformation_scheme Scheme to use when transforming domain. See Pyomo documentation for supported schemes.

finite_elements Number of finite elements to use in transformation (equivalent to Pyomo nfe argument).

collocation_points Number of collocation points to use (equivalent to Pyomo ncp argument).

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (ControlVolume1DBlock) New instance

class `idaes.core.control_volume1d.ControlVolume1DBlockData` (*component*)

1-Dimensional ControlVolume Class

This class forms the core of all 1-D IDAES models. It provides methods to build property and reaction blocks, and add mass, energy and momentum balances. The form of the terms used in these constraints is specified in the chosen property package.

add_geometry (*length_domain=None*, *length_domain_set=[0.0, 1.0]*,
flow_direction=<FlowDirection.forward: 1>)

Method to create spatial domain and volume Var in ControlVolume.

Parameters

- *length_domain_set* – domain for the ControlVolume. If not provided, a new ContinuousSet will be created (default=None). ContinuousSet should be normalized to run between 0 and 1.
- – a new ContinuousSet if length_domain is not provided (default = [0.0, 1.0]).
- **argument indicating direction of material flow** (*flow_direction*) –

relative to length domain. Valid values:

- FlowDirection.forward (default), flow goes from 0 to 1.
- FlowDirection.backward, flow goes from 1 to 0

Returns None

add_phase_component_balances (*has_rate_reactions=False*, *has_equilibrium_reactions=False*,
has_phase_equilibrium=False, *has_mass_transfer=False*,
custom_molar_term=None, *custom_mass_term=None*)

This method constructs a set of 1D material balances indexed by time, length, phase and component.

Parameters

- **has_rate_reactions** – whether default generation terms for rate reactions should be included in material balances
- **has_equilibrium_reactions** – whether generation terms should for chemical equilibrium reactions should be included in material balances
- **has_phase_equilibrium** – whether generation terms should for phase equilibrium behaviour should be included in material balances
- **has_mass_transfer** – whether generic mass transfer terms should be included in material balances
- **custom_molar_term** – a Pyomo Expression representing custom terms to be included in material balances on a molar basis. Expression must be indexed by time, length domain, phase list and component list
- **custom_mass_term** – a Pyomo Expression representing custom terms to be included in material balances on a mass basis. Expression must be indexed by time, length domain, phase list and component list

Returns Constraint object representing material balances

add_phase_energy_balances (**args*, ***kwargs*)

Method for adding energy balances (including kinetic energy) indexed by phase to the control volume.

See specific control volume documentation for details.

add_phase_enthalpy_balances (*args, **kwargs)

Method for adding enthalpy balances indexed by phase to the control volume.

See specific control volume documentation for details.

add_phase_momentum_balances (*args, **kwargs)

Method for adding momentum balances indexed by phase to the control volume.

See specific control volume documentation for details.

add_phase_pressure_balances (*args, **kwargs)

Method for adding pressure balances indexed by phase to the control volume.

See specific control volume documentation for details.

add_reaction_blocks (has_equilibrium=None)

This method constructs the reaction block for the control volume.

Parameters

- **has_equilibrium** – indicates whether equilibrium calculations will be required in reaction block
- **package_arguments** – dict-like object of arguments to be passed to reaction block as construction arguments

Returns None

add_state_blocks (information_flow=<FlowDirection.forward: 1>, has_phase_equilibrium=None)

This method constructs the state blocks for the control volume.

Parameters

- **information_flow** – a FlowDirection Enum indicating whether information flows from inlet-to-outlet or outlet-to-inlet
- **has_phase_equilibrium** – indicates whether equilibrium calculations will be required in state blocks
- **package_arguments** – dict-like object of arguments to be passed to state blocks as construction arguments

Returns None

add_total_component_balances (has_rate_reactions=False, has_equilibrium_reactions=False, has_phase_equilibrium=False, has_mass_transfer=False, custom_molar_term=None, custom_mass_term=None)

This method constructs a set of 1D material balances indexed by time length and component.

Parameters

- **has_rate_reactions** – whether default generation terms for rate reactions should be included in material balances
- **has_equilibrium_reactions** – whether generation terms should for chemical equilibrium reactions should be included in material balances
- **has_phase_equilibrium** – whether generation terms should for phase equilibrium behaviour should be included in material balances
- **has_mass_transfer** – whether generic mass transfer terms should be included in material balances

- **custom_molar_term** – a Pyomo Expression representing custom terms to be included in material balances on a molar basis. Expression must be indexed by time, length domain and component list
- **custom_mass_term** – a Pyomo Expression representing custom terms to be included in material balances on a mass basis. Expression must be indexed by time, length domain and component list

Returns Constraint object representing material balances

add_total_element_balances (*has_rate_reactions=False, has_equilibrium_reactions=False, has_phase_equilibrium=False, has_mass_transfer=False, custom_elemental_term=None*)

This method constructs a set of 1D element balances indexed by time and length.

Parameters

- **whether default generation terms for rate**
(*has_rate_reactions*) – reactions should be included in material balances
- **whether generation terms should for** (*has_equilibrium_reactions*)
– chemical equilibrium reactions should be included in material balances
- **whether generation terms should for phase**
(*has_phase_equilibrium*) – equilibrium behaviour should be included in material balances
- **whether generic mass transfer terms should be**
(*has_mass_transfer*) – included in material balances
- **a Pyomo Expression representing custom**
(*custom_elemental_term*) – terms to be included in material balances on a molar elemental basis. Expression must be indexed by time, length and element list

Returns Constraint object representing material balances

add_total_energy_balances (**args, **kwargs*)

Method for adding a total energy balance (including kinetic energy) to the control volume.

See specific control volume documentation for details.

add_total_enthalpy_balances (*has_heat_of_reaction=False, has_heat_transfer=False, has_work_transfer=False, custom_term=None*)

This method constructs a set of 1D enthalpy balances indexed by time and phase.

Parameters

- **whether terms for heat of reaction should**
(*has_heat_of_reaction*) – be included in enthalpy balance
- **whether terms for heat transfer should be**
(*has_heat_transfer*) – included in enthalpy balances
- **whether terms for work transfer should be**
(*has_work_transfer*) – included in enthalpy balances
- **a Pyomo Expression representing custom terms to**
(*custom_term*) – be included in enthalpy balances. Expression must be indexed by time, length and phase list

Returns Constraint object representing enthalpy balances

add_total_material_balances (**args, **kwargs*)

Method for adding a total material balance to the control volume.

See specific control volume documentation for details.

add_total_momentum_balances (*args, **kwargs)

Method for adding a total momentum balance to the control volume.

See specific control volume documentation for details.

add_total_pressure_balances (has_pressure_change=False, custom_term=None)

This method constructs a set of 1D pressure balances indexed by time.

Parameters

- **whether terms for pressure change should be** (has_pressure_change) – included in enthalpy balances
- **a Pyomo Expression representing custom terms to** (custom_term) – be included in pressure balances. Expression must be indexed by time and length domain

Returns Constraint object representing pressure balances

apply_transformation ()

Method to apply DAE transformation to the Control Volume length domain. Transformation applied will be based on the Control Volume configuration arguments.

build ()

Build method for ControlVolume1DBlock blocks.

Returns None

initialize (state_args=None, outlvl=0, optarg=None, solver='ipopt', hold_state=True)

Initialization routine for 1D control volume (default solver ipopt)

Keyword Arguments

- **state_args** – a dict of arguments to be passed to the property package(s) to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default=None)
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')
- **hold_state** – flag indicating whether the initialization routine should unfix any state variables fixed during initialization, **default** - True. **Valid values:** **True** - states variables are not unfixed, and a dict of returned containing flags for which states were fixed during initialization, **False** - state variables are unfixed after initialization by calling the release_state method.

Returns If hold_states is True, returns a dict containing flags for which states were fixed during initialization else the release state is triggered.

model_check ()

This method executes the model_check methods on the associated state blocks (if they exist). This method is generally called by a unit model as part of the unit's model_check method.

Parameters None –

Returns None

release_state (flags, outlvl=0)

Method to release state variables fixed during initialization.

Keyword Arguments

- **flags** – dict containing information of which state variables were fixed during initialization, and should now be unfixed. This dict is returned by initialize if hold_state = True.
- **outlvl** – sets output level of logging

Returns None**report** (*time_point=0, dof=False, ostream=None, prefix=""*)

No report method defined for ControlVolume1D class. This is due to the difficulty of presenting spatially discretized data in a readable form without plotting.

ControlVolume1DBlock Equations

This section documents the variables and constraints created by each of the methods provided by the ControlVolume0DBlock class.

- *t* indicates time index
- *x* indicates spatial (length) index
- *p* indicates phase index
- *j* indicates component index
- *e* indicates element index
- *r* indicates reaction name index

Most terms within the balance equations written by ControlVolume1DBlock are on a basis of per unit length (e.g. $\text{mol}/\text{m} \cdot \text{s}$).

add_geometry

The add_geometry method creates the normalized length domain for the control volume (or a reference to an external domain). All constraints in ControlVolume1DBlock assume a normalized length domain, with values between 0 and 1.

This method also adds variables and constraints to describe the geometry of the control volume. ControlVolume1DBlock does not support varying dimensions of the control volume with time at this stage.

Variables

Variable Name	Symbol	Indices	Conditions
length_domain	x	None	None
volume	V	None	None
area	A	None	None
length	L	None	None

Constraints*geometry_constraint:*

$$V = A \times L$$

add_phase_component_balances

Material balances are written for each component in each phase (e.g. separate balances for liquid water and steam). Physical property packages may include information to indicate that certain species do not appear in all phases, and material balances will not be written in these cases (if *has_holdup* is True holdup terms will still appear for these species, however these will be set to 0).

Variables

Variable Name	Symbol	Indices	Conditions
material_holdup	$M_{t,x,p,j}$	t, x, p, j	has_holdup = True
phase_fraction	$\phi_{t,x,p}$	t, x, p	has_holdup = True
material_accumulation	$\frac{\partial M_{t,x,p,j}}{\partial t}$	t, x, p, j	dynamic = True
_flow_terms	$F_{t,x,p,j}$	t, x, p, j	None
material_flow_dx	$\frac{\partial F_{t,x,p,j}}{\partial x}$	t, x, p, j	None
rate_reaction_generation	$N_{kinetic,t,x,p,j}$	t, x, p, j	has_rate_reactions = True
rate_reaction_extent	$X_{kinetic,t,x,r}$	t, x, r	has_rate_reactions = True
equilibrium_reaction_generation	$N_{equilibrium,t,x,p,j}$	t, x, p, j	has_equilibrium_reactions = True
equilibrium_reaction_extent	$X_{equilibrium,t,x,r}$	t, x, r	has_equilibrium_reactions = True
phase_equilibrium_generation	$N_{pe,t,x,p,j}$	t, x, p, j	has_phase_equilibrium = True
mass_transfer_term	$N_{transfer,t,x,p,j}$	t, x, p, j	has_mass_transfer = True

Constraints

material_balances(t, x, p, j):

$$L \times \frac{\partial M_{t,x,p,j}}{\partial t} = fd \times \frac{\partial F_{t,x,p,j}}{\partial x} + L \times N_{kinetic,t,x,p,j} + L \times N_{equilibrium,t,x,p,j} + L \times N_{pe,t,x,p,j} + L \times N_{transfer,t,x,p,j} + L \times N_{custom,t,x,p,j}$$

fd is a flow direction term, which allows for material flow to be defined in either direction. If material flow is defined as *forward*, *fd* = -1, otherwise *fd* = 1.

The $N_{custom,t,x,p,j}$ term allows the user to provide custom terms (variables or expressions) in both mass and molar basis which will be added into the material balances, which will be converted as necessary to the same basis as the material balance (by multiplying or dividing by the component molecular weight). The basis of the material balance is determined by the physical property package, and if undefined (or not mass or mole basis), an Exception will be returned.

material_flow_linking_constraints(t, x, p, j):

This constraint is an internal constraint used to link the extensive material flow terms in the StateBlocks into a single indexed variable. This is required as Pyomo.DAE requires a single indexed variable to create the associated DerivativeVars and their numerical expansions.

If *has_holdup* is True, *material_holdup_calculation(t, x, p, j):*

$$M_{t,x,p,j} = \rho_{t,x,p,j} \times A \times \phi_{t,x,p}$$

where $\rho_{t,x,p,j}$ is the density of component *j* in phase *p* at time *t* and location *x*.

If *dynamic* is True:

Numerical discretization of the derivative terms, $\frac{\partial M_{t,x,p,j}}{\partial t}$, will be performed by Pyomo.DAE.

If *has_rate_reactions* is True, *rate_reaction_stoichiometry_constraint(t, x, p, j):*

$$N_{kinetic,t,x,p,j} = \alpha_{r,p,j} \times X_{kinetic,t,x,r}$$

where $\alpha_{r,p,j}$ is the stoichiometric coefficient of component j in phase p for reaction r (as defined in the PhysicalParameterBlock).

If `has_equilibrium_reactions` argument is True, `equilibrium_reaction_stoichiometry_constraint(t, x, p, j)`:

$$N_{equilibrium,t,x,p,j} = \alpha_{r,p,j} \times X_{equilibrium,t,x,r}$$

where $\alpha_{r,p,j}$ is the stoichiometric coefficient of component j in phase p for reaction r (as defined in the PhysicalParameterBlock).

add_total_component_balances

Material balances are written for each component across all phases (e.g. one balance for both liquid water and steam). Physical property packages may include information to indicate that certain species do not appear in all phases, and material balances will not be written in these cases (if `has_holdup` is True holdup terms will still appear for these species, however these will be set to 0).

Variables

Variable Name	Symbol	Indices	Conditions
material_holdup	$M_{t,x,p,j}$	t, x, p, j	has_holdup = True
phase_fraction	$\phi_{t,x,p}$	t, x, p	has_holdup = True
material_accumulation	$\frac{\partial M_{t,x,p,j}}{\partial t}$	t, x, p, j	dynamic = True
_flow_terms	$F_{t,x,p,j}$	t, x, p, j	None
material_flow_dx	$\frac{\partial F_{t,x,p,j}}{\partial x}$	t, x, p, j	None
rate_reaction_generation	$N_{kinetic,t,x,p,j}$	t, x, p, j	has_rate_reactions = True
rate_reaction_extent	$X_{kinetic,t,x,r}$	t, x, r	has_rate_reactions = True
equilibrium_reaction_generation	$N_{equilibrium,t,x,p,j}$	t, x, p, j	has_equilibrium_reactions = True
equilibrium_reaction_extent	$X_{equilibrium,t,x,r}$	t, x, r	has_equilibrium_reactions = True
mass_transfer_term	$N_{transfer,t,x,p,j}$	t, x, p, j	has_mass_transfer = True

Constraints

`material_balances(t, x, p, j)`:

$$L \times \sum_p \frac{\partial M_{t,x,p,j}}{\partial t} = fd \times \sum \frac{\partial F_{t,x,p,j}}{\partial x} + L \times \sum_p N_{kinetic,t,x,p,j} + L \times \sum_p N_{equilibrium,t,x,p,j} + L \times \sum_p N_{transfer,t,x,p,j} + L \times$$

fd is a flow direction term, which allows for material flow to be defined in either direction. If material flow is defined as *forward*, $fd = -1$, otherwise $fd = 1$.

The $N_{custom,t,x,j}$ term allows the user to provide custom terms (variables or expressions) in both mass and molar basis which will be added into the material balances, which will be converted as necessary to the same basis as the material balance (by multiplying or dividing by the component molecular weight). The basis of the material balance is determined by the physical property package, and if undefined (or not mass or mole basis), an Exception will be returned.

`material_flow_linking_constraints(t, x, p, j)`:

This constraint is an internal constraint used to link the extensive material flow terms in the StateBlocks into a single indexed variable. This is required as Pyomo.DAE requires a single indexed variable to create the associated DerivativeVars and their numerical expansions.

If `has_holdup` is True, `material_holdup_calculation(t, x, p, j)`:

$$M_{t,x,p,j} = \rho_{t,x,p,j} \times A \times \phi_{t,x,p}$$

where $\rho_{t,x,p,j}$ is the density of component j in phase p at time t and location x .

If *dynamic* is True:

Numerical discretization of the derivative terms, $\frac{\partial M_{t,x,p,j}}{\partial t}$, will be performed by Pyomo.DAE.

If *has_rate_reactions* is True, *rate_reaction_stoichiometry_constraint*(t, x, p, j):

$$N_{kinetic,t,x,p,j} = \alpha_{r,p,j} \times X_{kinetic,t,x,r}$$

where $\alpha_{r,p,j}$ is the stoichiometric coefficient of component j in phase p for reaction r (as defined in the PhysicalParameterBlock).

If *has_equilibrium_reactions* argument is True, *equilibrium_reaction_stoichiometry_constraint*(t, x, p, j):

$$N_{equilibrium,t,x,p,j} = \alpha_{r,p,j} \times X_{equilibrium,t,x,r}$$

where $\alpha_{r,p,j}$ is the stoichiometric coefficient of component j in phase p for reaction r (as defined in the PhysicalParameterBlock).

add_total_element_balances

Material balances are written for each element in the mixture.

Variables

Variable Name	Symbol	Indices	Conditions
element_holdup	$M_{t,x,e}$	t, x, e	has_holdup = True
phase_fraction	$\phi_{t,x,p}$	t, x, p	has_holdup = True
element_accumulation	$\frac{\partial M_{t,x,e}}{\partial t}$	t, x, e	dynamic = True
elemental_mass_transfer_term	$N_{transfer,t,x,e}$	t, x, e	has_mass_transfer = True
elemental_flow_term	$F_{t,x,e}$	t, x, e	None

Constraints

elemental_flow_constraint(t, x, e):

$$F_{t,x,e} = \sum_p \sum_j F_{t,x,p,j} \times n_{j,e}$$

where $n_{j,e}$ is the number of moles of element e in component j .

element_balances(t, x, e):

$$L \times \frac{\partial M_{t,x,e}}{\partial t} = fd \times \frac{\partial F_{t,x,e}}{\partial x} + L \times N_{transfer,t,p,j} + L \times N_{custom,t,e}$$

fd is a flow direction term, which allows for material flow to be defined in either direction. If material flow is defined as *forward*, $fd = -1$, otherwise $fd = 1$.

The $N_{custom,t,x,e}$ term allows the user to provide custom terms (variables or expressions) which will be added into the material balances.

If *has_holdup* is True, *elemental_holdup_calculation*(t, x, e):

$$M_{t,x,e} = \rho_{t,x,p,j} \times A \times \phi_{t,x,p}$$

where $\rho_{t,x,p,j}$ is the density of component j in phase p at time t and location x .

If *dynamic* is True:

Numerical discretization of the derivative terms, $\frac{\partial M_{t,x,p,j}}{\partial t}$, will be performed by Pyomo.DAE.

add_total_enthalpy_balances

A single enthalpy balance is written for the entire mixture at each point in the spatial domain.

Variables

Variable Name	Symbol	Indices	Conditions
enthalpy_holdup	$E_{t,x,p}$	t, x, p	has_holdup = True
phase_fraction	$\phi_{t,x,p}$	t, x, p	has_holdup = True
enthalpy_accumulation	$\frac{\partial E_{t,x,p}}{\partial t}$	t, x, p	dynamic = True
_enthalpy_flow	$H_{t,x,p}$	t, x, p	None
enthalpy_flow_dx	$\frac{\partial H_{t,x,p}}{\partial x}$	t, x, p	None
heat	$Q_{t,x}$	t, x	has_heat_transfer = True
work	$W_{t,x}$	t, x	has_work_transfer = True

Expressions

heat_of_reaction(t, x):

$$Q_{rxn,t,x} = \text{sum}_r X_{kinetic,t,x,r} \times \Delta H_{rxn,r} + \text{sum}_r X_{equilibrium,t,x,r} \times \Delta H_{rxn,r}$$

where $Q_{rxn,t,x}$ is the total enthalpy released by both kinetic and equilibrium reactions, and $\Delta H_{rxn,r}$ is the specific heat of reaction for reaction r .

Parameters

Parameter Name	Symbol	Default Value
scaling_factor_energy	s_{energy}	1E-6

Constraints

enthalpy_balance(t):

$$s_{energy} \times L \times \sum_p \frac{\partial E_{t,x,p}}{\partial t} = s_{energy} \times fd \times \sum_p \frac{\partial H_{t,x,p}}{\partial x} + s_{energy} \times L \times Q_{t,x} + s_{energy} \times L \times W_{t,x} + s_{energy} \times L \times Q_{rxn,t,x}$$

fd is a flow direction term, which allows for material flow to be defined in either direction. If material flow is defined as *forward*, $fd = -1$, otherwise $fd = 1$.

The $E_{custom,t,x}$ term allows the user to provide custom terms which will be added into the energy balance.

enthalpy_flow_linking_constraints(t, x, p):

This constraint is an internal constraint used to link the extensive enthalpy flow terms in the StateBlocks into a single indexed variable. This is required as Pyomo.DAE requires a single indexed variable to create the associated DerivativeVars and their numerical expansions.

If *has_holdup* is True, *enthalpy_holdup_calculation(t, x, p):*

$$E_{t,x,p} = h_{t,x,p} \times A \times \phi_{t,x,p}$$

where $h_{t,x,p}$ is the enthalpy density (specific enthalpy) of phase p at time t and location x .

If *dynamic* is True:

Numerical discretization of the derivative terms, $\frac{\partial E_{t,x,p}}{\partial t}$, will be performed by Pyomo.DAE.

add_total_pressure_balances

A single pressure balance is written for the entire mixture at all points in the spatial domain.

Variables

Variable Name	Symbol	Indices	Conditions
pressure	$P_{t,x}$	t, x	None
pressure_dx	$\frac{\partial P_{t,x}}{\partial x}$	t, x	None
deltaP	$\Delta P_{t,x}$	t, x	has_pressure_change = True

Parameters

Parameter Name	Symbol	Default Value
scaling_factor_pressure	$s_{pressure}$	1E-4

Constraints

pressure_balance(t, x):

$$0 = s_{pressure} \times fd \times \frac{\partial P_{t,x}}{\partial x} + s_{pressure} \times L \times \Delta P_{t,x} + s_{pressure} \times L \times \Delta P_{custom,t,x}$$

fd is a flow direction term, which allows for material flow to be defined in either direction. If material flow is defined as *forward*, $fd = -1$, otherwise $fd = 1$.

The $\Delta P_{custom,t,x}$ term allows the user to provide custom terms which will be added into the pressure balance.

pressure_linking_constraint(t, x):

This constraint is an internal constraint used to link the pressure terms in the StateBlocks into a single indexed variable. This is required as Pyomo.DAE requires a single indexed variable to create the associated DerivativeVars and their numerical expansions.

Control Volumes are the center of the IDAES process modeling framework, and serve as the fundamental building block of all unit operations. Control Volumes represent a single, well-defined volume of material over which material, energy and/or momentum balances will be performed.

The IDAES Control Volume classes are designed to facilitate the construction of these balance equations by providing the model developer with a set of pre-built methods to perform the most common tasks in developing models of unit operations. The Control Volume classes contain methods for creating and linking the necessary property calculations and writing common forms of the balance equations so that the model developer can focus their time on the aspects that make each unit model unique.

The IDAES process modeling framework currently supports two types of Control Volume:

- *ControlVolume0DBlock* represents a single well-mixed volume of material with a single inlet and a single outlet. This type of control volume is sufficient to model most inlet-outlet type unit operations which do not require spatial discretization.
- *ControlVolume1DBlock* represents a volume with spatial variation in one dimension parallel to the material flow. This type of control volume is useful for representing flow in pipes and simple 1D flow reactors.

Common Control Volume Tasks

All of the IDAES Control Volume classes are built on a common core (*ControlVolumeBlockData*) which defines a set of common tasks required for all Control Volumes. The more specific Control Volume classes then build upon these common tasks to provide tools appropriate for their specific application.

All Control Volume classes begin with the following tasks:

- Determine if the `ControlVolume` should be steady-state or dynamic.
- Get the time domain.
- Determine whether material and energy holdups should be calculated.
- Collect information necessary for creating `StateBlocks` and `ReactionBlocks`.
- Create references to `phase_list` and `component_list` Sets in the `PhysicalParameterBlock`.

More details on these steps is *provided later*.

Setting up the time domain

The first common task the Control Volume block performs is to determine if it should be dynamic or steady-state and to collect the time domain from the `UnitModel`. Control Volume blocks have an argument `dynamic` which can be provided during construction which specifies if the Control Volume should be dynamic (`dynamic=True`) or steady-state (`dynamic=False`). If the argument is not provided, the Control Volume block will inherit this argument from its parent `UnitModel`.

Finally, the Control Volume checks that the `has_holdup` argument is consistent with the `dynamic` argument, and raises a `ConfigurationError` if it is not.

Getting Property Package Information

If a reference to a property package was not provided by the `UnitModel` as an argument, the Control Volume first checks to see if the `UnitModel` has a `property_package` argument set, and uses this if present. Otherwise, the Control Volume block begins searching up the model tree looking for an argument named `default_property_package` and uses the first of these that it finds. If no `default_property_package` is found, a `ConfigurationError` is returned.

Collecting Indexing Sets for Property Package

The final common step for all Control Volumes is to collect any required indexing sets from the physical property package (for example component and phase lists). These are used by the Control Volume for determining what balance equations need to be written, and what terms to create.

The indexing sets the Control Volume looks for are:

- `component_list` - used to determine what components are present, and thus what material balances are required
- `phase_list` - used to determine what phases are present, and thus what balance equations are required

ControlVolume and ControlVolumeBlockData Classes

A key purpose of Control Volumes is to automate as much of the task of writing a unit model as possible. For this purpose, Control Volumes support a number of methods for common tasks model developers may want to perform. The specifics of these methods will be different between different types of Control Volumes, and certain methods may not be applicable to some types of Control Volumes (in which case a `NotImplementedError` will be returned). A full list of potential methods is provided here, however users should check the documentation for the specific Control Volume they are using for more details on what methods are supported in that specific Control Volume.


```
class idaes.core.control_volume_base.ControlVolume(*args, **kwargs)
```

This class is not usually used directly. Use ControlVolume0DBlock or ControlVolume1DBlock instead.

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic, **default** - useDefault. **Valid values:** { **useDefault** - get flag from parent, **True** - set as a dynamic model, **False** - set as a steady-state model }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **True** - construct holdup terms, **False** - do not construct holdup terms }

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

reaction_package Reaction parameter object used to define reaction calculations, **default** - None. **Valid values:** { **None** - no reaction package, **ReactionParameterBlock** - a ReactionParameterBlock object. }

reaction_package_args A ConfigBlock with arguments to be passed to a reaction block(s) and used when constructing these, **default** - None. **Valid values:** { see reaction package for documentation. }

auto_construct If set to True, this argument will trigger the auto_construct method which will attempt to construct a set of material, energy and momentum balance equations based on the parent unit’s config block. The parent unit must have a config block which derives from CONFIG_Base, **default** - False. **Valid values:** { **True** - use automatic construction, **False** - do not use automatic construction. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (ControlVolume) New instance

```
class idaes.core.control_volume_base.ControlVolumeBlockData(component)
```

The ControlVolumeBlockData Class forms the base class for all IDAES ControlVolume models. The purpose of this class is to automate the tasks common to all control volume blockss and ensure that the necessary attributes of a control volume block are present.

The most significant role of the ControlVolumeBlockData class is to set up the construction arguments for the control volume block, automatically link to the time domain of the parent block, and to get the information about the property and reaction packages.

add_energy_balances (*balance_type*=<*EnergyBalanceType.useDefault: -1*>, ***kwargs*)

General method for adding energy balances to a control volume. This method makes calls to specialised sub-methods for each type of energy balance.

Parameters

- **balance_type** (*EnergyBalanceType*) – Enum indicating which type of energy balance should be constructed.
- **has_heat_of_reaction** (*bool*) – whether terms for heat of reaction should be included in energy balance
- **has_heat_transfer** (*bool*) – whether generic heat transfer terms should be included in energy balances
- **has_work_transfer** (*bool*) – whether generic mass transfer terms should be included in energy balances
- **custom_term** (*Expression*) – a Pyomo Expression representing custom terms to be included in energy balances

Returns Constraint objects constructed by sub-method

add_geometry (**args*, ***kwargs*)

Method for defining the geometry of the control volume.

See specific control volume documentation for details.

add_material_balances (*balance_type*=<*MaterialBalanceType.useDefault: -1*>, ***kwargs*)

General method for adding material balances to a control volume. This method makes calls to specialised sub-methods for each type of material balance.

Parameters

- – **MaterialBalanceType** Enum indicating which type of (*balance_type*) – material balance should be constructed.
- – **whether default generation terms for rate** (*has_rate_reactions*) – reactions should be included in material balances
- – **whether generation terms should for** (*has_equilibrium_reactions*) – chemical equilibrium reactions should be included in material balances
- – **whether generation terms should for phase** (*has_phase_equilibrium*) – equilibrium behaviour should be included in material balances
- – **whether generic mass transfer terms should be** (*has_mass_transfer*) – included in material balances
- – **a Pyomo Expression representing custom terms to** (*custom_mass_term*) – be included in material balances on a molar basis.
- – **a Pyomo Expression representing custom terms to** – be included in material balances on a mass basis.

Returns Constraint objects constructed by sub-method

add_momentum_balances (*balance_type*=<*MomentumBalanceType.pressureTotal: 1*>, ***kwargs*)

General method for adding momentum balances to a control volume. This method makes calls to specialised sub-methods for each type of momentum balance.

Parameters

- **balance_type** (*MomentumBalanceType*) – Enum indicating which type of momentum balance should be constructed. Default = *MomentumBalanceType.pressureTotal*.
- **has_pressure_change** (*bool*) – whether default generation terms for pressure change should be included in momentum balances
- **custom_term** (*Expression*) – a Pyomo Expression representing custom terms to be included in momentum balances

Returns Constraint objects constructed by sub-method

add_phase_component_balances (**args, **kwargs*)

Method for adding material balances indexed by phase and component to the control volume.

See specific control volume documentation for details.

add_phase_energy_balances (**args, **kwargs*)

Method for adding energy balances (including kinetic energy) indexed by phase to the control volume.

See specific control volume documentation for details.

add_phase_enthalpy_balances (**args, **kwargs*)

Method for adding enthalpy balances indexed by phase to the control volume.

See specific control volume documentation for details.

add_phase_momentum_balances (**args, **kwargs*)

Method for adding momentum balances indexed by phase to the control volume.

See specific control volume documentation for details.

add_phase_pressure_balances (**args, **kwargs*)

Method for adding pressure balances indexed by phase to the control volume.

See specific control volume documentation for details.

add_reaction_blocks (**args, **kwargs*)

Method for adding ReactionBlocks to the control volume.

See specific control volume documentation for details.

add_state_blocks (**args, **kwargs*)

Method for adding StateBlocks to the control volume.

See specific control volume documentation for details.

add_total_component_balances (**args, **kwargs*)

Method for adding material balances indexed by component to the control volume.

See specific control volume documentation for details.

add_total_element_balances (**args, **kwargs*)

Method for adding total elemental material balances indexed to the control volume.

See specific control volume documentation for details.

add_total_energy_balances (**args, **kwargs*)

Method for adding a total energy balance (including kinetic energy) to the control volume.

See specific control volume documentation for details.

add_total_enthalpy_balances (**args, **kwargs*)

Method for adding a total enthalpy balance to the control volume.

See specific control volume documentation for details.

add_total_material_balances (*args, **kwargs)

Method for adding a total material balance to the control volume.

See specific control volume documentation for details.

add_total_momentum_balances (*args, **kwargs)

Method for adding a total momentum balance to the control volume.

See specific control volume documentation for details.

add_total_pressure_balances (*args, **kwargs)

Method for adding a total pressure balance to the control volume.

See specific control volume documentation for details.

build()

General build method for Control Volumes blocks. This method calls a number of sub-methods which automate the construction of expected attributes of all ControlVolume blocks.

Inheriting models should call *super().build*.

Parameters None –

Returns None

Auto-Construct Method

To reduce the demands on unit model developers even further, Control Volumes have an optional auto-construct feature that will attempt to populate the Control Volume based on a set of instructions provided at the Unit Model level. If the `auto_construct` configuration argument is set to *True*, the following methods are called automatically in the following order when instantiating the Control Volume.

1. `add_geometry`
2. `add_state_blocks`
3. `add_reaction_blocks`
4. `add_material_balances`
5. `add_energy_balances`
6. `add_momentum_balances`
7. `apply_transformation`

To determine what terms are required for the balance equations, the Control Volume expects the Unit Model to have the following configuration arguments, which are used as arguments to the methods above.

- `dynamic`
- `has_holdup`
- `material_balance_type`
- `energy_balance_type`
- `momentum_balance_type`
- `has_rate_reactions`
- `has_equilibrium_reactions`
- `has_phase_equilibrium`
- `has_mass_transfer`

- `has_heat_of_reaction`
- `has_heat_transfer`
- `has_work_transfer`
- `has_pressure_change`
- `property_package`
- `property_package_args`
- `reaction_package`
- `reaction_package_args`

For convenience, a template `ConfigBlock` (named *CONFIG_Template*) is available in the `control_volume_base.py` module which contains all the necessary arguments which can be inherited by unit models wishing to use the auto-construct feature.

Utility Methods

Utilities for Dynamic Flowsheets

These are utility functions for working with dynamic IDAES flowsheets.

Methods

This module contains utility functions for dynamic IDAES models.

`idaes.core.util.dyn_utils.copy_non_time_indexed_values` (*fs_tgt*, *fs_src*,
copy_fixed=True)

Function to set the values of all variables that are not (implicitly or explicitly) indexed by time to their values in a different flowsheet.

Parameters

- **fs_tgt** – Flowsheet into which values will be copied.
- **fs_src** – Flowsheet from which values will be copied.
- **copy_fixed** – Bool marking whether or not to copy over fixed variables in the target flowsheet.

Returns

None

`idaes.core.util.dyn_utils.copy_values_at_time` (*fs_tgt*, *fs_src*, *t_target*, *t_source*,
copy_fixed=True, *outlvl=0*)

Function to set the values of all (explicitly or implicitly) time-indexed variables in a flowsheet to similar values (with the same name) but at different points in time and (potentially) in different flowsheets.

Parameters

- **fs_tgt** – Target flowsheet, whose variables' values will get set
- **fs_src** – Source flowsheet, whose variables' values will be used to set those of the target flowsheet. Could be the target flowsheet
- **t_target** – Target time point
- **t_source** – Source time point
- **copy_fixed** – Bool of whether or not to copy over fixed variables in target model

- **outlvl** – IDAES logger output level

Returns None

`idaes.core.util.dyn_utils.deactivate_constraints_unindexed_by(b, time)`

Searches block *b* for and constraints not indexed by time and deactivates them.

Parameters

- **b** – Block to search
- **time** – Set with respect to which to find unindexed constraints

Returns List of constraints deactivated

`idaes.core.util.dyn_utils.deactivate_model_at(b, cset, pts, outlvl=0)`

Finds any block or constraint in block *b*, indexed explicitly (and not implicitly) by *cset*, and deactivates it at points specified. Implicitly indexed components are excluded because one of their parent blocks will be deactivated, so deactivating them too would be redundant.

Parameters

- **b** – Block to search
- **cset** – ContinuousSet of interest
- **pts** – Value or list of values, in ContinuousSet, to deactivate at

Returns A dictionary mapping points in *pts* to lists of component data that have been deactivated there

`idaes.core.util.dyn_utils.fix_vars_unindexed_by(b, time)`

Searches block *b* for variables not indexed by time and fixes them.

Parameters

- **b** – Block to search
- **time** – Set with respect to which to find unindexed variables

Returns List of variables fixed

`idaes.core.util.dyn_utils.get_activity_dict(b)`

Function that builds a dictionary telling whether or not each ConstraintData and BlockData object in a model is active. Uses the objects' ids as the hash.

Parameters **b** – A Pyomo Block to be searched for active components

Returns A dictionary mapping id of constraint and block data objects to a bool indicating if they are active

`idaes.core.util.dyn_utils.get_derivatives_at(b, time, pts)`

Finds derivatives with respect to time at points specified. No distinction made for multiple derivatives or mixed partials.

Parameters

- **b** – Block to search for derivatives
- **time** – ContinuousSet to look for derivatives with respect to
- **pts** – Value or list of values in time set at which to return derivatives

Returns Dictionary mapping time points to lists of derivatives at those points

`idaes.core.util.dyn_utils.get_index_set_except(comp, *sets)`

Function for getting indices of a component over a product of its indexing sets other than those specified. Indices for the specified sets can be used to construct indices of the proper dimension for the original component via the `index_getter` function.

Parameters

- **comp** – Component whose indexing sets are to be manipulated
- **sets** – Sets to omit from the `set_except` product

Returns A dictionary. Maps ‘`set_except`’ to a Pyomo Set or SetProduct of `comp`’s index set, excluding those in `sets`. Maps ‘`index_getter`’ to a function that returns an index of the proper dimension for `comp`, given an element of `set_except` and a value for each set excluded. These values must be provided in the same order their Sets were provided in the `sets` argument.

`idaes.core.util.dyn_utils.is_explicitly_indexed_by(comp, *sets)`

Function for determining whether a pyomo component is indexed by a set or group of sets.

Parameters

- **comp** – some Pyomo component, possibly indexed
- **sets** – Pyomo Sets to check indexing by

Returns A bool that is True if `comp` is directly indexed each set in `sets`.

`idaes.core.util.dyn_utils.is_implicitly_indexed_by(comp, s, stop_at=None)`

Function for determining whether a component is contained in a block that is indexed by a particular set.

Parameters

- **comp** – Component whose parent blocks are checked
- **s** – Set for which indices are checked
- **stop_at** – Block at which to stop searching if reached, regardless of whether or not it is indexed by `s`

Returns Bool that is true if `comp` is contained in a block indexed by `s`

`idaes.core.util.dyn_utils.path_from_block(comp, blk, include_comp=False)`

Returns a list of tuples with (local_name, index) pairs required to locate `comp` from `blk`

Parameters

- **comp** – Component(Data) object to locate
- **blk** – Block(Data) to locate `comp` from
- **include_comp** – Bool of whether or not to include the local_name, index of the component itself

Returns A list of string, index tuples that can be used to locate `comp` from `blk`

Homotopy Meta-Solver

The IDAES homotopy meta-solver is useful for cases where a user has a feasible solution to a well-defined (i.e. square) problem at one set of conditions (i.e. value of fixed variables), and wishes to find a feasible solution to the same problem at a different set of conditions. In many situations this can be achieved by directly changing the values of the fixed variables to their new values and solving the problem, but cases exist where this is challenging. Homotopy solvers try to find a feasible path to the new solution by taking smaller steps in the value of the fixed variables to progressively find a solution at the new point.

Note: A homotopy solver should not be considered a fix to a poorly posed or ill-conditioned problem, and users should first consider whether their problem can be reformulated for better performance.

Homotopy Routine

The IDAES homotopy routine starts from a feasible solution to the problem at the initial values for the fixed variables (v_0) and a set of target values for these (t). The routine then calculates a set of new values for the fixed variables during the first homotopy evaluation based on an initial step size s_0 such that:

$$v_1 = t \times s_0 + v_0 \times (1 - s_0)$$

The problem is then passed to Ipopt to try to find a solution at the current values for the fixed variables. Based on the success or failure of the solver step, the following occurs:

1. If the solver returns an optimal solution, the step is accepted and the solution to the current state of the model is saved (to provide a feasible point to revert to in case a future step fails). If the current meta-solver progress is 1 (i.e. it has converged to the target values), the meta-solver terminates otherwise the meta-solver progress (p_i) is then updated, $p_i = p_{i-1} + s_i$, and the size of the next homotopy step is then calculated based on an adaptive step size method such that:

$$s_{i+1} = s_i \times \left(1 + a \times \left[\frac{I_t}{I_a} - 1 \right] \right)$$

where I_a is the number of solver iterations required in the current homotopy step, I_t is the desired number of solver iterations per homotopy step (an input parameter to the homotopy routine) and a is a step size acceleration factor (another input parameter). As such, the size of the homotopy step is adjusted to try to achieve a desired number of solver iterations per step as a proxy for difficulty in solving each step. If new step would overshoot the target values, then the step size is cut back to match the target values. The user can also specify a maximum and/or minimum size for the homotopy which can be used to limit the homotopy step.

A new set of values for the fixed variables is calculated using $v_{i+1} = t \times (p_i + s_{i+1}) + v_0 \times (1 - (p_i + s_{i+1}))$ and the process repeated.

2. If the solver fails to find an optimal solution (for any reason), the current step is rejected and solution to the previous successful step is reloaded. If the last homotopy step was equal to the minimum homotopy step size, the meta-solver terminates, otherwise, a reduced homotopy step is calculated using:

$$s_{i+1} = s_i \times c$$

where c is a step cut factor (an input parameter between 0.1 and 0.9). If the new step homotopy step is less than the minimum homotopy step size, the minimum step is used instead.

A new set of fixed variable values are then calculated and another attempt to solve the problem is made.

Possible Termination Conditions

The homotopy meta-solver has the following possible termination conditions (using the Pyomo *TerminationCondition* Enum):

- *TerminationCondition.optimal* - meta-solver successfully converged at the target values for the fixed variables.
- *TerminationCondition.other* - the meta-solver successfully converged at the target values for the fixed variables, but with regularization of during final step. Users are recommended to discard this solution.
- *TerminationCondition.minStepLength* - the meta-solver was unable to find a feasible path to the target values, as the solver failed to find a solution using the minimum homotopy step size.

- *TerminationCondition.maxEvaluations* - the meta-solver terminated due to reaching the maximum allowed number of attempted homotopy steps
- *TerminationCondition.infeasible* - could not find feasible solution to the problem at the initial values for the fixed variables.

Available Methods

IDAES Homotopy meta-solver routine.

```
idaes.core.util.homotopy.homotopy(model, variables, targets, max_solver_iterations=50,
                                   max_solver_time=10, step_init=0.1, step_cut=0.5,
                                   iter_target=4, step_accel=0.5, max_step=1,
                                   min_step=0.05, max_eval=200)
```

Homotopy meta-solver routine using Ipopt as the non-linear solver. This routine takes a model along with a list of fixed variables in that model and a list of target values for those variables. The routine then tries to iteratively move the values of the fixed variables to their target values using an adaptive step size.

Parameters

- **model** – model to be solved
- **variables** – list of Pyomo Var objects to be varied using homotopy. Variables must be fixed.
- **targets** – list of target values for each variable
- **max_solver_iterations** – maximum number of solver iterations per homotopy step (default=50)
- **max_solver_time** – maximum cpu time for the solver per homotopy step (default=10)
- **step_init** – initial homotopy step size (default=0.1)
- **step_cut** – factor by which to reduce step size on failed step (default=0.5)
- **step_accel** – acceleration factor for adjusting step size on successful step (default=0.5)
- **iter_target** – target number of solver iterations per homotopy step (default=4)
- **max_step** – maximum homotopy step size (default=1)
- **min_step** – minimum homotopy step size (default=0.05)
- **max_eval** – maximum number of homotopy evaluations (both successful and unsuccessful) (default=200)

Returns

A Pyomo TerminationCondition Enum indicating how the meta-solver terminated (see documentation)

Solver Progress [a fraction indication how far the solver progressed] from the initial values to the target values

Number of Iterations [number of homotopy evaluations before solver] terminated

Return type Termination Condition

Initialization Methods

The IDAES toolset contains a number of utility functions to assist users with initializing models.

Available Methods

This module contains utility functions for initialization of IDAES models.

`idaes.core.util.initialization.fix_state_vars` (*blk*, *state_args*={})

Method for fixing state variables within StateBlocks. Method takes an optional argument of values to use when fixing variables.

Parameters

- **blk** – An IDAES StateBlock object in which to fix the state variables
- **state_args** – a dict containing values to use when fixing state variables. Keys must match with names used in the `define_state_vars` method, and indices of any variables must agree.

Returns A dict keyed by block index, state variable name (as defined by `define_state_variables`) and variable index indicating the fixed status of each variable before the `fix_state_vars` method was applied.

`idaes.core.util.initialization.initialize_by_time_element` (*fs*, *time*, ***kwargs*)

Function to initialize Flowsheet *fs* element-by-element along ContinuousSet time. Assumes sufficient initialization/correct degrees of freedom such that the first finite element can be solved immediately and each subsequent finite element can be solved by fixing differential and derivative variables at the initial time point of that finite element.

Parameters

- **fs** – Flowsheet to initialize
- **time** – Set whose elements will be solved for individually
- **solver** – Pyomo solver object initialized with user's desired options
- **outlvl** – IDAES logger outlvl
- **ignore_dof** – Bool. If True, checks for square problems will be skipped.

Returns None

`idaes.core.util.initialization.propagate_state` (*stream*, *direction*='forward')

This method propagates values between Ports along Arcs. Values can be propagated in either direction using the *direction* argument.

Parameters

- **stream** – Arc object along which to propagate values
- **direction** – direction in which to propagate values. Default = 'forward' Valid value: 'forward', 'backward'.

Returns None

`idaes.core.util.initialization.revert_state_vars` (*blk*, *flags*)

Method to revert the fixed state of the state variables within an IDAES StateBlock based on a set of flags of the previous state.

Parameters

- **blk** – an IDAES StateBlock
- **flags** – a dict of bools indicating previous state with keys in the form (StateBlock index, state variable name (as defined by `define_state_vars`), var indices).

Returns None

`idaes.core.util.initialization.solve_indexed_blocks(solver, blocks, **kws)`

This method allows for solving of Indexed Block components as if they were a single Block. A temporary Block object is created which is populated with the contents of the objects in the blocks argument and then solved.

Parameters

- **solver** – a Pyomo solver object to use when solving the Indexed Block
- **blocks** – an object which inherits from Block, or a list of Blocks
- **kws** – a dict of arguments to be passed to the solver

Returns A Pyomo solver results object

Model State Serialization

The IDAES framework has some utility functions for serializing the state of a Pyomo model. These functions can save and load attributes of Pyomo components, but cannot reconstruct the Pyomo objects (it is not a replacement for pickle). It does have some advantages over pickle though. Not all Pyomo models are picklable. Serialization and deserialization of the model state to/from json is more secure in that it only deals with data and not executable code. It should be safe to use the `from_json()` function with data from untrusted sources, while, unpickling an object from an untrusted source is not secure. Storing a model state using these functions is also probably more robust against Python and Python package version changes, and possibly more suitable for long-term storage of results.

Below are a few example use cases for this module.

- Some models are very complex and may take minutes to initialize. Once a model is initialized it's state can be saved. For future runs, the initialized state can be reloaded instead of rerunning the initialization procedure.
- Results can be stored for later evaluation without needing to rerun the model. These results can be archived in a data management system if needed later.
- These functions may be useful in writing initialization procedures. For example, a model may be constructed and ready to run but first it may need to be initialized. Which components are active and which variables are fixed can be stored. The initialization can change which variables are fixed and which components are active. The original state can be read back after initialization, but where only values of variables that were originally fixed are read back in. This is an easy way to ensure that whatever the initialization procedure may do, the result is exactly the same problem (with only better initial values for unfixed variables).
- These functions can be used to send and receive model data to/from JavaScript user interface components.

Examples

This section provides a few very simple examples of how to use these functions.

Example Models

This section provides some boilerplate and functions to create a couple simple test models. The second model is a little more complicated and includes suffixes.

```
from pyomo.environ import *
from idaes.core.util import to_json, from_json, StoreSpec

def setup_model01():
    model = ConcreteModel()
    model.b = Block([1,2,3])
```

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```

a = model.b[1].a = Var(bounds=(-100, 100), initialize=2)
b = model.b[1].b = Var(bounds=(-100, 100), initialize=20)
model.b[1].c = Constraint(expr=b==10*a)
a.fix(2)
return model

def setup_model02():
    model = ConcreteModel()
    a = model.a = Param(default=1, mutable=True)
    b = model.b = Param(default=2, mutable=True)
    c = model.c = Param(initialize=4)
    x = model.x = Var([1,2], initialize={1:1.5, 2:2.5}, bounds=(-10,10))
    model.f = Objective(expr=(x[1] - a)**2 + (x[2] - b)**2)
    model.g = Constraint(expr=x[1] + x[2] - c >= 0)
    model.dual = Suffix(direction=Suffix.IMPORT)
    model.ipopt_zL_out = Suffix(direction=Suffix.IMPORT)
    model.ipopt_zU_out = Suffix(direction=Suffix.IMPORT)
    return model

```

Serialization

These examples can be appended to the boilerplate code above.

The first example creates a model, saves the state, changes a value, then reads back the initial state.

```

model = setup_model01()
to_json(model, fname="ex.json.gz", gz=True, human_read=True)
model.b[1].a = 3000.4
from_json(model, fname="ex.json.gz", gz=True)
print(value(model.b[1].a))

```

2

This next example show how to save only suffixes.

```

model = setup_model02()
# Suffixes here are read back from solver, so to have suffix data,
# need to solve first
solver = SolverFactory("ipopt")
solver.solve(model)
store_spec = StoreSpec.suffix()
to_json(model, fname="ex.json", wts=store_spec)
# Do something and now I want my suffixes back
from_json(model, fname="ex.json", wts=store_spec)

```

to_json

Despite the name of the `to_json` function it is capable of creating Python dictionaries, json files, gzipped json files, and json strings. The function documentation is below. A *StoreSpec* object provides the function with details on what to store and how to handle special cases of Pyomo component attributes.

```

idaes.core.util.model_serializer.to_json(o, fname=None, human_read=False, wts=None,
                                         metadata={}, gz=None, return_dict=False, re-
                                         turn_json_string=False)

```

Save the state of a model to a Python dictionary, and optionally dump it to a json file. To load a model state, a model with the same structure must exist. The model itself cannot be recreated from this.

Parameters

- **o** – The Pyomo component object to save. Usually a Pyomo model, but could also be a subcomponent of a model (usually a sub-block).
- **fname** – json file name to save model state, if None only create python dict
- **gz** – If fname is given and gv is True gzip the json file. The default is True if the file name ends with '.gz' otherwise False.
- **human_read** – if True, add indents and spacing to make the json file more readable, if false cut out whitespace and make as compact as possible
- **metadata** – A dictionary of additional metadata to add.
- **wts** – is What To Save, this is a StoreSpec object that specifies what object types and attributes to save. If None, the default is used which saves the state of the complete model state.
- **metadata** – additional metadata to save beyond the standard format_version, date, and time.
- **return_dict** – default is False if true returns a dictionary representation
- **return_json_string** – default is False returns a json string

Returns If return_dict is True returns a dictionary serialization of the Pyomo component. If return_dict is False and return_json_string is True returns a json string dump of the dict. If fname is given the dictionary is also written to a json file. If gz is True and fname is given, writes a gzipped json file.

from_json

The from_json function puts data from Python dictionaries, json files, gzipped json files, and json strings back into a Pyomo model. The function documentation is below. A [StoreSpec](#) object provides the function with details on what to read and how to handle special cases of Pyomo component attributes.

```
idaes.core.util.model_serializer.from_json(o, sd=None, fname=None, s=None,
                                           wts=None, gz=None)
```

Load the state of a Pyomo component state from a dictionary, json file, or json string. Must only specify one of sd, fname, or s as a non-None value. This works by going through the model and loading the state of each sub-component of o. If the saved state contains extra information, it is ignored. If the save state doesn't contain an entry for a model component that is to be loaded an error will be raised, unless ignore_missing = True.

Parameters

- **o** – Pyomo component to for which to load state
- **sd** – State dictionary to load, if None, check fname and s
- **fname** – JSON file to load, only used if sd is None
- **s** – JSON string to load only used if both sd and fname are None
- **wts** – StoreSpec object specifying what to load
- **gz** – If True assume the file specified by fname is gzipped. The default is True if fname ends with '.gz' otherwise False.

Returns Dictionary with some performance information. The keys are “etime_load_file”, how long in seconds it took to load the json file “etime_read_dict”, how long in seconds it took to read models state “etime_read_suffixes”, how long in seconds it took to read suffixes

StoreSpec

StoreSpec is a class for objects that tell the `to_json()` and `from_json()` functions how to read and write Pyomo component attributes. The default initialization provides an object that would load and save attributes usually needed to save a model state. There are several other class methods that provide canned objects for specific uses. Through initialization arguments, the behavior is highly customizable. Attributes can be read or written using callback functions to handle attributes that can not be directly read or written (e.g. a variable lower bound is set by calling `setlb()`). See the class documentation below.

```
class idaes.core.util.model_serializer.StoreSpec (classes=((<class      'py-
omo.core.base.param.Param'>,
('_mutable', )), (<class      'py-
omo.core.base.var.Var'>,
()), (<class      'py-
omo.core.base.expression.Expression'>,
()), (<class      'py-
omo.core.base.component.Component'>,
('active', )), data_classes=((<class
'pyomo.core.base.var._VarData'>,
('fixed',      'stale',      'value',
'lb',      'ub')), (<class      'py-
omo.core.base.param._ParamData'>,
('value', )), (<class      'int'>,
('value', )), (<class      'float'>,
('value', )), (<class      'py-
omo.core.base.expression._ExpressionData'>,
()), (<class      'py-
omo.core.base.component.ComponentData'>,
('active', )),
skip_classes=(<class      'py-
omo.core.base.external.ExternalFunction'>,
<class      'pyomo.core.base.set.Set'>,
<class      'pyomo.network.port.Port'>,
<class      'py-
omo.core.base.expression.Expression'>,
<class      'py-
omo.core.base.set.RangeSet'>),
ignore_missing=True, suffix=True,
suffix_filter=None)
```

A StoreSpec object tells the serializer functions what to read or write. The default settings will produce a StoreSpec configured to load/save the typical attributes required to load/save a model state.

Parameters

- **classes** – A list of classes to save. Each class is represented by a list (or tuple) containing the following elements: (1) class (compared using `isinstance`) (2) attribute list or None, an empty list store the object, but none of its attributes, None will not store objects of this class type (3) optional load filter function. The load filter function returns a list of attributes to read based on the state of an object and its saved state. The allows, for example, loading values for unfixed variables, or only loading values whose current value is less than one. The filter function only applies to load not save. Filter functions take two arguments

(a) the object (current state) and (b) the dictionary containing the saved state of an object. More specific classes should come before more general classes. For example if an object is a HeatExchanger and a UnitModel, and HeatExchanger is listed first, it will follow the HeatExchanger settings. If UnitModel is listed first in the classes list, it will follow the UnitModel settings.

- **data_classes** – This takes the same form as the classes argument. This is for component data classes.
- **skip_classes** – This is a list of classes to skip. If a class appears in the skip list, but also appears in the classes argument, the classes argument will override skip_classes. The use for this is to specifically exclude certain classes that would get caught by more general classes (e.g. UnitModel is in the class list, but you want to exclude HeatExchanger which is derived from UnitModel).
- **ignore_missing** – If True will ignore a component or attribute that exists in the model, but not in the stored state. If false an exception will be raised for things in the model that should be loaded but aren't in the stored state. Extra items in the stored state will not raise an exception regardless of this argument.
- **suffix** – If True store suffixes and component ids. If false, don't store suffixes.
- **suffix_filter** – None to store all suffixes if suffix=True, or a list of suffixes to store if suffix=True

classmethod bound()

Returns a StoreSpec object to store variable bounds only.

get_class_attr_list(o)

Look up what attributes to save/load for an Component object. :param o: Object to look up attribute list for.

Returns A list of attributes and a filter function for object type

get_data_class_attr_list(o)

Look up what attributes to save/load for an ComponentData object. :param o: Object to look up attribute list for.

Returns A list of attributes and a filter function for object type

classmethod isfixed()

Returns a StoreSpec object to store if variables are fixed.

set_read_callback(attr, cb=None)

Set a callback to set an attribute, when reading from json or dict.

set_write_callback(attr, cb=None)

Set a callback to get an attribute, when writing to json or dict.

classmethod value()

Returns a StoreSpec object to store variable values only.

classmethod value_isfixed(only_fixed)

Return a StoreSpec object to store variable values and if fixed.

Parameters only_fixed – Only load fixed variable values

classmethod value_isfixed_isactive(only_fixed)

Return a StoreSpec object to store variable values, if variables are fixed and if components are active.

Parameters only_fixed – Only load fixed variable values

Structure

Python dictionaries, json strings, or json files are generated, in any case the structure of the data is the same. The current data structure version is 3.

The example json below shows the top-level structure. The "top_level_component" would be the name of the Pyomo component that is being serialized. The top level component is the only place where the component name does not matter when reading the serialized data.

```
{
  "__metadata__": {
    "format_version": 3,
    "date": "2018-12-21",
    "time": "11:34:39.714323",
    "other": {
    },
    "__performance__": {
      "n_components": 219,
      "etime_make_dict": 0.003
    }
  },
  "top_level_component": {
    "...": "..."
  },
}
```

The data structure of a Pyomo component is shown below. Here "attribute_1" and "attribute_2" are just examples the actual attributes saved depend on the "wts" argument to `to_json()`. Scalar and indexed components have the same structure. Scalar components have one entry in "data" with an index of "None". Only components derived from Pyomo's `_BlockData` have a "`__pyomo_components__`" field, and components appearing there are keyed by their name. The data structure duplicates the hierarchical structure of the Pyomo model.

Suffixes store extra attributes for Pyomo components that are not stored on the components themselves. Suffixes are a Pyomo structure that comes from the AMPL solver interface. If a component is a suffix, keys in the data section are the serial integer component IDs generated by `to_json()`, and the value is the value of the suffix for the corresponding component.

```
{
  "__type__": "<class 'some.class'>",
  "__id__": 0,
  "data": {
    "index_1": {
      "__type__": "<usually a component class but for params could be float, int, .
→...>",
      "__id__": 1,
      "__pyomo_components__": {
        "child_component_1": {
          "...": "..."
        }
      },
      "attribute_1": "... could be any number of attributes like 'value': 1.0,",
      "attribute_2": "..."
    }
  },
  "attribute_1": "... could be any number of attributes like 'active': true,",
  "attribute_2": "..."
}
```

As a more concrete example, here is the json generated for example model 2 in [Examples](#). This code can be appended

to the *example boilerplate above*. To generate the example json shown.

```
model = setup_model02()
solver = SolverFactory("ipopt")
solver.solve(model)
to_json(model, fname="ex.json")
```

The resulting json is shown below. The top-level component in this case is given as “unknown,” because the model was not given a name. The top level object name is not needed when reading back data, since the top level object is specified in the call to `from_json()`. Types are not used when reading back data, they may have some future application, but at this point they just provide a little extra information.

```
{
  "__metadata__":{
    "format_version":3,
    "date":"2019-01-02",
    "time":"10:22:25.833501",
    "other":{
    },
    "__performance__":{
      "n_components":18,
      "etime_make_dict":0.0009555816650390625
    }
  },
  "unknown":{
    "__type__":"<class 'pyomo.core.base.PyomoModel.ConcreteModel'>",
    "__id__":0,
    "active":true,
    "data":{
      "None":{
        "__type__":"<class 'pyomo.core.base.PyomoModel.ConcreteModel'>",
        "__id__":1,
        "active":true,
        "__pyomo_components__":{
          "a":{
            "__type__":"<class 'pyomo.core.base.param.SimpleParam'>",
            "__id__":2,
            "_mutable":true,
            "data":{
              "None":{
                "__type__":"<class 'pyomo.core.base.param.SimpleParam'>",
                "__id__":3,
                "value":1
              }
            }
          }
        },
        "b":{
          "__type__":"<class 'pyomo.core.base.param.SimpleParam'>",
          "__id__":4,
          "_mutable":true,
          "data":{
            "None":{
              "__type__":"<class 'pyomo.core.base.param.SimpleParam'>",
              "__id__":5,
              "value":2
            }
          }
        }
      }
    }
  },
}
```

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```

    "c": {
      "__type__": "<class 'pyomo.core.base.param.SimpleParam'>",
      "__id__": 6,
      "_mutable": false,
      "data": {
        "None": {
          "__type__": "<class 'pyomo.core.base.param.SimpleParam'>",
          "__id__": 7,
          "value": 4
        }
      }
    },
    "x": {
      "__type__": "<class 'pyomo.core.base.var.IndexedVar'>",
      "__id__": 8,
      "data": {
        "1": {
          "__type__": "<class 'pyomo.core.base.var._GeneralVarData'>",
          "__id__": 9,
          "fixed": false,
          "stale": false,
          "value": 1.5,
          "lb": -10,
          "ub": 10
        },
        "2": {
          "__type__": "<class 'pyomo.core.base.var._GeneralVarData'>",
          "__id__": 10,
          "fixed": false,
          "stale": false,
          "value": 2.5,
          "lb": -10,
          "ub": 10
        }
      }
    },
    "f": {
      "__type__": "<class 'pyomo.core.base.objective.SimpleObjective'>",
      "__id__": 11,
      "active": true,
      "data": {
        "None": { "__type__": "<class 'pyomo.core.base.objective.SimpleObjective'>"
        ↪,
          "__id__": 12,
          "active": true
        }
      }
    },
    "g": {
      "__type__": "<class 'pyomo.core.base.constraint.SimpleConstraint'>",
      "__id__": 13,
      "active": true,
      "data": {
        "None": {
          "__type__": "<class 'pyomo.core.base.constraint.SimpleConstraint'>",
          "__id__": 14,
          "active": true
        }
      }
    }
  }

```

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```

    }
},
"dual":{
  "__type__":"<class 'pyomo.core.base.suffix.Suffix'>",
  "__id__":15,
  "active":true,
  "data":{
    "14":0.9999999626149493
  }
},
"ipopt_zL_out":{
  "__type__":"<class 'pyomo.core.base.suffix.Suffix'>",
  "__id__":16,
  "active":true,
  "data":{
    "9":2.1791814146763388e-10,
    "10":2.004834508495852e-10
  }
},
"ipopt_zU_out":{
  "__type__":"<class 'pyomo.core.base.suffix.Suffix'>",
  "__id__":17,
  "active":true,
  "data":{
    "9":-2.947875485096964e-10,
    "10":-3.3408951850535573e-10
  }
}
}
}
}
}
```

Returns Number of degrees of freedom in block.

Report Statistics Method

The `report_statistics` method provides the user with a summary of the contents of their model, including the degrees of freedom and a break down of the different `Variables`, `Constraints`, `Objectives`, `Blocks` and `Expressions`. This method also includes numbers of deactivated components for the user to use in debugging complex models.

Note: This method only considers Pyomo components in activated `Blocks`. The number of deactivated `Blocks` is reported, but any components within these `Blocks` are not included.

Example Output

Model Statistics

Degrees of Freedom: 0

Total No. Variables: 52

 No. Fixed Variables: 12

 No. Unused Variables: 0 (Fixed: 0)

 No. Variables only in Inequalities: 0 (Fixed: 0)

Total No. Constraints: 40

 No. Equality Constraints: 40 (Deactivated: 0)

 No. Inequality Constraints: 0 (Deactivated: 0)

No. Objectives: 0 (Deactivated: 0)

No. Blocks: 14 (Deactivated: 0)

No. Expressions: 2

```
idaes.core.util.model_statistics.report_statistics(block, ostream=None)
```

Method to print a report of the model statistics for a Pyomo Block

Parameters

- **block** – the Block object to report statistics from
- **ostream** – output stream for printing (defaults to `sys.stdout`)

Returns Printed output of the model statistics

Other Statistics Methods

In addition to the methods discussed above, the `model_statistics` module also contains a number of methods for quantifying model statistics which may be of use to the user in debugging models. These methods come in three types:

- Number methods (start with `number_`) return the number of components which meet a given criteria, and are useful for quickly quantifying different types of components within a model for determining where problems may exist.

- Set methods (end with `_set`) return a Pyomo `ComponentSet` containing all components which meet a given criteria. These methods are useful for determining where a problem may exist, as the `ComponentSet` indicates which components may be causing a problem.
- Generator methods (end with `_generator`) contain Python generators which return all components which meet a given criteria.

Available Methods

This module contains utility functions for reporting structural statistics of IDAES models.

`idaes.core.util.model_statistics.activated_block_component_generator` (*block*, *ctype*)

Generator which returns all the components of a given ctype which exist in activated Blocks within a model.

Parameters

- **block** – model to be studied
- **ctype** – type of Pyomo component to be returned by generator.

Returns A generator which returns all components of ctype which appear in activated Blocks in block

`idaes.core.util.model_statistics.activated_blocks_set` (*block*)

Method to return a `ComponentSet` of all activated Block components in a model.

Parameters **block** – model to be studied

Returns A `ComponentSet` including all activated Block components in block (including block itself)

`idaes.core.util.model_statistics.activated_constraints_generator` (*block*)

Generator which returns all activated Constraint components in a model.

Parameters **block** – model to be studied

Returns A generator which returns all activated Constraint components block

`idaes.core.util.model_statistics.activated_constraints_set` (*block*)

Method to return a `ComponentSet` of all activated Constraint components in a model.

Parameters **block** – model to be studied

Returns A `ComponentSet` including all activated Constraint components in block

`idaes.core.util.model_statistics.activated_equalities_generator` (*block*)

Generator which returns all activated equality Constraint components in a model.

Parameters **block** – model to be studied

Returns A generator which returns all activated equality Constraint components block

`idaes.core.util.model_statistics.activated_equalities_set` (*block*)

Method to return a `ComponentSet` of all activated equality Constraint components in a model.

Parameters **block** – model to be studied

Returns A `ComponentSet` including all activated equality Constraint components in block

`idaes.core.util.model_statistics.activated_inequalities_generator` (*block*)

Generator which returns all activated inequality Constraint components in a model.

Parameters **block** – model to be studied

Returns A generator which returns all activated inequality Constraint components block

`idaes.core.util.model_statistics.activated_inequalities_set` (*block*)

Method to return a ComponentSet of all activated inequality Constraint components in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all activated inequality Constraint components in block

`idaes.core.util.model_statistics.activated_objectives_generator` (*block*)

Generator which returns all activated Objective components in a model.

Parameters `block` – model to be studied

Returns A generator which returns all activated Objective components block

`idaes.core.util.model_statistics.activated_objectives_set` (*block*)

Method to return a ComponentSet of all activated Objective components which appear in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all activated Objective components which appear in block

`idaes.core.util.model_statistics.active_variables_in_deactivated_blocks_set` (*block*)

Method to return a ComponentSet of any Var components which appear within an active Constraint but belong to a deactivated Block in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including any Var components which belong to a deactivated Block but appear in an active Constraint in block

`idaes.core.util.model_statistics.deactivated_blocks_set` (*block*)

Method to return a ComponentSet of all deactivated Block components in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all deactivated Block components in block (including block itself)

`idaes.core.util.model_statistics.deactivated_constraints_generator` (*block*)

Generator which returns all deactivated Constraint components in a model.

Parameters `block` – model to be studied

Returns A generator which returns all deactivated Constraint components block

`idaes.core.util.model_statistics.deactivated_constraints_set` (*block*)

Method to return a ComponentSet of all deactivated Constraint components in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all deactivated Constraint components in block

`idaes.core.util.model_statistics.deactivated_equalities_generator` (*block*)

Generator which returns all deactivated equality Constraint components in a model.

Parameters `block` – model to be studied

Returns A generator which returns all deactivated equality Constraint components block

`idaes.core.util.model_statistics.deactivated_equalities_set` (*block*)

Method to return a ComponentSet of all deactivated equality Constraint components in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all deactivated equality Constraint components in block

`idaes.core.util.model_statistics.deactivated_inequalities_generator` (*block*)

Generator which returns all deactivated inequality Constraint components in a model.

Parameters `block` – model to be studied

Returns A generator which returns all deactivated equality Constraint components block

`idaes.core.util.model_statistics.deactivated_inequalities_set` (*block*)

Method to return a ComponentSet of all deactivated inequality Constraint components in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all deactivated inequality Constraint components in block

`idaes.core.util.model_statistics.deactivated_objectives_generator` (*block*)

Generator which returns all deactivated Objective components in a model.

Parameters `block` – model to be studied

Returns A generator which returns all deactivated Objective components block

`idaes.core.util.model_statistics.deactivated_objectives_set` (*block*)

Method to return a ComponentSet of all deactivated Objective components which appear in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all deactivated Objective components which appear in block

`idaes.core.util.model_statistics.derivative_variables_set` (*block*)

Method to return a ComponentSet of all DerivativeVar components which appear in a model. Users should note that DerivativeVars are converted to ordinary Vars when a DAE transformation is applied. Thus, this method is useful for detecting any DerivativeVars which were do transformed.

Parameters `block` – model to be studied

Returns A ComponentSet including all DerivativeVar components which appear in block

`idaes.core.util.model_statistics.expressions_set` (*block*)

Method to return a ComponentSet of all Expression components which appear in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all Expression components which appear in block

`idaes.core.util.model_statistics.fixed_unused_variables_set` (*block*)

Method to return a ComponentSet of all fixed Var components which do not appear within any activated Constraint in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all fixed Var components which do not appear within any Constraints in block

`idaes.core.util.model_statistics.fixed_variables_generator` (*block*)

Generator which returns all fixed Var components in a model.

Parameters `block` – model to be studied

Returns A generator which returns all fixed Var components block

`idaes.core.util.model_statistics.fixed_variables_in_activated_equalities_set` (*block*)

Method to return a ComponentSet of all fixed Var components which appear within an equality Constraint in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all fixed Var components which appear within activated equality Constraints in block

`idaes.core.util.model_statistics.fixed_variables_only_in_inequalities(block)`
Method to return a ComponentSet of all fixed Var components which appear only within activated inequality Constraints in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all fixed Var components which appear only within activated inequality Constraints in block

`idaes.core.util.model_statistics.fixed_variables_set(block)`
Method to return a ComponentSet of all fixed Var components in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all fixed Var components in block

`idaes.core.util.model_statistics.large_residuals_set(block, tol=1e-05)`
Method to return a ComponentSet of all Constraint components with a residual greater than a given threshold which appear in a model.

Parameters

- `block` – model to be studied
- `tol` – residual threshold for inclusion in ComponentSet

Returns A ComponentSet including all Constraint components with a residual greater than `tol` which appear in block

`idaes.core.util.model_statistics.number_activated_blocks(block)`
Method to return the number of activated Block components in a model.

Parameters `block` – model to be studied

Returns Number of activated Block components in block (including block itself)

`idaes.core.util.model_statistics.number_activated_constraints(block)`
Method to return the number of activated Constraint components in a model.

Parameters `block` – model to be studied

Returns Number of activated Constraint components in block

`idaes.core.util.model_statistics.number_activated_equalities(block)`
Method to return the number of activated equality Constraint components in a model.

Parameters `block` – model to be studied

Returns Number of activated equality Constraint components in block

`idaes.core.util.model_statistics.number_activated_inequalities(block)`
Method to return the number of activated inequality Constraint components in a model.

Parameters `block` – model to be studied

Returns Number of activated inequality Constraint components in block

`idaes.core.util.model_statistics.number_activated_objectives(block)`
Method to return the number of activated Objective components which appear in a model.

Parameters `block` – model to be studied

Returns Number of activated Objective components which appear in block

`idaes.core.util.model_statistics.number_active_variables_in_deactivated_blocks` (*block*)
 Method to return the number of Var components which appear within an active Constraint but belong to a deactivated Block in a model.

Parameters `block` – model to be studied

Returns Number of Var components which belong to a deactivated Block but appear in an activate Constraint in block

`idaes.core.util.model_statistics.number_deactivated_blocks` (*block*)
 Method to return the number of deactivated Block components in a model.

Parameters `block` – model to be studied

Returns Number of deactivated Block components in block (including block itself)

`idaes.core.util.model_statistics.number_deactivated_constraints` (*block*)
 Method to return the number of deactivated Constraint components in a model.

Parameters `block` – model to be studied

Returns Number of deactivated Constraint components in block

`idaes.core.util.model_statistics.number_deactivated_equalities` (*block*)
 Method to return the number of deactivated equality Constraint components in a model.

Parameters `block` – model to be studied

Returns Number of deactivated equality Constraint components in block

`idaes.core.util.model_statistics.number_deactivated_inequalities` (*block*)
 Method to return the number of deactivated inequality Constraint components in a model.

Parameters `block` – model to be studied

Returns Number of deactivated inequality Constraint components in block

`idaes.core.util.model_statistics.number_deactivated_objectives` (*block*)
 Method to return the number of deactivated Objective components which appear in a model.

Parameters `block` – model to be studied

Returns Number of deactivated Objective components which appear in block

`idaes.core.util.model_statistics.number_derivative_variables` (*block*)
 Method to return the number of DerivativeVar components which appear in a model. Users should note that DerivativeVars are converted to ordinary Vars when a DAE transformation is applied. Thus, this method is useful for detecting any DerivativeVars which were do transformed.

Parameters `block` – model to be studied

Returns Number of DerivativeVar components which appear in block

`idaes.core.util.model_statistics.number_expressions` (*block*)
 Method to return the number of Expression components which appear in a model.

Parameters `block` – model to be studied

Returns Number of Expression components which appear in block

`idaes.core.util.model_statistics.number_fixed_unused_variables` (*block*)
 Method to return the number of fixed Var components which do not appear within any activated Constraint in a model.

Parameters `block` – model to be studied

Returns Number of fixed Var components which do not appear within any activated Constraints in block

`idaes.core.util.model_statistics.number_fixed_variables(block)`

Method to return the number of fixed Var components in a model.

Parameters `block` – model to be studied

Returns Number of fixed Var components in block

`idaes.core.util.model_statistics.number_fixed_variables_in_activated_equalities(block)`

Method to return the number of fixed Var components which appear within activated equality Constraints in a model.

Parameters `block` – model to be studied

Returns Number of fixed Var components which appear within activated equality Constraints in block

`idaes.core.util.model_statistics.number_fixed_variables_only_in_inequalities(block)`

Method to return the number of fixed Var components which only appear within activated inequality Constraints in a model.

Parameters `block` – model to be studied

Returns Number of fixed Var components which only appear within activated inequality Constraints in block

`idaes.core.util.model_statistics.number_large_residuals(block, tol=1e-05)`

Method to return the number Constraint components with a residual greater than a given threshold which appear in a model.

Parameters

- `block` – model to be studied
- `tol` – residual threshold for inclusion in ComponentSet

Returns Number of Constraint components with a residual greater than tol which appear in block

`idaes.core.util.model_statistics.number_total_blocks(block)`

Method to return the number of Block components in a model.

Parameters `block` – model to be studied

Returns Number of Block components in block (including block itself)

`idaes.core.util.model_statistics.number_total_constraints(block)`

Method to return the total number of Constraint components in a model.

Parameters `block` – model to be studied

Returns Number of Constraint components in block

`idaes.core.util.model_statistics.number_total_equalities(block)`

Method to return the total number of equality Constraint components in a model.

Parameters `block` – model to be studied

Returns Number of equality Constraint components in block

`idaes.core.util.model_statistics.number_total_inequalities(block)`

Method to return the total number of inequality Constraint components in a model.

Parameters `block` – model to be studied

Returns Number of inequality Constraint components in block

`idaes.core.util.model_statistics.number_total_objectives` (*block*)

Method to return the number of Objective components which appear in a model

Parameters `block` – model to be studied

Returns Number of Objective components which appear in block

`idaes.core.util.model_statistics.number_unfixed_variables` (*block*)

Method to return the number of unfixed Var components in a model.

Parameters `block` – model to be studied

Returns Number of unfixed Var components in block

`idaes.core.util.model_statistics.number_unfixed_variables_in_activated_equalities` (*block*)

Method to return the number of unfixed Var components which appear within activated equality Constraints in a model.

Parameters `block` – model to be studied

Returns Number of unfixed Var components which appear within activated equality Constraints in block

`idaes.core.util.model_statistics.number_unused_variables` (*block*)

Method to return the number of Var components which do not appear within any activated Constraint in a model.

Parameters `block` – model to be studied

Returns Number of Var components which do not appear within any activated Constraints in block

`idaes.core.util.model_statistics.number_variables` (*block*)

Method to return the number of Var components in a model.

Parameters `block` – model to be studied

Returns Number of Var components in block

`idaes.core.util.model_statistics.number_variables_in_activated_constraints` (*block*)

Method to return the number of Var components that appear within active Constraints in a model.

Parameters `block` – model to be studied

Returns Number of Var components which appear within active Constraints in block

`idaes.core.util.model_statistics.number_variables_in_activated_equalities` (*block*)

Method to return the number of Var components which appear within activated equality Constraints in a model.

Parameters `block` – model to be studied

Returns Number of Var components which appear within activated equality Constraints in block

`idaes.core.util.model_statistics.number_variables_in_activated_inequalities` (*block*)

Method to return the number of Var components which appear within activated inequality Constraints in a model.

Parameters `block` – model to be studied

Returns Number of Var components which appear within activated inequality Constraints in block

`idaes.core.util.model_statistics.number_variables_near_bounds` (*block*,
tol=0.0001)

Method to return the number of all Var components in a model which have a value within tol (relative) of a bound.

Parameters

- `block` – model to be studied
- `tol` – relative tolerance for inclusion in generator (default = 1e-4)

Returns Number of components block that are close to a bound

`idaes.core.util.model_statistics.number_variables_only_in_inequalities` (*block*)

Method to return the number of Var components which appear only within activated inequality Constraints in a model.

Parameters *block* – model to be studied

Returns Number of Var components which appear only within activated inequality Constraints in block

`idaes.core.util.model_statistics.total_blocks_set` (*block*)

Method to return a ComponentSet of all Block components in a model.

Parameters *block* – model to be studied

Returns A ComponentSet including all Block components in block (including block itself)

`idaes.core.util.model_statistics.total_constraints_set` (*block*)

Method to return a ComponentSet of all Constraint components in a model.

Parameters *block* – model to be studied

Returns A ComponentSet including all Constraint components in block

`idaes.core.util.model_statistics.total_equalities_generator` (*block*)

Generator which returns all equality Constraint components in a model.

Parameters *block* – model to be studied

Returns A generator which returns all equality Constraint components block

`idaes.core.util.model_statistics.total_equalities_set` (*block*)

Method to return a ComponentSet of all equality Constraint components in a model.

Parameters *block* – model to be studied

Returns A ComponentSet including all equality Constraint components in block

`idaes.core.util.model_statistics.total_inequalities_generator` (*block*)

Generator which returns all inequality Constraint components in a model.

Parameters *block* – model to be studied

Returns A generator which returns all inequality Constraint components block

`idaes.core.util.model_statistics.total_inequalities_set` (*block*)

Method to return a ComponentSet of all inequality Constraint components in a model.

Parameters *block* – model to be studied

Returns A ComponentSet including all inequality Constraint components in block

`idaes.core.util.model_statistics.total_objectives_generator` (*block*)

Generator which returns all Objective components in a model.

Parameters *block* – model to be studied

Returns A generator which returns all Objective components block

`idaes.core.util.model_statistics.total_objectives_set` (*block*)

Method to return a ComponentSet of all Objective components which appear in a model.

Parameters *block* – model to be studied

Returns A ComponentSet including all Objective components which appear in block

`idaes.core.util.model_statistics.unfixed_variables_generator (block)`

Generator which returns all unfixed Var components in a model.

Parameters `block` – model to be studied

Returns A generator which returns all unfixed Var components block

`idaes.core.util.model_statistics.unfixed_variables_in_activated_equalities_set (block)`

Method to return a ComponentSet of all unfixed Var components which appear within an activated equality Constraint in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all unfixed Var components which appear within activated equality Constraints in block

`idaes.core.util.model_statistics.unfixed_variables_set (block)`

Method to return a ComponentSet of all unfixed Var components in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all unfixed Var components in block

`idaes.core.util.model_statistics.unused_variables_set (block)`

Method to return a ComponentSet of all Var components which do not appear within any activated Constraint in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all Var components which do not appear within any Constraints in block

`idaes.core.util.model_statistics.variables_in_activated_constraints_set (block)`

Method to return a ComponentSet of all Var components which appear within a Constraint in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all Var components which appear within activated Constraints in block

`idaes.core.util.model_statistics.variables_in_activated_equalities_set (block)`

Method to return a ComponentSet of all Var components which appear within an equality Constraint in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all Var components which appear within activated equality Constraints in block

`idaes.core.util.model_statistics.variables_in_activated_inequalities_set (block)`

Method to return a ComponentSet of all Var components which appear within an inequality Constraint in a model.

Parameters `block` – model to be studied

Returns A ComponentSet including all Var components which appear within activated inequality Constraints in block

`idaes.core.util.model_statistics.variables_near_bounds_generator (block, tol=0.0001)`

Generator which returns all Var components in a model which have a value within tol (relative) of a bound.

Parameters

- `block` – model to be studied
- `tol` – relative tolerance for inclusion in generator (default = 1e-4)

Returns A generator which returns all Var components block that are close to a bound

`idaes.core.util.model_statistics.variables_near_bounds_set (block, tol=0.0001)`

Method to return a ComponentSet of all Var components in a model which have a value within tol (relative) of a bound.

Parameters

- **block** – model to be studied
- **tol** – relative tolerance for inclusion in generator (default = 1e-4)

Returns A ComponentSet including all Var components block that are close to a bound

`idaes.core.util.model_statistics.variables_only_in_inequalities (block)`

Method to return a ComponentSet of all Var components which appear only within inequality Constraints in a model.

Parameters **block** – model to be studied

Returns A ComponentSet including all Var components which appear only within inequality Constraints in block

`idaes.core.util.model_statistics.variables_set (block)`

Method to return a ComponentSet of all Var components in a model.

Parameters **block** – model to be studied

Returns A ComponentSet including all Var components in block

Scaling

This section describes scaling utility functions and methods.

Standard Practice

Scaling factors can be specified for any variable or constraint. Pyomo and many solvers support the `scaling_factor` suffix. IDAES, as described below, also supports the `scaling_expression` suffix which can be used to calculate `scaling_factor` values (e.g. based on state block units of measure).

To eliminate the possibility of defining, conflicting scaling factors in various places in the model the IDAES standard is to define the `scaling_factor` and `scaling_expression` suffixes in the same block as the variable or constraint that they are scaling. This ensures that each scale factor is defined in only one place, and is organized based on the model block structure.

Scaling factors in IDAES (and Pyomo) are multiplied by the variable or constraint they scale. For example, a Pressure variable in Pa units may be expected to have a magnitude of around 1×10^6 for a specific process. To scale the variable to a more reasonable magnitude the scale factor for the variable could be defined to be 1×10^{-5} .

Specifying Variable Scaling

Suffixes are used to specify scaling factors for IDAES models. Some solvers, such as Ipopt, support supplying scale factors. Pyomo also supplies scaling transformations for models when solver scaling is not supported.

To supply variable and constraint scaling factors, a suffix called `scaling_factor` should be created in the same block as the variable or constraint. For example:

```

from pyomo.environ import Suffix, ConcreteModel, Var

m = ConcreteModel()
m.scaling_factor = Suffix(direction=Suffix.EXPORT)
m.P = Var(initialize=1e6, doc="Pressure [Pa]")
m.conc = Var(["Na+", "Cl-"], initialize=1e-4)
m.scaling_factor[m.P] = 1e-5
m.scaling_factor[m.conc["Na+"]] = 1e3
m.scaling_factor[m.conc["Cl-"]] = 1e3

```

Variable scaling in state blocks is provided by the developer of a state block and can be used as a basis for scaling other model variables and constraints. Scaling factors can be modified by users to better represent the process they are modeling.

Specifying Scaling Factor Expressions

Scaling factors for variables and constraints can be calculated based on variable scaling factors, bounds, or values that have been provided. The calculation for a scaling factor can be provided as a python expression using model variables in the `scaling_expression` suffix. For variables, generally the expression should only depend on variables where scaling factors have been defined.

The `calculate_scaling_factors(m, basis)` function replaces the variables in the scaling expression with the specified basis values, calculates the scaling factors, and puts the scaling factor in the `scaling_factor` suffix.

```

from pyomo.environ import Suffix, ConcreteModel, Var, Constraint
from idaes.core.util.scaling import (
    ScalingBasis,
    calculate_scaling_factors,
)

m = ConcreteModel()
m.scaling_factor = Suffix(direction=Suffix.EXPORT)
m.scaling_expression = Suffix(direction=Suffix.LOCAL)

m.x = Var(initialize=1e6)
m.y = Var(initialize=1e6)
m.z = Var(initialize=1e12)

m.scaling_factor[m.x] = 1e-5
m.scaling_factor[m.y] = 1e-5
m.scaling_expression[m.z] = 1/(m.x*m.y)

m.c = Constraint(expr=m.z == m.x*m.y)
m.scaling_expression[m.c] = 1/(m.x*m.y)

calculate_scaling_factors(m, basis=ScalingBasis.InverseVarScale)

# Show that the constraint scaling factor is 1/((1/1e-5)*(1/1e-5))
assert(m.scaling_factor[m.c] - 1e-10 < 1e-12)
# Show that the z variable scaling factor is 1/((1/1e-5)*(1/1e-5))
assert(m.scaling_factor[m.z] - 1e-10 < 1e-12)

```

In the scaling expression the general guideline is that a scaling factor is being calculated based on the expected magnitude of the variable values. The magnitude could be estimated in different ways, but the most common way should be the inverse variable scale. The list below shows variable scaling bases that are provided.

ScalingBasis.InverseVarScale: Use the inverse variable scaling factors in scaling expressions.

ScalingBasis.Value: Use the current variable values in scaling expressions.

ScalingBasis.Mid: Use the mid-point between the upper and lower bounds in scaling expressions.

ScalingBasis.Lower: Use the lower bound of variables in scaling expressions.

ScalingBasis.Upper: Use the lower bound of variables in scaling expressions.

ScalingBasis.VarScale: This is less common, but it uses the variable scales directly. This can be used if you are using alternative scaling methods with divide by the scaling factor.

```
idaes.core.util.scaling.calculate_scaling_factors(m, basis=(<ScalingBasis.InverseVarScale: 3>, <ScalingBasis.Mid: 6>, <ScalingBasis.Value: 1>))
```

Set scale factors for variables and constraints from expressions stored in the `scaling_expression` suffix. The variables and Expressions in the scaling expressions are replaced by the scaling basis values before calculating the scaling factor. Variable scale factors are calculated first, and variable scaling expressions should be based on variables whose scale factors are supplied directly. Constraint scaling expressions can be based on any variables.

Parameters

- **m** (*Block*) – A Pyomo model or block to apply the scaling expressions to.
- **basis** – (ScalingBasis or List-like of ScalingBasis): Value to use when evaluating scaling expressions. A list-like of ScalingBasis can be used to provide fall-back values in the event that the first choice is not available. If none of the bases are available, 1 is used.

Returns None

Scaling Utility Functions

IDAES includes some utility functions to help evaluate model scaling and to auto-scale constraints.

```
idaes.core.util.scaling.badly_scaled_var_generator(blk, large=10000.0, small=0.001, zero=1e-10)
```

This provides a rough check for variables with poor scaling based on their current scale factors and values. For each potentially poorly scaled variable it returns the var and its current scaled value.

Parameters

- **large** – Magnitude that is considered to be too large
- **small** – Magnitude that is considered to be too small
- **zero** – Magnitude that is considered to be zero, variables with a value of zero are okay, and not reported.

Yields variable data object, current absolute value of scaled value

```
idaes.core.util.scaling.grad_fd(c, scaled=False, h=1e-06)
```

Finite difference the gradient for a constraint, objective or named expression. This is only for use in examining scaling. For faster more accurate gradients refer to `pynumero`.

Parameters

- **c** – constraint to evaluate
- **scaled** – if True calculate the scaled grad (default=False)
- **h** – step size for calculating finite differnced derivatives

Returns

(list of gradient values, list for variables in the constraint) The order of the variables corresponds to the gradient values.

`idaes.core.util.scaling.scale_constraint(c, v=None)`

This transforms a constraint with its scaling factor or a given scaling factor value. If it uses the scaling factor suffix value, the scaling factor suffix is set to 1 to avoid double scaling the constraint. This can be used when to scale constraints before sending the model to the solver.

Parameters

- **c** – Pyomo constraint
- **v** – Scale factor. If None, use value from scaling factor suffix and set suffix value to 1.

Returns None

`idaes.core.util.scaling.constraint_fd_autoscale(c, min_scale=1e-06, max_grad=100)`

Autoscale constraints so that if there maximum partial derivative with respect to any variable is greater than `max_grad` at the current variable values, the method will attempt to assign a scaling factor to the constraint that makes the maximum derivative `max_grad`. The `min_scale` value provides a lower limit allowed for constraint scaling factors. If the calculated scaling factor to make the maximum derivative `max_grad` is less than `min_scale`, `min_scale` is used instead. Derivatives are approximated using finite difference.

Parameters

- **c** – constraint object
- **max_grad** – the largest derivative after scaling subject to `min_scale`
- **min_scale** – the minimum scale factor allowed

Returns None

`idaes.core.util.scaling.set_scaling_factor(c, v)`

Set a scaling factor for a model component. This function creates the `scaling_factor` suffix if needed.

Parameters

- **c** – component to supply scaling factor for
- **v** – scaling factor

Returns None

Scaling with Ipopt

To use the supplied scaling factors with Ipopt the `nlp_scaling_method` solver option should be set to “user-scaling.”

Table Methods

The IDAES toolset contains a number of methods for generating and displaying summary tables of data in the form of pandas DataFrames.

Available Methods

`idaes.core.util.tables.arcs_to_stream_dict(blk, descend_into=True)`

Creates a stream dictionary from the Arcs in a model, using the Arc names as keys. This can be used to

automate the creation of the streams dictionary needed for the `create_stream_table_dataframe()` and `stream_states_dict()` functions.

Parameters

- **blk** (*pyomo.environ._BlockData*) – Pyomo model to search for Arcs
- **descend_into** (*bool*) – If True, search subblocks for Arcs as well. The default is True.

Returns Dictionary with Arc names as keys and the Arcs as values.

```
idaes.core.util.tables.create_stream_table_dataframe(streams, true_state=False,
                                                    time_point=0, orient='columns')
```

Method to create a stream table in the form of a pandas dataframe. Method takes a dict with name keys and stream values. Use an OrderedDict to list the streams in a specific order, otherwise the dataframe can be sorted later.

Parameters

- **streams** – dict with name keys and stream values. Names will be used as display names for stream table, and streams may be Arcs, Ports or StateBlocks.
- **true_state** – indicated whether the stream table should contain the display variables define in the StateBlock (False, default) or the state variables (True).
- **time_point** – point in the time domain at which to generate stream table (default = 0)
- **orient** – orientation of stream table. Accepted values are 'columns' (default) where streams are displayed as columns, or 'index' where stream are displayed as rows.

Returns A pandas DataFrame containing the stream table data.

```
idaes.core.util.tables.generate_table(blocks, attributes, heading=None)
```

Create a Pandas DataFrame that contains a list of user-defined attributes from a set of Blocks.

Parameters

- **blocks** (*dict*) – A dictionary with name keys and BlockData objects for values. Any name can be associated with a block. Use an OrderedDict to show the blocks in a specific order, otherwise the dataframe can be sorted later.
- **attributes** (*list or tuple of strings*) – Attributes to report from a Block, can be a Var, Param, or Expression. If an attribute doesn't exist or doesn't have a valid value, it will be treated as missing data.
- **heading** (*list or tuple of strings*) – A list of strings that will be used as column headings. If None the attribute names will be used.

Returns A Pandas dataframe containing a data table

Return type (DataFrame)

```
idaes.core.util.tables.stream_states_dict(streams, time_point=0)
```

Method to create a dictionary of state block representing stream states. This takes a dict with stream name keys and stream values.

Parameters

- **streams** – dict with name keys and stream values. Names will be used as display names for stream table, and streams may be Arcs, Ports or StateBlocks.
- **time_point** – point in the time domain at which to generate stream table (default = 0)

Returns A pandas DataFrame containing the stream table data.

`idaes.core.util.tables.stream_table_dataframe_to_string(stream_table, **kwargs)`
 Method to print a stream table from a dataframe. Method takes any argument understood by `DataFrame.to_string`

4.7.2 Core Overview

All components of the IDAES process modeling framework are built of Pyomo Block components (see Pyomo documentation).

The `ProcessBlock` class is the base class of IDAES models, and provides the common foundation for all other components.

`FlowsheetModel` objects represent the top level of the IDAES modeling hierarchy, and contain connected networks of unit models, or even contain other flowsheet models, which are connected by Pyomo Arcs.

Physical property packages supply information about a material's state including physical properties and flow rates. Reaction property packages are used in systems where chemical reactions may take place, and supply information on reaction rates and stoichiometry, based on a material's state.

Equipment models are derived from `UnitModel`. Unit models contain control volumes and have ports which can be used to connect material and energy flows between unit models. On top of the balance equations usually contained in control volumes unit models contain additional performance equations that may calculate things like heat and mass transfer or efficiency curves.

`ControlVolumes` are the basic building block used to construct unit models that contain material and energy holdup and flows in and out. These blocks contain energy, mass, and momentum balances, as well as state and reaction blocks associated with the material within the control volume.

More detail on the different types of modeling objects is available in the Modeling Concepts section.

4.8 Transformations

Transformations offer a convenient way to make systematic changes to a model.

4.8.1 Variable Replacement

There are a number of cases where it can be convenient to replace one variable for another. IDAES offers a convenient variable replacement transformation. This transformation is not reversible and can significantly alter the model structure.

An example use of this transformation, is a parameter estimation problem where a model contains several instances of a particular sub-model and each model contains a variable (β) for a model parameter to be estimated. In many cases β should be the same across all sub-models. One approach to this problem would be to add equality constraints to equate all the β 's. Another approach would be to use the variable replacement transformation to replace the individual β 's with a single global β variable.

Example

The following example demonstrates the basic usage of the transformation.

```
import idaes.core.plugins # Load IDAES plugins
import pyomo.environ as pyo

# Use Pyomo's transformation factory to create the transformation object
```

(continues on next page)

(continued from previous page)

```

rp = pyo.TransformationFactory("replace_variables")

# Create an example model
m = pyo.ConcreteModel()
m.x = pyo.Var({1,2,3}, initialize=2)
m.new_x = pyo.Var({1,2,3}, initialize=3)
m.e1 = pyo.Expression(expr=sum(m.x[i] for i in m.x))

# Apply the transformation to the model, the substitute argument contains a list
# of replacements, each element is a list-like object where the first element is
# a variable to be replaced by the second element.
rp.apply_to(m, substitute=[(m.x, m.new_x)])

# See that the variable was replaced
print(pyo.value(m.e1)) # since new_x has a value of 3 the expression value is 9

```

Output:

9

Usage

There are three basic steps to using the variable replacement transformation.

1. Import anything from the `idaes` package; this will cause the IDAES plugins to be loaded.
2. Use Pyomo's transformation factory to create a variable replacement transformation object (e.g. `rp = TransformationFactory("replace_variables")`).
3. Call the transformation object's `apply_to()` method to apply the transformation.

The `apply_to(instance, substitute)` method takes two arguments `instance` and `substitute`. The `instance` argument is a model or block to apply the transformation to. The `substitute` argument is a list-like object with substitutions. Each element is a two-element list-like object where the first element is a Pyomo Var, IndexedVar element or Reference to the variable to replace and the second element is a Pyomo Var, IndexedVar element or Reference to replace the first element with.

Indexed variables are allowed. The index set of the variable to replace must be a subset of the index set of the variable to replace it with. It can also be useful to use a Pyomo Reference to emulate an indexed variable, so this is also supported.

ReplaceVariables Class

The transformation object class is `ReplaceVariables`.

```
class idaes.core.plugins.variable_replace.ReplaceVariables (**kws)
```

Replace variables in a model or block with other variables.

Keyword arguments below are specified for the `apply_to(instance, **kwargs)` method.

Keyword Arguments `substitute` – List-like of tuples where the first item in a tuple is a Pyomo variable to be replaced and the second item in the tuple is a Pyomo variable to replace it with. This transformation is not reversible.

4.9 IDAES Model Libraries

The IDAES toolset contains a number of libraries of models for different application areas. All models within these libraries are built upon the core IDAES modeling framework, but are specialised for the needs of different applications. In many cases these models can be used together in the same flowsheet, however some applications may make specific assumptions which are not compatible with other application libraries.

4.9.1 Contents

Core IDAES Model Library

This library contains a suite of generic models that are applicable across most process applications. This library also forms the foundation for many of the specialized application libraries which build off these core models.

Contents

Property Model Library

Cubic Equations of State

This property package implements a general form of a cubic equation of state which can be used for most cubic-type equations of state. This package supports phase equilibrium calculations with a smooth phase transition formulation that makes it amenable for equation oriented optimization. The following equations of state are currently supported:

- Peng-Robinson
- Soave-Redlich-Kwong

Flow basis: Molar

Units: SI units

State Variables:

The state block uses the following state variables:

Inputs

When instantiating the parameter block that uses this particular state block, 1 optional argument can be passed:

The `valid_phase` argument denotes the valid phases for a given set of inlet conditions. For example, if the user knows a priori that it will only be a single phase (for example liquid only), then it is best not to include the complex flash equilibrium constraints in the model. If the user does not specify any option, then the package defaults to a 2 phase assumption meaning that the constraints to compute the phase equilibrium will be computed.

Degrees of Freedom

In general, the general cubic equation of state has a number of degrees of freedom equal to $2 +$ the number of components in the system (total flow rate, temperature, pressure and $N-1$ mole fractions). In some cases (primarily inlets to units), this is increased by 1 due to the removal of a constraint on the sum of mole fractions.

General Cubic Equation of State

All equations come from “The Properties of Gases and Liquids, 4th Edition” by Reid, Prausnitz and Poling. The general cubic equation of state is represented by the following equations:

$$0 = Z^3 - (1 + B - uB)Z^2 + (A - uB - (u - w)B^2)Z - AB - wB^2 - wB^3$$

$$A = \frac{a_m P}{R^2 T^2}$$

$$B = \frac{b_m P}{RT}$$

where Z is the compressibility factor of the mixture, a_m and b_m are properties of the mixture and u and w are parameters which depend on the specific equation of state being used as show in the table below.

Equation	u	w	Ω_A	Ω_B	κ_j
Peng-Robinson	2	-1	0.45724	0.07780	$(1 + (1 - T_r^2)(0.37464 + 1.54226\omega_j - 0.26992\omega_j^2))^2$
Soave-Redlich-Kwong	1	0	0.42748	0.08664	$(1 + (1 - T_r^2)(0.48 + 1.574\omega_j - 0.176\omega_j^2))^2$

The properties a_m and b_m are calculated from component specific properties a_j and b_j as shown below:

$$a_j = \frac{\Omega_A R^2 T_{c,j}^2}{P_{c,j}} \kappa_j$$

$$b_j = \frac{\Omega_B R T_{c,j}}{P_{c,j}}$$

$$a_m = \sum_i \sum_j y_i y_j (a_i a_j)^{1/2} (1 - k_{ij})$$

$$b_m = \sum_i y_i b_i$$

where $P_{c,j}$ and $T_{c,j}$ are the component critical pressures and temperatures, y_j is the mole fraction of component j , k_{ij} are a set of binary interaction parameters which are specific to the equation of state and Ω_A , Ω_B and κ_j are taken from the table above. ω_j is the Pitzer acentric factor of each component.

The cubic equation of state is solved for each phase via a call to an external function which automatically identifies the correct root of the cubic and returns the value of Z as a function of A and B along with the first and second partial derivatives.

VLE Model with Smooth Phase Transition

The flash equations consists of the following equations:

$$F^{in} = F^{liq} + F^{vap}$$

$$z_i^{in} F^{in} = x_i^{liq} F^{liq} + y_i^{vap} F^{vap}$$

At the equilibrium condition, the fugacity of the vapor and liquid phase are defined as follows:

$$\ln f_i^{vap} = \ln f_i^{liq}$$

$$f_i^{phase} = y_i^{phase} \phi_i^{phase} P$$

$$\ln \phi_i = \frac{b_i}{b_m} (Z - 1) - \ln (Z - B) + \frac{A}{B\sqrt{u^2 - 4w}} \left(\frac{b_i}{b_m} - \delta_i \right) \ln \left(\frac{2Z + B(u + \sqrt{u^2 - 4w})}{2Z + B(u - \sqrt{u^2 - 4w})} \right)$$

$$\delta_i = \frac{2a_i^{1/2}}{a_m} \sum_j x_j a_j^{1/2} (1 - k_{ij})$$

The cubic equation of state is solved to find Z for each phase subject to the composition of that phase. Typically, the flash calculations are computed at a given temperature, T . However, the flash calculations become trivial if the given conditions do not fall in the two phase region. For simulation only studies, the user may know a priori the condition of the stream but when the same set of equations are used for optimization, there is a high probability that the specifications can transcend the phase envelope and hence the flash equations included may be trivial in the single phase region (i.e. liquid or vapor only). To circumvent this problem, property packages in IDAES that support VLE will compute the flash calculations at an “equilibrium” temperature T_{eq} . The equilibrium temperature is computed as follows:

$$T_1 = \max(T_{bubble}, T)$$

$$T_{eq} = \min(T_1, T_{dew})$$

where T_{eq} is the equilibrium temperature at which flash calculations are computed, T is the stream temperature, T_1 is the intermediate temperature variable, T_{bubble} is the bubble point temperature of mixture, and T_{dew} is the dew point temperature of the mixture. Note that, in the above equations, approximations are used for the max and min functions as follows:

$$T_1 = 0.5[T + T_{bubble} + \sqrt{(T - T_{bubble})^2 + \epsilon_1^2}]$$

$$T_{eq} = 0.5[T_1 + T_{dew} - \sqrt{(T_1 - T_{dew})^2 + \epsilon_2^2}]$$

where ϵ_1 and ϵ_2 are smoothing parameters (mutable). The default values are 0.01 and 0.0005 respectively. It is recommended that $\epsilon_1 > \epsilon_2$. Please refer to reference 4 for more details. Therefore, it can be seen that if the stream temperature is less than that of the bubble point temperature, the VLE calculations will be computed at the bubble point. Similarly, if the stream temperature is greater than the dew point temperature, then the VLE calculations are computed at the dew point temperature. For all other conditions, the equilibrium calculations will be computed at the actual temperature.

Other Constraints

Additional constraints are included in the model to compute the thermodynamic properties based on the cubic equation of state, such as enthalpies and entropies. Please note that, these constraints are added only if the variable is called for when building the model. This eliminates adding unnecessary constraints to compute properties that are not needed in the model.

All thermophysical properties are calculated using an ideal and residual term, such that:

$$p = p^0 + p^r$$

The residual term is derived from the partial derivatives of the cubic equation of state, whilst the ideal term is determined using empirical correlations.

Enthalpy

The ideal enthalpy term is given by:

$$h_i^0 = \int_{298.15}^T (A + BT + CT^2 + DT^3) dT + \Delta h_{form}^{298.15K}$$

The residual enthalpy term is given by:

$$h_i^r b_m \sqrt{u^2 - 4w} = \left(T \frac{da}{dT} - a_m \right) \ln \left(\frac{2Z + B(u + \sqrt{u^2 - 4w})}{2Z + B(u - \sqrt{u^2 - 4w})} \right) + RT(Z - 1)b_m \sqrt{u^2 - 4w}$$

$$\frac{da}{dT} \sqrt{T} = -\frac{R}{2} \sqrt{\Omega_A} \sum_i \sum_j y_i y_j (1 - k_{ij}) \left(f_{w,j} \sqrt{a_i \frac{T_{c,j}}{P_{c,j}}} + f_{w,i} \sqrt{a_j \frac{T_{c,i}}{P_{c,i}}} \right)$$

Entropy

The ideal entropy term is given by:

$$s_i^0 = \int_{298.15}^T \frac{(A + BT + CT^2 + DT^3)}{T} dT + \Delta s_{form}^{298.15K}$$

The residual entropy term is given by:

$$s_i^r b_m \sqrt{u^2 - 4w} = R \ln \frac{Z - B}{Z} b_m \sqrt{u^2 - 4w} + R \ln \frac{Z P^{ref}}{P} b_m \sqrt{u^2 - 4w} + \frac{da}{dT} \ln \left(\frac{2Z + B(u + \sqrt{u^2 - 4w})}{2Z + B(u - \sqrt{u^2 - 4w})} \right)$$

Fugacity

Fugacity is calculated from the system pressure, mole fractions and fugacity coefficients as follows:

$$f_{i,p} = x_{i,p} \phi_{i,p} P$$

Fugacity Coefficient

The fugacity coefficient is calculated from the departure function of the cubic equation of state as shown below:

$$\ln \phi_i = \frac{b_i}{b_m} (Z - 1) - \ln (Z - B) + \frac{A}{B \sqrt{u^2 - 4w}} \left(\frac{b_i}{b_m} - \delta_i \right) \ln \left(\frac{2Z + B(u + \sqrt{u^2 - 4w})}{2Z + B(u - \sqrt{u^2 - 4w})} \right)$$

$$\delta_i = \frac{2a_i^{1/2}}{a_m} \sum_j x_j a_j^{1/2} (1 - k_{ij})$$

Gibbs Energy

The Gibbs energy of the system is calculated using the definition of Gibbs energy:

$$g_i = h_i - T \Delta s_i$$

List of Variables

Variable Name	Description	Units
flow_mol	Total molar flow rate	mol/s
mole_frac_comp	Mixture mole fraction indexed by component	None
temperature	Temperature	K
pressure	Pressure	Pa
flow_mol_phase	Molar flow rate indexed by phase	mol/s
mole_frac_phase_comp	Mole fraction indexed by phase and component	None
pressure_sat	Saturation or vapor pressure indexed by component	Pa
dens_mol_phase	Molar density indexed by phase	mol/m ³
dens_mass_phase	Mass density indexed by phase	kg/m ³
enth_mol_phase	Molar enthalpy indexed by phase	J/mol
enth_mol	Molar enthalpy of mixture	J/mol
entr_mol_phase	Molar entropy indexed by phase	J/mol.K
entr_mol	Molar entropy of mixture	J/mol.K
fug_phase_comp	Fugacity indexed by phase and component	Pa
fug_coeff_phase_comp	Fugacity coefficient indexed by phase and component	None
gibbs_mol_phase	Molar Gibbs energy indexed by phase	J/mol
mw	Molecular weight of mixture	kg/mol
mw_phase	Molecular weight by phase	kg/mol
temperature_bubble	Bubble point temperature	K
temperature_dew	Dew point temperature	K
pressure_bubble	Bubble point pressure	Pa
pressure_dew	Dew point pressure	Pa
_teq	Temperature at which the VLE is calculated	K

List of Parameters

Parameter Name	Description	Units
cubic_type	Type of cubic equation of state to use, from CubicEoS Enum	None
pressure_ref	Reference pressure	Pa
temperature_ref	Reference temperature	K
omega	Pitzer acentricity factor	None
kappa	Binary interaction parameters for EoS (note that parameters are specific for a given EoS)	None
mw_comp	Component molecular weights	kg/mol
cp_ig	Parameters for calculating component heat capacities	varies
dh_form	Component standard heats of formation (used for enthalpy at reference state)	J/mol
ds_form	Component standard entropies of formation (used for entropy at reference state)	J/mol.K
antoine	Component Antoine coefficients (used to initialize bubble and dew point calculations)	bar, K

Config Block Documentation

class `idaes.generic_models.properties.cubic_eos.cubic_prop_pack.CubicParameterData` (*component*)
 General Property Parameter Block Class

build()

Callable method for Block construction.

classmethod define_metadata (*obj*)

Define properties supported and units.

class `idaes.generic_models.properties.cubic_eos.cubic_prop_pack.CubicStateBlock` (**args*,
***kwargs*)

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

parameters A reference to an instance of the Property Parameter Block associated with this property package.

defined_state Flag indicating whether the state should be considered fully defined, and thus whether constraints such as sum of mass/mole fractions should be included, **default** - False. **Valid values:** { **True** - state variables will be fully defined, **False** - state variables will not be fully defined. }

has_phase_equilibrium Flag indicating whether phase equilibrium constraints should be constructed in this state block, **default** - True. **Valid values:** { **True** - StateBlock should calculate phase equilibrium, **False** - StateBlock should not calculate phase equilibrium. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (CubicStateBlock) New instance

class `idaes.generic_models.properties.cubic_eos.cubic_prop_pack.CubicStateBlockData` (*components*)
An general property package for cubic equations of state with VLE.

build()

Callable method for Block construction.

define_display_vars()

Method used to specify components to use to generate stream tables and other outputs. Defaults to `define_state_vars`, and developers should overload as required.

define_state_vars()

Define state vars.

get_energy_density_terms (*p*)

Create energy density terms.

get_enthalpy_flow_terms (*p*)

Create enthalpy flow terms.

get_material_density_terms (*p, j*)

Create material density terms.

get_material_flow_basis()

Method which returns an Enum indicating the basis of the material flow term.

get_material_flow_terms(p, j)

Create material flow terms for control volume.

model_check()

Model checks for property block.

Vapor-Liquid Equilibrium Property Models (Ideal Gas - Non-ideal Liquids)

This property package supports phase equilibrium calculations with a smooth phase transition formulation that makes it amenable for equation oriented optimization. The gas phase is assumed to be ideal and for the liquid phase, the package supports an ideal liquid or a non-ideal liquid using an activity coefficient model. To compute the activity coefficient, the package currently supports the Non Random Two Liquid Model (NRTL) or the Wilson model. Therefore, this property package supports the following combinations for gas-liquid mixtures for VLE calculations:

1. Ideal (vapor) - Ideal (liquid)
2. Ideal (vapor) - NRTL (liquid)
3. Ideal (vapor) - Wilson (liquid)

Flow basis: Molar

Units: SI units

State Variables:

The state block supports the following two sets of state variables:

Option 1 - “FTPz”:

Option 2 - “FcTP”:

The user can specify the choice of state variables while instantiating the parameter block. See the Inputs section for more details.

Support for other combinations of state variables will be made available in the future.

Inputs

When instantiating the parameter block that uses this particular state block, 2 arguments can be passed:

The `valid_phase` argument denotes the valid phases for a given set of inlet conditions. For example, if the user knows a priori that it will only be a single phase (for example liquid only), then it is best not to include the complex flash equilibrium constraints in the model. If the user does not specify any option, then the package defaults to a 2 phase assumption meaning that the constraints to compute the phase equilibrium will be computed.

The `activity_coeff_model` denotes the liquid phase assumption to be used. If the user does not specify any option, then the package defaults to assuming an ideal liquid assumption.

The `state_vars` denotes the preferred set of state variables to be used. If the user does not specify any option, then the package defaults to using the total flow, mixture mole fraction, temperature and pressure as the state variables.

Degrees of Freedom

The number of degrees of freedom that need to be fixed to yield a square problem (i.e. degrees of freedom = 0) depends on the options selected. The following table provides a summary of the variables to be fixed and also the corresponding variable names in the model.

Property Model Type	State variables	Additional Variables	Total number of variables
Ideal (vapor) - Ideal (liquid)	flow_mol, temperature, pressure, mole_frac_comp	None	$3 + N_c$
Ideal (vapor) - NRTL (liquid)	flow_mol, temperature, pressure, mole_frac_comp	alpha, tau	$3 + N_c + 2N_c^2$
Ideal (vapor) - Wilson (liquid)	flow_mol, temperature, pressure, mole_frac_comp	vol_mol_comp, tau	$3 + N_c + 2N_c^2$

Please refer to reference 3 for recommended values for tau.

VLE Model with Smooth Phase Transition

The flash equations consists of the following equations depending on the choice of state variables selected by the user.

If the state variables are total flow, mole fraction, temperature, and pressure, then the following constraints are implemented:

$$F^{in} = F^{liq} + F^{vap}$$

$$z_i^{in} F^{in} = x_i^{liq} F^{liq} + y_i^{vap} F^{vap}$$

If the state variables are component flow rates, temperature, and pressure, then the following constraints are implemented:

$$F_i^{in} = F_i^{liq} + F_i^{vap}$$

The equilibrium condition, the fugacity of the vapor and liquid phase are defined as follows:

$$f_i^{vap} = f_i^{liq}$$

$$f_i^{vap} = y_i \phi_i P$$

$$f_i^{liq} = x_i p_i^{sat} \nu_i$$

The equilibrium constraint is written as a generic constraint such that it can be extended easily for non-ideal gases and liquids. As this property package only supports an ideal gas, the fugacity coefficient (ϕ_i) for the vapor phase is 1 and hence the expression reduces to $y_i P$. For the liquid phase, if the ideal option is selected then the activity coefficient (ν_i) is 1. If an activity coefficient model is selected then corresponding constraints are added to compute the activity coefficient.

Typically, the flash calculations are computed at a given temperature, T . However, the flash calculations become trivial if the given conditions do not fall in the two phase region. For simulation only studies, the user may know a priori the

condition of the stream but when the same set of equations are used for optimization, there is a high probability that the specifications can transcend the phase envelope and hence the flash equations included may be trivial in the single phase region (i.e. liquid or vapor only). To circumvent this problem, property packages in IDAES that support VLE will compute the flash calculations at an “equilibrium” temperature T_{eq} . The equilibrium temperature is computed as follows:

$$T_1 = \max(T_{bubble}, T)$$

$$T_{eq} = \min(T_1, T_{dew})$$

where T_{eq} is the equilibrium temperature at which flash calculations are computed, T is the stream temperature, T_1 is the intermediate temperature variable, T_{bubble} is the bubble point temperature of mixture, and T_{dew} is the dew point temperature of the mixture. Note that, in the above equations, approximations are used for the max and min functions as follows:

$$T_1 = 0.5[T + T_{bubble} + \sqrt{(T - T_{bubble})^2 + \epsilon_1^2}]$$

$$T_{eq} = 0.5[T_1 + T_{dew} - \sqrt{(T_1 - T_{dew})^2 + \epsilon_2^2}]$$

where ϵ_1 and ϵ_2 are smoothing parameters(mutable). The default values are 0.01 and 0.0005 respectively. It is recommended that $\epsilon_1 > \epsilon_2$. Please refer to reference 4 for more details. Therefore, it can be seen that if the stream temperature is less than that of the bubble point temperature, the VLE calculations will be computed at the bubble point. Similarly, if the stream temperature is greater than the dew point temperature, then the VLE calculations are computed at the dew point temperature. For all other conditions, the equilibrium calculations will be computed at the actual temperature.

Additional constraints are included in the model to compute the thermodynamic properties such as component saturation pressure, enthalpy, specific heat capacity. Please note that, these constraints are added only if the variable is called for when building the model. This eliminates adding unnecessary constraints to compute properties that are not needed in the model.

The saturation or vapor pressure (`pressure_sat`) for component i is computed using the following correlation[1]:

$$\log \frac{P^{sat}}{P_c} = \frac{Ax + Bx^{1.5} + Cx^3 + Dx^6}{1 - x}$$

$$x = 1 - \frac{T_{eq}}{T_c}$$

where P_c is the critical pressure, T_c is the critical temperature of the component and T_{eq} is the equilibrium temperature at which the saturation pressure is computed. Please note that when using this expression, $T_{eq} < T_c$ is required and when violated it results in a negative number raised to the power of a fraction.

The specific enthalpy (`enthalpy_comp_liq`) for component i is computed using the following expression for the liquid phase:

$$h_i^{liq} = \Delta h_{form,Liq,i} + \int_{298.15}^T (A + BT + CT^2 + DT^3 + ET^4) dT$$

The specific enthalpy (`enthalpy_comp_vap`) for component i is computed using the following expression for the vapor phase:

$$h_i^{vap} = \Delta h_{form,Vap,i} + \int_{298.15}^T (A + BT + CT^2 + DT^3 + ET^4) dT$$

The mixture specific enthalpies (`enthalpy_liq` & `enthalpy_vap`) are computed using the following expressions for the liquid and vapor phase respectively:

$$H^{liq} = \sum_i h_i^{liq} x_i$$

$$H^{vap} = \sum_i h_i^{vap} y_i$$

Similarly, specific entropies are calculated as follows. The specific entropy (`entropy_comp_liq`) for component i is computed using the following expression for the liquid phase:

$$s_i^{liq} = \Delta s_{form,Liq,i} + \int_{298.15}^T (A/T + B + CT + DT^2 + ET^3) dT$$

The specific entropy (`entropy_comp_vap`) for component i is computed using the following expression for the vapor phase:

$$s_i^{vap} = \Delta s_{form,Vap,i} + \int_{298.15}^T (A/T + B + CT + DT^2 + ET^3) dT$$

Please refer to references 1 and 2 to get parameters for different components.

Activity Coefficient Model - NRTL

The activity coefficient for component i is computed using the following equations when using the Non-Random Two Liquid model [3]:

$$\log \gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ij}}{\sum_k x_k G_{kj}} \left[\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right]$$

$$G_{ij} = \exp(-\alpha_{ij} \tau_{ij})$$

where α_{ij} is the non-randomness parameter and τ_{ij} is the binary interaction parameter for the NRTL model. Note that in the IDAES implementation, these are declared as variables that allows for more flexibility and the ability to use these in a parameter estimation problem. These NRTL model specific variables need to be either fixed for a given component set or need to be estimated from VLE data.

The bubble point is computed by enforcing the following condition:

$$\sum_i [z_i p_i^{sat}(T_{bubble}) \nu_i] - P = 0$$

Activity Coefficient Model - Wilson

The activity coefficient for component i is computed using the following equations when using the Wilson model [3]:

$$\log \gamma_i = 1 - \log \sum_j x_j G_{ji} - \sum_j \frac{x_j G_{ij}}{\sum_k x_k G_{kj}}$$

$$G_{ij} = (v_i/v_j) \exp(-\tau_{ij})$$

where v_i is the molar volume of component i and τ_{ij} is the binary interaction parameter. These are Wilson model specific variables that either need to be fixed for a given component set or need to be estimated from VLE data.

The bubble point is computed by enforcing the following condition:

$$\sum_i [z_i p_i^{sat}(T_{bubble}) \nu_i] - P = 0$$

List of Variables

Variable Name	Description	Units
flow_mol	Total molar flow rate	mol/s
mole_frac_comp	Mixture mole fraction indexed by component	None
temperature	Temperature	K
pressure	Pressure	Pa
flow_mol_phase	Molar flow rate indexed by phase	mol/s
mole_frac_phase_comp	Mole fraction indexed by phase and component	None
pressure_sat	Saturation or vapor pressure indexed by component	Pa
density_mol_phase	Molar density indexed by phase	mol/m3
ds_vap	Molar entropy of vaporization	J/mol.K
enthalpy_comp_liq	Liquid molar enthalpy indexed by component	J/mol
enthalpy_comp_vap	Vapor molar enthalpy indexed by component	J/mol
enthalpy_liq	Liquid phase enthalpy	J/mol
enthalpy_vap	Vapor phase enthalpy	J/mol
entropy_comp_liq	Liquid molar entropy indexed by component	J/mol
entropy_comp_vap	Vapor molar entropy indexed by component	J/mol
entolpy_liq	Liquid phase entropy	J/mol
entropy_vap	Vapor phase entropy	J/mol
temperature_bubble	Bubble point temperature	K
temperature_dew	Dew point temperature	K
_temperature_equilibrium	Temperature at which the VLE is calculated	K

Table 2: NRTL model specific variables

Variable Name	Description	Units
alpha	Non-randomness parameter indexed by component and component	None
tau	Binary interaction parameter indexed by component and component	None
activity_coeff_comp	Activity coefficient indexed by component	None

Table 3: Wilson model specific variables

Variable Name	Description	Units
vol_mol_comp	Molar volume of component indexed by component	None
tau	Binary interaction parameter indexed by component and component	None
activity_coeff_comp	Activity coefficient indexed by component	None

Initialization

Config Block Documentation

```
class idaes.generic_models.properties.activity_coeff_models.activity_coeff_prop_pack.Activ
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”

- **default** (*dict*) – Default ProcessBlockData config

Keys

default_arguments Default arguments to use with Property Package

activity_coeff_model Flag indicating the activity coefficient model to be used for the non-ideal liquid, and thus corresponding constraints should be included, **default** - Ideal liquid. **Valid values:** { “NRTL” - Non Random Two Liquid Model, “Wilson” - Wilson Liquid Model, }

state_vars Flag indicating the choice for state variables to be used for the state block, and thus corresponding constraints should be included, **default** - FTPz **Valid values:** { “FTPx” - Total flow, Temperature, Pressure and Mole fraction, “FcTP” - Component flow, Temperature and Pressure }

valid_phase Flag indicating the valid phase for a given set of conditions, and thus corresponding constraints should be included, **default** - (“Vap”, “Liq”). **Valid values:** { “Liq” - Liquid only, “Vap” - Vapor only, (“Vap”, “Liq”) - Vapor-liquid equilibrium, (“Liq”, “Vap”) - Vapor-liquid equilibrium, }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (ActivityCoeffParameterBlock) New instance

class `idaes.generic_models.properties.activity_coeff_models.activity_coeff_prop_pack.ActivityCoeffParameterBlock`

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

parameters A reference to an instance of the Property Parameter Block associated with this property package.

defined_state Flag indicating whether the state should be considered fully defined, and thus whether constraints such as sum of mass/mole fractions should be included, **default** - False. **Valid values:** { **True** - state variables will be fully defined, **False** - state variables will not be fully defined. }

has_phase_equilibrium Flag indicating whether phase equilibrium constraints should be constructed in this state block, **default** - True. **Valid values:** { **True** - StateBlock should calculate phase equilibrium, **False** - StateBlock should not calculate phase equilibrium. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (ActivityCoeffStateBlock) New instance

```
class idaes.generic_models.properties.activity_coeff_models.activity_coeff_prop_pack.Activ
    An example property package for ideal VLE.

    build()
        Callable method for Block construction.

    define_state_vars()
        Define state vars.

    get_energy_density_terms(p)
        Create enthalpy density terms.

    get_enthalpy_flow_terms(p)
        Create enthalpy flow terms.

    get_material_density_terms(p,j)
        Create material density terms.

    get_material_flow_basis()
        Declare material flow basis.

    get_material_flow_terms(p,j)
        Create material flow terms for control volume.

    model_check()
        Model checks for property block.
```

References

1. “The properties of gases and liquids by Robert C. Reid”
2. “Perry’s Chemical Engineers Handbook by Robert H. Perry”.
3. H. Renon and J.M. Prausnitz, “Local compositions in thermodynamic excess functions for liquid mixtures.”, AIChE Journal Vol. 14, No.1, 1968.
4. AP Burgard, JP Eason, JC Eslick, JH Ghouse, A Lee, LT Biegler, DC Miller. “A Smooth, Square Flash Formulation for Equation Oriented Flowsheet Optimization”, Computer Aided Chemical Engineering 44, 871-876, 2018

Water/Steam - IAPWS95

Accurate and thermodynamically consistent steam properties are provided for the IDAES framework by implementing the International Association for the Properties of Water and Steam’s “*Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use.*” Non-analytic terms designed to improve accuracy very near the critical point were omitted, because they cause a singularity at the critical point, a feature which is undesirable in optimization problems. The IDAES implementation provides features which make the water and steam property calculations amenable to rigorous mathematical optimization.

Example

Theses modules can be imported as:

```
from idaes.generic_models.properties import iapws95
```

The Heater unit model *example*, provides a simple example for using water properties.

```
import pyomo.environ as pe # Pyomo environment
from idaes.core import FlowsheetBlock, MaterialBalanceType
from idaes.generic_models.unit_models import Heater
from idaes.generic_models.properties import iapws95

# Create an empty flowsheet and steam property parameter block.
model = pe.ConcreteModel()
model.fs = FlowsheetBlock(default={"dynamic": False})
model.fs.properties = iapws95.Iapws95ParameterBlock(default={
    "phase_presentation": iapws95.PhaseType.LG,
    "state_vars": iapws95.StateVars.PH})

# Add a Heater model to the flowsheet.
model.fs.heater = Heater(default={
    "property_package": model.fs.properties,
    "material_balance_type": MaterialBalanceType.componentTotal})

# Setup the heater model by fixing the inputs and heat duty
model.fs.heater.inlet[:].enth_mol.fix(4000)
model.fs.heater.inlet[:].flow_mol.fix(100)
model.fs.heater.inlet[:].pressure.fix(101325)
model.fs.heater.heat_duty[:].fix(100*20000)

# Initialize the model.
model.fs.heater.initialize()
```

Since all properties except the state variables are Pyomo Expressions in the water properties module, after solving the problem any property can be calculated in any state block. Continuing from the heater example, to get the viscosity of both phases, the lines below could be added.

```
mu_l = pe.value(model.fs.heater.control_volume.properties_out[0].visc_d_phase["Liq"])
mu_v = pe.value(model.fs.heater.control_volume.properties_out[0].visc_d_phase["Vap"])
```

For more information about how StateBlocks and PropertyParameterBlocks work see the [StateBlock documentation](#).

Units

The iapws95 property module uses SI units (m, kg, s, J, mol) for all public variables and expressions. Temperature is in K. Note that this means molecular weight is in the unusual unit of kg/mol.

A few expressions intended to be used internally and all external function calls use units of kg, kJ, kPa, and K. These generally are not needed by the end user.

Methods

These methods use the IAPWS-95 formulation for scientific use for thermodynamic properties ([Wagner and Pruss, 2002](#); [IAPWS, 2016](#)). To solve the phase equilibrium, the method of [Akasaka \(2008\)](#) was used. For solving these equations, some relations from the IAPWS-97 formulation for industrial use are used as initial values ([Wagner et al., 2002](#)). The industrial formulation is slightly discontinuous between different regions, so it may not be suitable for optimization. In addition to thermodynamic quantities, viscosity and thermal conductivity are calculated ([IAPWS, 2008](#); [IAPWS, 2011](#)).

External Functions

The IAPWS-95 formulation uses density and temperature as state variables. For most applications those state variables are not the most convenient choices. Using other state variables requires solving equations to get density and temperature from the chosen state variables. These equations can have numerous solutions only one of which is physically meaningful. Rather than solve these equations as part of the full process simulation, external functions were developed that can solve the equations required to change state variables and guarantee the correct roots.

The external property functions are written in C++ and compiled such that they can be called by AMPL solvers. See the [Installation](#) page for information about compiling these functions. The external functions provide both first and second derivatives for all property function calls, however at phase transitions some of these functions may be non-smooth.

IDAES Framework Wrapper

A wrapper for the external functions is provided for compatibility with the IDAES framework. Most properties are available as Pyomo Expressions from the wrapper. Only the state variables are model variables. Benefits of using mostly expressions in the property package are: no initialization is required specifically for the property package, the model has fewer equations, and all properties can be easily calculated after the model is solved from the state variable values even if they were not used in the model. Calls to the external functions are used within expressions so users do not need to directly call any functions. The potential downside of the extensive use of expressions here is that combining the expressions to form constraints could yield equations that are more difficult to solve than, they would have been if an equivalent system of equations was written with more variables and simpler equations. Quantifying the effect of writing larger equations with fewer variables is difficult. Experience suggests in this particular case more expressions and fewer variables is better.

Although not generally used, the wrapper provides direct access to the `ExternalFunctions`, including intermediate functions. For more information see section [ExternalFunctions](#). These are mostly available for testing purposes.

Phase Presentation

The property package wrapper can present fluid phase information to the IDAES framework in different ways. See the [class reference](#) for details on how to set these options. The `phase_presentation=PhaseType.MIX` option looks like one phase called “Mix” to the IDAES framework. The property package will calculate a phase fraction. This will bypass any two phase handling equations written for unit models, and should work with any unit model options as long as you do not want to separate the phases. The benefit of this option is that it can potentially lead to a simpler set of equations.

The `phase_presentation=PhaseType.LG` option appears to the IDAES framework to be two phases “Vap” and “Liq”. This option requires one of two unit model options to be set. You can use the total material balance option for unit models, to specify that only one material balance equation should be written not one per phase. The other possible option is to specify `has_phase_equilibrium=True`. This will still write a material balance per phase, but will add a phase generation term to the model. For the IAPWS-95 package, it is generally recommended that specifying total material balances is best because it results in a problem with fewer variables.

There are also two single phase options `phase_presentation=PhaseType.L` and `phase_presentation=PhaseType.G`, these present a single phase “Liq” or “Vap” to the framework. The vapor fraction will also always return 0 or 1 as appropriate. These options can be used when the phase of a fluid is known for certain to only be liquid or only be vapor. For the temperature-pressure-vapor fraction formulation, this eliminates the complementarity constraint, but for the enthalpy-pressure formulation, where the vapor fraction is always calculated, the single phase options probably do not provide any real benefit.

Pressure-Enthalpy Formulation

The advantage of this choice of state variables is that it is very robust when phase changes occur, and is especially useful when it is not known if a phase change will occur. The disadvantage of this choice of state variables is that for equations like heat transfer equations that are highly dependent on temperature, a model could be harder to solve near regions with phase change. Temperature is a non-smooth function with non-smoothness when transitioning from the single-phase to the two-phase region. Temperature also has a zero derivative with respect to enthalpy in the two-phase region, so near the two-phase region solving a constraint that specifies a specific temperature may not be possible.

The variables for this form are `flow_mol` (mol/s), `pressure` (Pa), and `enth_mol` (J/mol).

Since temperature and vapor fraction are not state variables in this formulation, they are provided by expressions, and cannot be fixed. For example, to set a temperature to a specific value, a constraint could be added which says the temperature expression equals a fixed value.

These expressions are specific to the P-H formulation:

temperature Expression that calculates temperature by calling an ExternalFunction of enthalpy and pressure. This expression is non-smooth in the transition from single-phase to two-phase and has a zero derivative with respect to enthalpy in the two-phase region.

vapor_frac Expression that calculates vapor fraction by calling an ExternalFunction of enthalpy and pressure. This expression is non-smooth in the transition from single-phase to two-phase and has a zero derivative with respect to enthalpy in the single-phase region, where the value is 0 (liquid) or 1 (vapor).

Temperature-Pressure-Vapor Fraction

This formulation uses temperature (K), pressure (Pa), and vapor fraction as state variables. When a single phase option is given, the vapor fraction is fixed to the appropriate value and not included in the state variable set. For single phase, the complementarity constraint is also deactivated.

A complementarity constraint is required for the T-P-x formulation. First, two expressions are defined below where P^- is pressure under saturation pressure and P^+ is pressure over saturation pressure. The max function is provided by an IDAES utility function which provides a smooth max expression.

$$P^- = \max(0, P_{\text{sat}} - P)$$

$$P^+ = \max(0, P - P_{\text{sat}})$$

With the pressure over and pressure under saturated pressure expressions a complementarity constraint can be written. If the pressure under saturation is more than zero, only vapor exists. If the pressure over saturation is greater than zero only a liquid exists. If both are about zero two phases can exist. The saturation pressure function maxes out at the critical pressure and any temperature above the critical temperature will yield a saturation pressure that is the critical pressure, so supercritical fluids will be classified as liquids as the convention for this property package.

$$0 = xP^+ - (1 - x)P^-$$

Assuming the vapor fraction (x) is positive and noting that only one of P^+ and P^- can be nonzero (approximately), the complementarity equation above requires x to be 0 when P^+ is not zero (liquid) or x to be 1 when P^- is not zero (vapor). When both P^+ and P^- are about 0, the complementarity constraint says nothing about x , but it does provide another constraint, that $P = P_{\text{sat}}$. When two phases are present x can be found by the unit model energy balance and the temperature will be T_{sat} .

An alternative approach is sometimes useful. If you know for certain that you have two phases, the complementarity constraint can be deactivated and a $P = P_{\text{sat}}$ or $T = T_{\text{sat}}$ constraint can be added.

Using the T-P-x formulation requires better initial guesses than the P-H form. It is not strictly necessary but it is best to try to get an initial guess that is in the correct phase region for the expected result model.

Expressions

Unless otherwise noted, the property expressions are common to both the T-P-x and P-H formulations. For phase specific properties, valid phase indexes are "Liq" and "Vap"

Expression	Description
mw	Molecular weight (kg/mol)
tau	Critical temperature divided by temperature (unitless)
temperature	Temperature (K) if PH form
temperature_red	Reduced temperature, temperature divided by critical temperature (unitless)
temperature_sat	Saturation temperature (K)
tau_sat	Critical temperature divided by saturation temperature (unitless)
pressure_sat	Saturation pressure (Pa)
dens_mass_phase[phase]	Density phase (kg/m ³)
dens_phase_red[phase]	Phase reduced density (δ), mass density divided by critical density (unitless)
dens_mass	Total mixed phase mass density (kg/m ³)
dens_mol	Total mixed phase mole density (kg/m ³)
flow_vol	Total volumetric flow rate (m ³ /s)
enth_mass	Mass enthalpy (J/kg)
enth_mol_sat_phase[phase]	Saturation enthalpy of phase, enthalpy at P and T _{sat} (J/mol)
enth_mol	Molar enthalpy (J/mol) if TPx form
enth_mol_phase[phase]	Molar enthalpy of phase (J/mol)
energy_internal_mol	molar internal energy (J/mol)
energy_internal_mol_phase[phase]	Molar internal energy of phase (J/mol)
entr_mol_phase	Molar entropy of phase (J/mol/K)
entr_mol	Total mixed phase entropy (J/mol/K)
cp_mol_phase[phase]	Constant pressure molar heat capacity of phase (J/mol/K)
cv_mol_phase[phase]	Constant pressure volume heat capacity of phase (J/mol/K)
cp_mol	Total mixed phase constant pressure heat capacity (J/mol/K)
cv_mol	Total mixed phase constant volume heat capacity (J/mol/K)
heat_capacity_ratio	cp_mol/cv_mol
speed_sound_phase[phase]	Speed of sound in phase (m/s)
dens_mol_phase[phase]	Mole density of phase (mol/m ³)
therm_cond_phase[phase]	Thermal conductivity of phase (W/K/m)
vapor_frac	Vapor fraction, if PH form
visc_d_phase[phase]	Viscosity of phase (Pa/s)
visc_k_phase[phase]	Kinimatic viscosity of phase (m ² /s)
phase_frac[phase]	Phase fraction
flow_mol_comp["H2O"]	Same as total flow since only water (mol/s)
P_under_sat	Pressure under saturation pressure (kPa)
P_over_sat	Pressure over saturation pressure (kPa)

ExternalFunctions

This provides a list of ExternalFuctions available in the wrapper. These functions do not use SI units and are not usually called directly. If these functions are needed, they should be used with caution. Some of these are used in the property expressions, some are just provided to allow easier testing with a Python framework.

All of these functions provide first and second derivative and are generally suited to optimization (including the ones that return derivatives of Helmholtz free energy). Some functions may have non-smoothness at phase transitions. The delta_vap and delta_liq functions return the same values in the critical region. They will also return real values

when a phase doesn't exist, but those values do not necessarily have physical meaning.

There are a few variables that are common to a lot of these functions, so they are summarized here τ is the critical temperature divided by the temperature $\frac{T_c}{T}$, δ is density divided by the critical density $\frac{\rho}{\rho_c}$, and ϕ is Helmholtz free energy divided by the ideal gas constant and temperature $\frac{f}{RT}$.

Pyomo Function	C Function	Returns	Arguments
func_p	p	pressure (kPa)	δ, τ
func_u	u	internal energy (kJ/kg)	δ, τ
func_s	s	entropy (kJ/K/kg)	δ, τ
func_h	h	enthalpy (kJ/kg)	δ, τ
func_hvpt	hvpt	vapor enthalpy (kJ/kg)	P (kPa), τ
func_hlpt	hlpt	liquid enthalpy (kJ/kg)	P (kPa), τ
func_tau	tau	τ (unitless)	h (kJ/kg), P (kPa)
func_vf	vf	vapor fraction (unitless)	h (kJ/kg), P (kPa)
func_g	g	Gibbs free energy (kJ/kg)	δ, τ
func_f	f	Helmholtz free energy (kJ/kg)	δ, τ
func_cv	cv	const. volume heat capacity (kJ/K/kg)	δ, τ
func_cp	cp	const. pressure heat capacity (kJ/K/kg)	δ, τ
func_w	w	speed of sound (m/s)	δ, τ
func_delta_liq	delta_liq	liquid δ (unitless)	P (kPa), τ
func_delta_vap	delta_vap	vapor δ (unitless)	P (kPa), τ
func_delta_sat_l	delta_sat_l	sat. liquid δ (unitless)	τ
func_delta_sat_v	delta_sat_v	sat. vapor δ (unitless)	τ
func_p_sat	p_sat	sat. pressure (kPa)	τ
func_tau_sat	tau_sat	sat. τ (unitless)	P (kPa)
func_phi0	phi0	ϕ idaes gas part (unitless)	δ, τ
func_phi0_delta	phi0_delta	$\frac{\partial \phi_0}{\partial \delta}$	δ
func_phi0_delta2	phi0_delta2	$\frac{\partial^2 \phi_0}{\partial \delta^2}$	δ
func_phi0_tau	phi0_tau	$\frac{\partial \phi_0}{\partial \tau}$	τ
func_phi0_tau2	phi0_tau2	$\frac{\partial^2 \phi_0}{\partial \tau^2}$	τ
func_phir	phir	ϕ real gas part (unitless)	δ, τ
func_phir_delta	phir_delta	$\frac{\partial \phi_r}{\partial \delta}$	δ, τ
func_phir_delta2	phir_delta2	$\frac{\partial^2 \phi_r}{\partial \delta^2}$	δ, τ
func_phir_tau	phir_tau	$\frac{\partial \phi_r}{\partial \tau}$	δ, τ
func_phir_tau2	phir_tau2	$\frac{\partial^2 \phi_r}{\partial \tau^2}$	δ, τ
func_phir_delta_tau	phir_delta_tau	$\frac{\partial^2 \phi_r}{\partial \delta \partial \tau}$	δ, τ

Initialization

The IAPWS-95 property functions do provide initialization functions for general compatibility with the IDAES framework, but as long as the state variables are specified to some reasonable value, initialization is not required. All required solves are handled by external functions.

References

International Association for the Properties of Water and Steam (2016). IAPWS R6-95 (2016), "Revised Release on the IAPWS Formulation 1995 for the Properties of Ordinary Water Substance for General Scientific Use," URL: <http://iapws.org/relguide/IAPWS95-2016.pdf>

Wagner, W., A. Pruss (2002). “The IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use.” J. Phys. Chem. Ref. Data, 31, 387-535.

Wagner, W. et al. (2000). “The IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam,” ASME J. Eng. Gas Turbines and Power, 122, 150-182.

Akasaka, R. (2008). “A Reliable and Useful Method to Determine the Saturation State from Helmholtz Energy Equations of State.” Journal of Thermal Science and Technology, 3(3), 442-451.

International Association for the Properties of Water and Steam (2011). IAPWS R15-11, “Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance,” URL: <http://iapws.org/relguide/ThCond.pdf>.

International Association for the Properties of Water and Steam (2008). IAPWS R12-08, “Release on the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance,” URL: <http://iapws.org/relguide/visc.pdf>.

Convenience Functions

`idaes.generic_models.properties.iapws95.htpx(T, P=None, x=None)`

Convenience function to calculate steam enthalpy from temperature and either pressure or vapor fraction. This function can be used for inlet streams and initialization where temperature is known instead of enthalpy.

User must provided values for one (and only one) of arguments P and x.

Parameters

- **T** – Temperature [K] (between 200 and 3000)
- **P** – Pressure [Pa] (between 1 and 1e9), None if saturated steam
- **x** – Vapor fraction [mol vapor/mol total] (between 0 and 1), None if
- **or subcooled** (*superheated*) –

Returns Total molar enthalpy [J/mol].

lapws95StateBlock Class

`class idaes.generic_models.properties.iapws95.Iapws95StateBlock(*args, **kwargs)`

This is some placeholder doc.

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

parameters A reference to an instance of the Property Parameter Block associated with this property package.

defined_state Flag indicating whether the state should be considered fully defined, and thus whether constraints such as sum of mass/mole fractions should be included, **default** - False. **Valid values:** { **True** - state variables will be fully defined, **False** - state variables will not be fully defined. }

has_phase_equilibrium Flag indicating whether phase equilibrium constraints should be constructed in this state block, **default** - True. **Valid values:** { **True** - StateBlock should calculate phase equilibrium, **False** - StateBlock should not calculate phase equilibrium. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (Iapws95StateBlock) New instance

lapws95StateBlockData Class

class `idaes.generic_models.properties.iapws95.Iapws95StateBlockData` (*component*)
This is a property package for calculating thermophysical properties of water.

build(*args)
Callable method for Block construction

lapws95ParameterBlock Class

[illegible]

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

default arguments Default arguments to use with Property Package

phase_presentation Set the way phases are presented to models. The MIX option appears to the framework to be a mixed phase containing liquid and/or vapor. The mixed option can simplify calculations at the unit model level since it can be treated as a single phase, but unit models such as flash vessels will not be able to treat the phases independently. The LG option presents as two separate phases to the framework. The L or G options can be used if it is known for sure that only one phase is present. **default** - PhaseType.MIX **Valid values:** { **PhaseType.MIX** - Present a mixed phase with liquid and/or vapor, **PhaseType.LG** - Present a liquid and vapor phase, **PhaseType.L** - Assume only liquid can be present, **PhaseType.G** - Assume only vapor can be present }

state_vars The set of state variables to use. Depending on the use, one state variable set or another may be better computationally. Usually pressure and enthalpy are the best choice because they are well behaved during a phase change. **default** - StateVars.PH
Valid values: { **StateVars.PH** - Pressure-Enthalpy, **StateVars.TPX** - Temperature-Pressure-Quality }

- **initialize**(*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.

- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (Iapws95ParameterBlock) New instance

Iapws95ParameterBlockData Class

```
class idaes.generic_models.properties.iapws95.Iapws95ParameterBlockData (component)
```

build()

General build method for PropertyParameterBlocks. Inheriting models should call super().build.

Parameters None –

Returns None

Generic Property Package Framework

Contents

Defining Property Packages

Contents

- *Defining Property Packages*
 - *Introduction*
 - *Configure*
 - *Build*
 - *Examples*

Introduction

In order to define a property package using the IDAES Generic Property Package Framework, users need to define a *Property Parameter Block* in order to describe their material and its properties. The class should inherit from the IDAES *GenericParameterData* class and contain two methods;

1. *configure*, which defines the users selection of sub-models, and
2. *build*, which defines the parameters necessary for the selected property methods.

A basic outline of a user defined Property Parameter Block is shown below.

```
@declare_process_block_class("UserParameterBlock")
class UserParameterData(GenericParameterData):
    def configure(self):
        # Set configuration options
    def build(self):
        # Define parameters
```

Users should populate the *configure* and *build* methods as discussed below.

Configure

The ‘configure’ method is used to select the sub-models and methods to be used when constructing the *StateBlocks* associated with this property package within a process model. These options define the behavior of the property package, and allow users to customize the property package to their needs.

Configuration options are set by assigning an appropriate method to *self.configure.option_name* within the *configure* method. A full list of the available property options is given [here](#).

Build

The *build* method is used to define and specify values for all the parameters associated with the property calculations. All property calculations depend on a set of empirically derived parameters to describe the behavior of the material. The list of parameters which need to be defined will depend upon the configuration options chosen, and the documentation for each method lists the expected parameters which need to be defined in this section. Users need only define those parameters required by the options they have chosen.

Property parameters can be defined as either Pyomo *Params* or *Vars* depending upon the application. Whilst *Params* would seem to be the logical choice, be aware that for parameter estimation problems, the parameters being estimated need to be defined as *Vars* so that the solver is free to vary them.

Note: If using *Params*, users should consider whether these should be *mutable* or not - *Params* that are not mutable have their value defined upon creation and this cannot be changed later.

If using *Vars*, remember that you will need to fix the value unless you are trying to estimate the value of that parameter.

Property parameters need to have the correct set of indices and follow the naming convention laid out in the [standard naming conventions](#) and described in the documentation for each property method. Property parameters are created using Pyomo code as shown below:

Param

```
self.parameter = Param([indices], initialize=value(s), mutable=True/False)
```

Var

```
self.parameter = Var([indices], initialize=value(s))
self.parameter.fix()
```

Examples

Examples of using the IDAES Generic Property Package Framework can be found in the *idaes/property_models/core/examples* folder.

Configuration Options

Contents

- *Configuration Options*
 - *Mandatory Configuration Options*
 - *Additional Configuration Options*
 - *Pure Component Property Options*

The following configuration options are available in the IDAES Generic Property Package Framework.

Mandatory Configuration Options

Users must provide a selection for the following options in all property packages.

Component List

Argument: *config.component_list*

The list of chemical species of interest in the material.

Phase List

Argument: *config.phase_list*

The list of thermodynamic phases that should be included in the model. Phases may or may not interact via phase equilibrium.

State Definition

Argument: *config.state_definition*

An IDAES state definition module which creates the desired set of state variables along with any necessary auxiliary variables.

Equation of State

Argument: *config.equation_of_state*

A *dict* indicating an equation of state to use for each phase in the property package. The expected form is:

```
config.equation_of_state = {'phase_1': eos_1, 'phase_2': eos_2, ...}
```

Each phase in *config.phase_list* must be assigned an equation of state, which should take the form of an IDAES equation of state module which defines methods for calculating all thermophysical and transport properties.

Additional Configuration Options

The following configuration options are not necessary, but are useful or required in some circumstances.

Phase Component Dictionary

Argument: *config.phase_component_dict*

The option allows users to specify different component lists for each phase in their system. This is useful in circumstances where certain species will only ever appear in a given phase (e.g. a non-condensable gas). The expected form of this argument is:

```
config.phase_component_dict = {'phase_1': [list of components in phase 1], 'phase_2':  
↪ [list of components in phase 2], ...}
```

Component lists for each phase must be a subset of *config.component_list*, and all components in *config.component_list* should appear in at least one phase.

State Bounds

Argument: *config.state_bounds*

The option allows users to specify custom bounds on the state variables in their property package during construction. This is important for bounding the resulting problem and ensuring solutions do not stray outside the regions over which property parameters were fitted. The expected form of this argument is:

```
config.state_bounds = {'state_var_1': (lower, upper), 'state_var_2': (lower, upper),  
↪ ..}
```

Users should consult the documentation for the state definition they are using to determine the state variables which can be bounded.

Phase Equilibrium Formulation

Argument: *config.phase_equilibrium_formulation*

The option allows users to specify the formulation to use for expressing phase equilibrium in their property package. This argument should be an IDAES phase equilibrium module which creates constraint describing the equilibria between phases. If the user wishes to include phase equilibria in their property package, both this argument and the *phase_equilibrium_dict* argument must be provided.

Phase Equilibrium Dictionary

Argument: *config.phase_equilibrium_dict*

The option allows users to specify which components in their system are in equilibrium between different phases. The expected form of this argument is:

```
config.phase_equilibrium_dict = {id1: [component, (phase_1, phase_2)], id2:  
↪ [component, (phase_1, phase_2)], ...}
```

Here the *id* is used to identify each phase equilibrium reaction, *component* identifies the component in equilibrium and *phase1* and *phase2* identify the two phases over which this component should be in equilibrium. For cases where a given component is in equilibrium across more than 2 phases, multiple entries for the component are required identifying each pair of phases which should be in equilibrium (this is the reason for the *id* to identify reactions rather than just component name).

If the user wishes to include phase equilibria in their property package, both this argument and the *phase_equilibrium_formulation* argument must be provided.

Bubble Temperature

Argument: *config.temperature_bubble*

This argument allows users to specify a method for calculating the bubble temperature of the mixture in their property package.

Dew Temperature

Argument: *config.temperature_dew*

This argument allows users to specify a method for calculating the dew temperature of the mixture in their property package.

Bubble Pressure

Argument: *config.pressure_bubble*

This argument allows users to specify a method for calculating the bubble pressure of the mixture in their property package.

Dew Pressure

Argument: *config.pressure_dew*

This argument allows users to specify a method for calculating the dew pressure of the mixture in their property package.

Pure Component Property Options

The remaining options allow users to select methods to use for calculating each pure component property, and users must provide a selection for every method that will be used within their process flowsheet. A full list of supported pure component properties can be found [here](#).

Defining State Variables

An important part of defining a set of property calculations is choosing the set of variables which will describe the state of the material. The set of state variables needs to include information on the extensive flow, composition and thermodynamic state of the material. However, there are many ways in which this information can be described, and the best choice of state variables depends on many factors.

Within the IDAES Generic Property Package Framework, the definition of state variables is done using sub-modules which create the necessary variables supporting information for the property package. A state definition sub-module may define any set of state variables the user feel appropriate, but must define the following components as either state variables or functions of the state variables:

- *temperature*
- *pressure*
- *mole_frac_phase_comp*
- *phase_frac*

The IDAES Generic Property Package Framework has a library of prebuilt state definition sub-modules for users to use which are listed below.

State Definition Libraries

FTP_x

Contents

- *FTP_x*
 - *State Definition*
 - *Application*
 - *Bounds*
 - *Supporting Variables and Constraints*
 - *Default Balance Types and Flow Basis*

State Definition

This approach describes the material state in terms of total flow (F : *flow_mol*), overall (mixture) mole fractions (x_j : *mole_frac_comp*), temperature (T : *temperature*) and pressure (P : *pressure*). As such, there are $3 + N_{components}$ state variables, however only $2 + N_{components}$ are independent as the mole fraction must sum to 1.

Application

This is the simplest approach to fully defining the state of a material, and one of the most easily accessible to the user as it is defined in terms of variables that are easily measured and understood. However, this approach has a number of limitations which the user should be aware of:

- If the property package is set up for multiphase flow, an equilibrium calculation is required at the inlet of each unit, as the state definition does not contain information on multiphase flow. This increases the number of complex equilibrium calculations that must be performed, which could be avoided by using a different state definition.
- State becomes ill-defined when only one component is present and multiphase behavior can occur, as temperature and pressure are insufficient to fully define the thermodynamic state under these conditions.

Bounds

The FTPx module supports bounding of the following variables through the *state_bounds* configuration argument:

- *flow_mol*
- *temperature*
- *pressure*

Note that mole fractions are automatically assigned a lower bound of 0, but the upper bound is left free as this is implicitly defined by the sum of mole fractions constraint.

Supporting Variables and Constraints

In addition to the state variables, this definition of state creates a number of supporting variables and constraints.

Variables

- *flow_mol_phase* ($F_{mol,p}$)
- *mole_frac_phase_comp* ($x_{p,j}$)
- *phase_frac* (ψ_p)

Constraints

In all cases, a constraint is written for the sum of the overall mole fractions.

$$\sum_j x_j = 1$$

Note: The sum of mole fractions constraint is not written at inlet states, as all mole fractions should be defined in the inlet stream.

If the property package supports only one phase:

$$F_{mol,p} = F_{mol}$$

$$x_{p,j} = x_j \text{ for all } j$$

$$\psi_p = 1$$

If the property package supports only two phases, the Rachford-Rice formulation is used:

$$\sum_p F_{mol,p} = F_{mol}$$

$$F_{mol} \times x_j = \sum_p F_{mol,p} \times x_{p,j} \text{ for all } j$$

$$\sum_j x_{\text{phase } 1,j} - \sum_j x_{\text{phase } 2,j} = 0$$

$$\psi_p \times F_{mol} = F_{mol,p} \text{ for all } p$$

If the property package supports more than two phases, the following general formulation is used:

$$F_{mol} \times x_j = \sum_p F_{mol,p} \times x_{p,j} \text{ for all } j$$

$$\sum_j x_{p,j} = 1 \text{ for all } p$$

$$\psi_p \times F_{mol} = F_{mol,p} \text{ for all } p$$

Default Balance Types and Flow Basis

The following defaults are specified for Unit Models using this state definition:

- Material balances: total component balances
- Material flow basis: molar flow
- Energy balances: total enthalpy

Equations of State

Equations of State (or equivalent methods) describe the relationship between different thermophysical properties and ensure that the behavior of these are thermodynamically consistent. A wide range of equations of state have been developed for different applications and levels of rigor. Equations of state generally start with ideal pure component properties, and provide a set of relationships which describe how these are combined and deviate from ideality in real mixtures. Equation of state packages within the IDAES Generic Property Package Framework need to implement equations (either *Constraints* or *Expressions*) for all of the mixture properties of interest to the user relating these to the pure component properties and state variables.

The IDAES Generic Property Package Framework provides a number of prebuilt equation of state packages for users to use, which are listed below.

Equation of State Libraries

Ideal Gases and Liquids

Contents

- *Ideal Gases and Liquids*
 - *Introduction*
 - *Mass Density by Phase*
 - *Molar Density by Phase*
 - *Molar Enthalpy by Phase*
 - *Component Molar Enthalpy by Phase*
 - *Molar Entropy by Phase*
 - *Component Molar Entropy by Phase*
 - *Component Fugacity by Phase*
 - *Component Fugacity Coefficient by Phase*

- *Molar Gibbs Energy by Phase*
- *Component Gibbs Energy by Phase*

Introduction

Ideal behavior represents the simplest possible equation of state that ensures thermodynamic consistency between different properties.

Mass Density by Phase

The following equation is used for both liquid and vapor phases, where p indicates a given phase:

$$\rho_{mass,p} = \rho_{mol,p} \times MW_p$$

where MW_p is the mixture molecular weight of phase p .

Molar Density by Phase

For the vapor phase, the Ideal Gas Equation is used to calculate the molar density;

$$\rho_{mol,Vap} = \frac{P}{RT}$$

whilst for the liquid phase the molar density is the weighted sum of the pure component liquid densities:

$$\rho_{mol,Liq} = \sum_j x_{Li,q,j} \times \rho_{Li,q,j}$$

where $x_{Li,q,j}$ is the mole fraction of component j in the liquid phase.

Molar Enthalpy by Phase

For both liquid and vapor phases, the molar enthalpy is calculated as the weighted sum of the component molar enthalpies for the given phase:

$$h_{mol,p} = \sum_j x_{p,j} \times h_{mol,p,j}$$

where $x_{p,j}$ is the mole fraction of component j in the phase p .

Component Molar Enthalpy by Phase

Component molar enthalpies by phase are calculated using the pure component method provided by the users in the property package configuration arguments.

Molar Entropy by Phase

For both liquid and vapor phases, the molar entropy is calculated as the weighted sum of the component molar entropies for the given phase:

$$s_{mol,p} = \sum_j x_{p,j} \times s_{mol,p,j}$$

where $x_{p,j}$ is the mole fraction of component j in the phase p .

Component Molar Entropy by Phase

Component molar entropies by phase are calculated using the pure component method provided by the users in the property package configuration arguments.

Component Fugacity by Phase

For the vapor phase, ideal behavior is assumed:

$$\Phi_{Vap,j} = x_{Vap,j} \times P$$

For the liquid phase, Raoult's Law is used:

$$\Phi_{Liq,j} = x_{Vap,j} \times P_{sat,j}$$

Component Fugacity Coefficient by Phase

Ideal behavior is assumed, so all $\phi_{p,j} = 1$ for all components and phases.

Molar Gibbs Energy by Phase

For both liquid and vapor phases, the molar Gibbs energy is calculated as the weighted sum of the component molar Gibbs energies for the given phase:

$$g_{mol,p} = \sum_j x_{p,j} \times g_{mol,p,j}$$

where $x_{p,j}$ is the mole fraction of component j in the phase p .

Component Gibbs Energy by Phase

Component molar Gibbs energies are calculated using the definition of Gibbs energy:

$$g_{mol,p,j} = h_{mol,p,j} - s_{mol,p,j} \times T$$

Defining Pure Component Properties

Most methods for calculating the thermophysical properties of materials start from estimating the properties of each component in its pure form, before applying mixing rules to determine the properties of the mixture. Pure component properties generally take the form of empirical correlations as a function of material state (generally temperature) derived from experimental data. Data and correlations for many components are readily available in literature. However due to the empirical nature of these correlations and the wide range of data available, different sources use different forms for their correlations.

Within the IDAES Generic Property Package Framework, pure component property correlations are provided in the form of Python methods which return a Pyomo expression relating the pure component property to the material state (using the *standard naming conventions*). IDAES provides a number of libraries containing common forms for these correlations, and a list of the libraries currently supported by IDAES is given below.

A list of all the pure component properties currently supported by the IDAES Generic Property Package Framework can be found after the list of pure component libraries.

Pure Component Libraries

NIST Webbook

Contents

- *NIST Webbook*
 - *Source*
 - *Ideal Gas Molar Heat Capacity (Constant Pressure)*
 - *Ideal Gas Molar Enthalpy*
 - *Ideal Gas Molar Entropy*
 - *Saturation (Vapor) Pressure*

Source

Pure component properties as used by the NIST WebBook

<https://webbook.nist.gov/chemistry/> Retrieved: September 13th, 2019

Ideal Gas Molar Heat Capacity (Constant Pressure)

NIST uses the Shomate equation for the ideal gas molar heat capacity, which is shown below:

$$c_{p,ig,j} = A + B \times t + C \times t^2 + D \times t^3 + \frac{E}{t^2}$$

where $t = \frac{T}{1000}$.

Parameters

Symbol	Parameter Name	Indices	Description
A, B, C, D, E	cp_mol_ig_comp_coeff	component, ['A', 'B', 'C', 'D', 'E']	

Ideal Gas Molar Enthalpy

The correlation for the ideal gas molar enthalpy is derived from the correlation for the molar heat capacity and is given below:

$$\frac{h_{ig,j} - h_{ig,ref,j}}{1000} = A \times (t - t_{ref}) + \frac{B}{2} \times (t^2 - t_{ref}^2) + \frac{C}{3} \times (t^3 - t_{ref}^3) + \frac{D}{4} \times (t^4 - t_{ref}^4) + E \times \left(\frac{1}{t} - \frac{1}{t_{ref}}\right) + F - H$$

Symbol	Parameter Name	Indices	Description
A, B, C, D, E, F, H	cp_mol_ig_comp_coeff	component, ['A', 'B', 'C', 'D', 'F', 'H']	
T_{ref}	temperature_ref	None	Temperature at reference state

Note: This correlation uses the same parameters as for the ideal gas heat capacity with additional parameters F and H . These parameters account for the enthalpy at the reference state defined by NIST. Users wanting to use a different reference state will need to update H .

Ideal Gas Molar Entropy

The correlation for the ideal gas molar entropy is derived from the correlation for the molar heat capacity and is given below:

$$s_{ig,j} = A \times \ln(t) + B \times t + \frac{C}{2} \times t^2 + \frac{D}{3} \times t^3 + \frac{E}{2 \times t^2} + G$$

Parameters

Symbol	Parameter Name	Indices	Description
A, B, C, D, E, G	cp_mol_ig_comp_coeff	component, ['A', 'B', 'C', 'D', 'E', 'G']	

Note: This correlation uses the same parameters as for the ideal gas heat capacity with additional parameter G , which accounts for the standard entropy at the reference state defined by NIST. Users wanting to use a different reference state will need to update G .

Saturation (Vapor) Pressure

NIST uses the Antoine equation to calculate the vapor pressure of a component, which is given below:

$$\log_{10}(P_{sat,j}) = A - \frac{B}{T + C}$$

Parameters

Symbol	Parameter Name	Indices	Description
A, B, C	pressure_sat_comp_coeff	component, ['A', 'B', 'C']	

Note: The Antoine equation is generally written with saturation pressure expressed in bars. The units of the correlation can be converted to Pascals by adding 5 to A .

Perry's Chemical Engineers' Handbook

Contents

- *Perry's Chemical Engineers' Handbook*
 - *Source*
 - *Ideal Liquid Molar Heat Capacity (Constant Pressure)*
 - *Ideal Liquid Molar Enthalpy*
 - *Ideal Liquid Molar Entropy*
 - *Liquid Molar Density*

Source

Methods for calculating pure component properties from:

Perry's Chemical Engineers' Handbook, 7th Edition Perry, Green, Maloney, 1997, McGraw-Hill

Ideal Liquid Molar Heat Capacity (Constant Pressure)

Perry's Handbook uses the following correlation for ideal liquid molar heat capacity:

$$\frac{c_{p, \text{liq}, j}}{1000} = C_1 + C_2 \times T + C_3 \times T^2 + C_4 \times T^3 + C_5 \times T^4$$

Parameters

Symbol	Parameter Name	Indices	Description
C_1, C_2, C_3, C_4, C_5	cp_mol_liq_comp_coeff	component, [1, 2, 3, 4, 5]	

Ideal Liquid Molar Enthalpy

The correlation for the ideal liquid molar enthalpy is derived from the correlation for the molar heat capacity and is given below:

$$\frac{h_{\text{liq}, j} - h_{\text{liq ref}, j}}{1000} = C_1 \times (T - T_{\text{ref}}) + \frac{C_2}{2} \times (T^2 - T_{\text{ref}}^2) + \frac{C_3}{3} \times (T^3 - T_{\text{ref}}^3) + \frac{C_4}{4} \times (T^4 - T_{\text{ref}}^4) + \frac{C_5}{5} \times (T^5 - T_{\text{ref}}^5) + \Delta h_{\text{form}}$$

Parameters

Symbol	Parameter Name	Indices	Description
C_1, C_2, C_3, C_4, C_5	cp_mol_liq_comp_coeff	component, [1, 2, 3, 4, 5]	
Δh_{form}	enth_mol_form_phase_comp_ref	phase, component	Molar heat of formation at reference state
T_{ref}	temperature_ref	None	Temperature at reference state

Note: This correlation uses the same parameters as for the ideal gas heat capacity.

Ideal Liquid Molar Entropy

The correlation for the ideal liquid molar entropy is derived from the correlation for the molar heat capacity and is given below:

$$s_{\text{liq},j} = C_1 \times \ln(T) + C_2 \times T + \frac{C_3}{2} \times T^2 + \frac{C_4}{3} \times T^3 + \frac{C_5}{4} \times T^4 + s_{\text{ref, Vap},j}$$

Parameters

Symbol	Parameter Name	Indices	Description
C_1, C_2, C_3, C_4, C_5	cp_mol_liq_comp_coeff	component, [1, 2, 3, 4, 5]	
s_{ref}	entr_mol_phase_comp_ref	phase, component	Standard molar entropy at reference state

Note: This correlation uses the same parameters as for the ideal gas heat capacity.

Liquid Molar Density

Perry's Handbook uses the following correlation for liquid molar density:

$$\rho_{\text{liq},j} = \frac{C_1}{C_2^{1+(1-\frac{T}{C_3})^{C_4}}}$$

Parameters

Symbol	Parameter Name	Indices	Description
C_1, C_2, C_3, C_4	dens_mol_comp_liq_coeff	component, [1, 2, 3, 4]	

Note: Currently, only the most common correlation form from Perry's Handbook is implemented. Some components use different forms which are not yet supported.

Properties of Gases and Liquids

Contents

- *Properties of Gases and Liquids*
 - *Source*
 - *Ideal Gas Molar Heat Capacity (Constant Pressure)*
 - *Ideal Gas Molar Enthalpy*
 - *Ideal Gas Molar Entropy*
 - *Saturation (Vapor) Pressure*

Source

Methods for calculating pure component properties from:

The Properties of Gases & Liquids, 4th Edition Reid, Prausnitz and Polling, 1987, McGraw-Hill

Ideal Gas Molar Heat Capacity (Constant Pressure)

Properties of Gases and Liquids uses the following correlation for the ideal gas molar heat capacity:

$$c_{p\text{ ig},j} = A + B \times T + C \times T^2 + D \times T^3$$

Parameters

Symbol	Parameter Name	Indices	Description
A, B, C, D	cp_mol_ig_comp_coeff	component, ['A', 'B', 'C', 'D']	

Ideal Gas Molar Enthalpy

The correlation for the ideal gas molar enthalpy is derived from the correlation for the molar heat capacity and is given below:

$$h_{\text{ig},j} - h_{\text{ig ref},j} = A \times (T - T_{\text{ref}}) + \frac{B}{2} \times (T^2 - T_{\text{ref}}^2) + \frac{C}{3} \times (T^3 - T_{\text{ref}}^3) + \frac{D}{4} \times (T^4 - T_{\text{ref}}^4) + \Delta h_{\text{form, Vap},j}$$

Parameters

Symbol	Parameter Name	Indices	Description
A, B, C, D	cp_mol_ig_comp_coeff	component, ['A', 'B', 'C', 'D']	
Δh_{form}	enth_mol_form_phase_comp_ref	phase, component	Molar heat of formation at reference state
T_{ref}	temperature_ref	None	Temperature at reference state

Note: This correlation uses the same parameters as the ideal gas heat capacity correlation.

Ideal Gas Molar Entropy

The correlation for the ideal gas molar entropy is derived from the correlation for the molar heat capacity and is given below:

$$s_{ig,j} = A \times \ln(T) + B \times T + \frac{C}{2} \times T^2 + \frac{D}{3} \times T^3 + s_{ref, Vap,j}$$

Parameters

Symbol	Parameter Name	Indices	Description
A, B, C, D	cp_mol_ig_comp_coeff	component, ['A', 'B', 'C', 'D']	
s_{ref}	entr_mol_phase_comp_ref	phase, component	Standard molar entropy at reference state

Note: This correlation uses the same parameters as the ideal gas heat capacity correlation .

Saturation (Vapor) Pressure

Properties of Gases and Liquids uses the following correlation to calculate the vapor pressure of a component:

$$\ln\left(\frac{P_{sat,j}}{P_{crit}}\right) \times (1 - x) = A \times x + B \times x^{1.5} + C \times x^3 + D \times x^6$$

where $x = 1 - \frac{T}{T_{crit}}$.

Symbol	Parameter Name	Indices	Description
A, B, C, D	pressure_sat_comp_coeff	component, ['A', 'B', 'C', 'D']	
P_{crit}	pressure_crit_comp	None	Critical pressure
T_{crit}	temperature_crit_comp	None	Critical temperature

Note: This correlation is only valid at temperatures **below** the critical temperature. Above this point, there is no real solution to the equation.

Supported Properties

The following pure component properties are supported by IDAES Generic Property Package Framework.

Property	Method	Arguments
Ideal Gas Molar Heat Capacity	cp_mol_ig_comp	component, temperature
Ideal Gas Molar Enthalpy	enth_mol_ig_comp	component, temperature
Ideal Gas Molar Entropy	entr_mol_ig_comp	component, temperature
Ideal Liquid Molar Heat Capacity	cp_mol_liq_comp	component, temperature
Ideal Liquid Molar Enthalpy	enth_mol_liq_comp	component, temperature
Ideal Liquid Molar Entropy	entr_mol_liq_comp	component, temperature
Liquid Molar Density	dens_mol_liq_comp	component, temperature
Saturation Pressure	pressure_sat_comp	component, temperature

Bubble and Dew Point Methods

Contents

- *Bubble and Dew Point Methods*
 - *Introduction*
 - *Ideal Assumptions*
 - * *Ideal Bubble Pressure*
 - * *Ideal Bubble Temperature*
 - * *Ideal Dew Pressure*
 - * *Ideal Dew Temperature*

Introduction

Bubble and dew points are often of interest to process engineers for designing process equipment, and appear in some calculations of other thermodynamic properties. Whilst calculation of the saturation pressure for single components is relatively simple, calculating the bubble and dew points of mixtures is more challenging due to the non-linear nature of the equations.

The IDAES Generic Property Package Framework has a number of prebuilt methods for calculating the bubble and dew points of mixtures which are listed below.

Ideal Assumptions

In the case where ideal behavior can be assumed, i.e. Raoult's Law holds, the bubble and dew points can be calculated directly from the saturation pressure using the following equations.

Ideal Bubble Pressure

This method is implemented as *bubble_press_ideal*.

$$P_{bub} = \sum_j x_j \times P_{sat,j}(T)$$

$$x_j(P_{bub}) \times P_{bub} = x_j \times P_{sat,j}(T)$$

where P_{bub} is the bubble pressure of the mixture, $P_{sat,j}(T)$ is the saturation pressure of component j at the system temperature, T , x_j is the overall mixture mole fraction and $x_j(P_{bub})$ is the mole fraction of the vapor phase at the bubble pressure.

Ideal Bubble Temperature

This method is implemented as *bubble_temp_ideal*.

$$\sum_j (x_j \times P_{sat,j}(T_{bub})) - P = 0$$

$$x_j(T_{bub}) \times P = x_j \times P_{sat,j}(T_{bub})$$

where P is the system pressure, $P_{sat,j}(T_{bub})$ is the saturation pressure of component j at the bubble temperature, T_{bub} , x_j is the overall mixture mole fraction and $x_j(T_{bub})$ is the mole fraction of the vapor phase at the bubble temperature.

Ideal Dew Pressure

This method is implemented as *dew_press_ideal*.

$$0 = 1 - P_{dew} \times \sum_j x_j \times P_{sat,j}(T)$$

$$x_j(P_{dew}) \times P_{sat,j}(T) = x_j \times P_{dew}$$

where P_{dew} is the dew pressure of the mixture, $P_{sat,j}(T)$ is the saturation pressure of component j at the system temperature, T , x_j is the overall mixture mole fraction and $x_j(P_{dew})$ is the mole fraction of the liquid phase at the dew pressure.

Ideal Dew Temperature

This method is implemented as *dew_temp_ideal*.

$$P \times \sum_j (x_j \times P_{sat,j}(T_{dew})) - 1 = 0$$

$$x_j(T_{dew}) \times P_{sat,j}(T_{dew}) = x_j \times P$$

where P is the system pressure, $P_{sat,j}(T_{dew})$ is the saturation pressure of component j at the dew temperature, T_{dew} , x_j is the overall mixture mole fraction and $y_j(T_{dew})$ is the mole fraction of the liquid phase at the dew temperature.

Phase Equilibrium Formulations

Phase equilibrium and separation is a key part of almost all chemical processes, and also represent some of the most complex and non-linear constraints in a model, especially when dealing with systems which may cross phase boundaries. As such, good formulations of these constraints is key to a robust and tractable model.

To assist users with formulating the phase equilibrium constraints in their models, the IDAES Generic Property Package Framework contains a library of different formulations for phase equilibrium.

Phase Equilibrium Libraries

Smooth Vapor-Liquid Equilibrium Formulation

Contents

- *Smooth Vapor-Liquid Equilibrium Formulation*
 - *Source*
 - *Introduction*
 - *Formulation*

Source

Burgard, A.P., Eason, J.P., Eslick, J.C., Ghouse, J.H., Lee, A., Biegler, L.T., Miller, D.C., 2018, A Smooth, Square Flash Formulation for Equation-Oriented Flowsheet Optimization. Proceedings of the 13th International Symposium on Process Systems Engineering – PSE 2018, July 1-5, 2018, San Diego.

Introduction

Typically, equilibrium calculations are only used when the user knows the current state is within the two-phase envelope. For simulation only studies, the user may know a priori the condition of the stream but when the same set of equations are used for optimization, there is a high probability that the specifications can transcend the phase envelope. In these situations, the equilibrium calculations become trivial, thus it is necessary to find a formulation that has non-trivial solutions at all states.

To address this, the smooth vapor-liquid equilibrium (VLE) formulation always solves the equilibrium calculations at a condition where a valid two-phase solution exists. In situations where only a single phase is present, the phase equilibrium is solved at the either the bubble or dew point, where the non-existent phase exists but in negligible amounts. In this way, a non-trivial solution is guaranteed but still gives near-zero material in the non-existent phase in the single phase regions.

Formulation

The approach used by the smooth VLE formulation is to define an “equilibrium temperature” (T_{eq}) at which the equilibrium calculations will be performed. The equilibrium temperature is computed as follows:

$$T_1 = \max(T_{bubble}, T)$$

$$T_{eq} = \min(T_1, T_{dew})$$

where T is the actual stream temperature, T_1 is an intermediate temperature variable and T_{bubble} and T_{dew} are the bubble and dew point temperature of mixture. In order to express the maximum and minimum operators in a tractable form, these equations are reformulated using the IDAES *smooth_max* and *smooth_min* operators which results in the following equations:

$$T_1 = 0.5 \left[T + T_{bubble} + \sqrt{(T - T_{bubble})^2 + \epsilon_1^2} \right]$$

$$T_{eq} = 0.5 \left[T_1 + T_{dew} - \sqrt{(T_1 - T_{dew})^2 + \epsilon_2^2} \right]$$

where ϵ_1 and ϵ_2 are smoothing parameters (mutable *Params* named *eps_1* and *eps_2*). The default values are 0.01 and 0.0005 respectively, and it is recommended that $\epsilon_1 > \epsilon_2$. It can be seen that if the stream temperature is less than that of the bubble point temperature, the VLE calculations will be computed at the bubble point. Similarly, if the stream temperature is greater than the dew point temperature, then the VLE calculations are computed at the dew point temperature. For all other conditions, the equilibrium calculations will be computed at the actual temperature.

Finally, the phase equilibrium is expressed using the following equation:

$$\Phi_{Vap,j}(T_{eq}) = \Phi_{Liq,j}(T_{eq})$$

where $\Phi_{p,j}(T_{eq})$ is the fugacity of component j in the phase p calculated at T_{eq} . The fugacities are calculated using methods defined by the equation of state chosen by the user for each phase.

Developing New Property Libraries

Information on how to develop new components for the IDAES Generic Property Package Framework are given in the following sections.

Contents

Developing Pure Component Methods

Contents

- *Developing Pure Component Methods*
 - *Naming Methods*
 - *Method Arguments*
 - *Method Parameters*
 - *Method Body*
 - *Example*

The most common task developers of new property packages will need to do is writing methods for new pure component property calculations. Most equation of state type approaches rely on a set of calculations for pure components under ideal conditions which are then modified to account for mixing and deviations from ideality. These pure component property calculations tend to be empirical correlations based on experimental data (generally as functions of temperature) and due to their empirical nature a wide range of forms have been used in literature.

In order to support different forms for these calculations, the IDAES Generic Property Package Framework uses Python methods to define the form of pure component property calculations. This allows developers and users to easily enter the form they wish to use for their application with a minimum amount of code.

Naming Methods

The IDAES Generic Property Package Framework supports two ways of providing pure component property methods:

1. Providing the method directly - users may directly provide their method of choice as a config argument (*config.property_name*) in the *PropertyParameterBlock*, in which case the method can use any name the user desires.
2. Providing a library module - alternatively, users can provide a module containing a library of methods as the config argument (*config.property_name*), in which case the framework searches the module for a method with the same name as the property (and the config argument). E.g., for the property *enth_mol_phase_comp* the method name would be *enth_mol_phase_comp* (as would the associated config argument).

Method Arguments

Note: Currently, the IDAES Generic Property Package Framework assumes pure component property calculations will be a function of only temperature. If additional functionality is required, please contact the IDAES Developers.

Currently, all pure component property methods in the IDAES Generic Property Package Framework take three arguments:

1. A reference to the *StateBlock* where the method will be used (generally *self*),
2. An element of a component list,
3. A pointer to the *temperature* variable to be used in the calculation. By using a pointer rather than an absolute reference (i.e. *self.temperature*), this allows the method to be applied at different temperatures as necessary (e.g. the reference temperature).

Method Parameters

Pure component property methods all depend on a number of parameters, often derived from empirical data. In order to avoid duplication of parameters and facilitate parameter estimation studies, all property parameters are stored in the *PropertyParameterBlock* and each *StateBlock* contains a reference to its associated parameter block (*self.params*).

For pure component property methods, parameter names are defined in the associated methods thus developers can choose any name they desire. However, the IDAES standard is to use the name of the property appended with *_coeff* and developers are encouraged to follow this convention.

Method Body

The body of the pure component property method should assemble an expression describing the specified quantity for the component given in the method arguments. This expression should involve Pyomo components from the *StateBlock* (i.e. *self*), the associated *PropertyParameterBlock* (*self.params*) and be returned in the final step of the method.

Example

Below is an example of a pure component property method for the molar heat capacity of a component in the (ideal) gas phase with the form $c_{p,ig,j} = A + B \times T$.

```
def cp_mol_ig_comp(self, component, temperature):
    # Method named using standard naming convention
    # Arguments are self, a component and temperature

    # Return an expression involving temperature and parameters
    return (self.params.cp_mol_ig_comp_coeff[component, "A"] +
            self.params.cp_mol_ig_comp_coeff[component, "B"]*temperature)
```

Note that the method only returns an expression representing the R.H.S. of the correlation.

Developing Equation of State Modules

Contents

- *Developing Equation of State Modules*
 - *Equations of State and Multiple Phases*
 - *General Structure*

- *Phase Equilibrium*
- *Accessing Pure Component Property Methods*
- *Common Methods*
- *Mixture Property Methods*
- *Example*

The central part of any property package are the equations of state or equivalent models which describe how the mixture behaves under the conditions of interest. For systems with multiple phases and phase equilibrium, each phase must have its own equation of state (or equivalent), which must provide information on phase equilibrium which is compatible with the other phases in the system.

Equations of State and Multiple Phases

The IDAES Generic Property Package Framework requires users to assign an equation of state module for each phase in their system, thus equations of state can be written for specific phases (e.g. an ideal gas equation of state). In some cases, developers may wish to write equations of state for multiple phases, and the generic framework supports this by indexing all properties by phase.

Developers are encouraged to add checks to their methods to ensure their equations of state are only applied to phases where they are appropriate (e.g. an ideal gas equation of state should raise an exception if the phase argument is not “Vap”).

General Structure

Equation of State Modules in the IDAES Generic Property Package Framework are files (modules) containing a number of methods which describe the behavior of the material. These methods define how each of the properties associated with a given phase should be calculated, and the list of properties supported for a given phase is limited by the methods provided by the developer of the equation of state.

Phase Equilibrium

When calculating phase equilibrium, the IDAES Generic Property Package Framework uses the general form $\Phi_{\text{phase } 1, j}^e = \Phi_{\text{phase } 2, j}^e$ where $\Phi_{p, j}^e$ is the fugacity of component j in phase p calculated at the equilibrium temperature (T_{eq} , variable name `self._teq`). The equilibrium temperature is calculated using the users’ choice of phase equilibrium formulation and determines how the property package will handle phase transitions.

All equation of state methods should contain a method for calculating fugacity if they are to support phase equilibrium calculations.

Accessing Pure Component Property Methods

In most cases, property calculations in the equation of state methods will require calculations of the pure component properties for the system. These can be accessed using `get_method` (imported from `idaes.property_models.core.generic.generic_property`) using the form `get_method(self, “property_name”)`. This will return the **method** defined by the user in the `PropertyParameterBlock` for the named property, which can then be used in the equation of state methods (note that users will need to call the method and provide it with the required arguments - generally `self`, component and a pointer to temperature).

Common Methods

For equations of state that support multiple phases, there may be certain calculations and/or variables that are common to all phases. To support this (and avoid duplication of these), equation of state methods should contain a method named *common* which implements any component which are common to multiple phases. This method should also contain checks to ensure that these components have not already been created for another phase in the system (to avoid duplication). In cases where there are no common components, this method can *pass*.

Mixture Property Methods

The main part of an equation of state method are a set of methods which describe properties of the mixture for a given phase. Any mixture property that the property package needs to support must be defined as a method in the equation of state module, which returns an expression for the given property (construction of the actual Pyomo component will be handled by the core framework code).

Mixture properties can be defined in any way the developer desires, and can cross-link and reference other mixture properties as required. Developers should recall that the State Definition method should have defined the following properties which can be used in mixture property correlations:

- pressure
- temperature
- mole_frac_phase_comp
- phase_frac

Other state variables **may** have been defined by the user's choice of State Definition, however this cannot be guaranteed. Developers may choose to assume that certain state variables will be present, but this will limit the application of their equation of state module to certain state definitions which should be clearly documented.

Example

Below is an example method for a method in an equation of state module for calculating molar density that supports both liquid and vapor phases.

```
def dens_mol_phase(b, phase):
    if phase == "Vap":
        return b.pressure / (b.params.gas_const * b.temperature)
    elif phase == "Liq":
        return sum(b.mole_frac_phase_comp[phase, j] *
                   get_method(b, "dens_mol_liq_comp")(b, j, b.temperature)
                   for j in b.params.component_list)
    else:
        raise PropertyNotSupportedError("Phase not supported")
```

Developing State Definitions

Contents

- *Developing State Definitions*
 - `define_state(self)`

```
* State Variables
* define_state_vars
* Auxiliary Variables
* Supporting Constraints
* always_flash
* get_material_flow_terms(phase, comp)
* get_enthalpy_flow_terms(phase)
* get_material_density_terms(phase, component)
* get_energy_density_terms(phase)
* get_material_flow_basis()
* default_material_balance_type()
* default_energy_balance_type()
* define_port_members()
* define_display_vars()
- state_initialization(self)
- self.do_not_initialize
```

The primary purpose of the State Definition method is to define the state variables which will be used to describe the state of the mixture in the property package. However, a number of other key aspects of the property package definition are tied to the choice of state variables and must be declared here as well.

State definitions are defined as Python modules with two methods and one list, which are describe below.

define_state(self)

The first method in a State Definition module is the *define_state* method. This method is used to define the state variables and associated components and methods. The *define_state* method must define the following things:

State Variables

The most important part of a State Definition module is the definition of the state variables that should be used in the resulting property package. The choice of state variables is up to the module developer, however the set of variables selected must contain sufficient information to fully define the extensive and intensive state of the material. That is, if all the state variables are fixed, the resulting set of variables and constraints should form a square problem (i.e. 0 degrees of freedom). Beyond this requirement however, developers may choose any combination of state variables they wish.

State variables should be defined as Pyomo *Vars* with names drawn from the IDAES naming standard, and should include initial values and bounds. The Generic Property Package Framework includes an optional user input of bounds for the state variables (*config.state_bounds*) which developers are encouraged to make use of when setting bounds and initializing variables.

define_state_vars

In order to inform the IDAES Process Modeling Framework of which variables should be considered state variable, developers are required to define a method named *define_state_vars*. This method should return a *dict* where the keys are a string identifier for each state variable and the values being pointers to the associated *Var* component. For example:

```
def define_state_vars_state_definition():
    return {"flow_mol": self.flow_mol,
            "mole_frac_comp": self.mole_frac_comp,
            "pressure": self.pressure,
            "temperature": self.temperature,}
self.define_state_vars = define_state_vars_state_definition
```

Auxiliary Variables

Whilst the developer is free to choose any set of state variable they wish to define their system, there are certain properties/quantities associated with material state that are frequently used in process models. For example, most property calculation methods drawn upon empirical correlations for pure component properties which are most commonly expressed as functions of temperature (and sometimes pressure). Additionally, multiphase systems often require knowledge of the volume fractions of each phase present.

To ensure that these properties/quantities are available when required, it is required that State Definition modules define the following quantities if they are not already one of the state variables chosen:

- *temperature* - the temperature of the mixture,
- *pressure* - the pressure of the mixture,
- *mole_frac_phase_comp* - mole fraction of the mixture by phase and component (even if only one phase is present),
- *phase_frac* - volume fractions of each phase (even if only one phase is present).

These quantities can be defined as either Pyomo *Vars* with associated *Constraints*, or as Pyomo *Expressions* as the developer desires. Developers may choose to include additional auxiliary variables as required by their needs (e.g. different forms of flow rates).

Supporting Constraints

Depending upon the choice of state and auxiliary variables, developers may need to include a number of supporting constraints in their State Definitions. Common examples include constraints for the sum of mole fractions in the system, and relationships between different types of flow rates. Any number of constraints can be included by the developer to suit their needs, subject to the limitations of degrees of freedom.

However, developers need to be aware of the difference between inlet and outlet states and how this affects which constraints can be written. In the case of inlet states, all state variables are defined by the upstream process and thus no constraint can be written that involves only state variables (e.g. sum of mole fractions). For outlet (and intermediate) states however, it is often necessary to include these types of constraints to fully define the system. The IDAES Process Modeling Framework uses the *config.defined_state* configuration argument to indicate situations where the state variables should be considered fully defined (e.g. inlets) which can be used in *if* statements to determine whether a constraint should be included.

always_flash

Whilst the set of state variables chosen must be sufficient for fully defining the state of the material, depending on the set of state variables chosen information of the phase separation (if applicable) may or may not be explicitly included. For example, using total flow rate and composition along with pressure and specific enthalpy is sufficient to define the state of the material, however it does not explicitly describe the phase fractions of the system. In these cases, it is necessary to perform a flash calculation at every state in the system to determine the phase fractions. However, If the state is defined in terms of flow rates by phase and component along with pressure and specific enthalpy, information on the phase separation is already included in the state definition and flash calculations are not required where the state is fully defined (i.e. `config.state_defined` is True).

To inform the Generic Property Package Framework of whether phase equilibrium calculations should be included when `config.state_defined` is True, all State Definitions are required to include a component named *always_flash* which is a boolean indicating whether equilibrium calculations should always be included (True) or only included when the state is not fully defined (False).

get_material_flow_terms(phase, comp)

In order to automate the construction of the material balance equations, the IDAES Process Modeling Framework expects property packages to provide expressions for the flow terms in these equations. This is done via the *get_material_flow_terms* method which should return an expression involving variables in the StateBlock which should be used as the flow term in the material balances.

There are many forms this expression can take depending upon the state variables chosen and how the developer wishes to formulate the material balance equations, and the framework endeavors to support as many of these as possible. Material flow terms are defined on a phase-component basis (i.e. a separate expression for each component in each phase). An example of a *get_material_flow_term* using flow rate and mole fractions by phase is shown below.

```
def get_material_flow_terms_definition(phase, component):  
    return self.flow_mol_phase[phase] * self.mole_frac_phase_comp[phase, component]  
self.get_material_flow_terms = get_material_flow_terms_definition
```

get_enthalpy_flow_terms(phase)

In the same way that *get_material_flow_terms* is used to automate construction of the material balance equations, automating the construction of the energy balance equations requires a *get_enthalpy_flow_terms* method. This method should return an expression for the enthalpy flow terms involving variables in the StateBlock.

There are many forms for the enthalpy flow terms as well, and developers may choose whichever best suits their needs. Enthalpy flow terms are defined on a phase basis, and an example is shown below using flow rate and specific enthalpy by phase.

```
def get_enthalpy_flow_terms_definition(phase):  
    return self.flow_mol_phase[phase] * self.enth_mol_phase[phase]  
self.get_enthalpy_flow_terms = get_enthalpy_flow_terms_definition
```

get_material_density_terms(phase, component)

For dynamic system, calculation of the material holdups also requires a material density term which is defined using the *get_material_density_terms* method. This method is defined in a similar fashion to the *get_material_flow_terms* method and is also defined on a phase-component basis.

get_energy_density_terms(phase)

For dynamic system, calculation of the energy holdups also requires an energy density term which is defined using the *get_energy_density_terms* method. This method is defined in a similar fashion to the *get_enthalpy_flow_terms* method and is also defined on a phase basis. Note however that the energy density term should only include internal energy contributions, and not the full enthalpy density (i.e. excluding the PV term).

get_material_flow_basis()

To automate generation of some terms in the balance equations, the IDAES Process Modeling Framework needs to know the basis (mass, mole or other) of the flow terms. This is defined in the State Definition by providing a *get_material_flow_basis* method which returns a *MaterialFlowBasis Enum* (importable from *idaes.core*). E.g.:

```
def get_material_flow_basis_definition():
    return MaterialFlowBasis.molar
self.get_material_flow_basis = get_material_flow_basis_definition
```

default_material_balance_type()

The IDAES Process Modeling Framework allows property packages to specify a default form for the material balance equations to be used if the modeler does not specify a form. Whilst not strictly required, developers are strongly encouraged to define a default form for the material balance equations.

To set the default material balance type, the State Definition must implement a method which returns a *MaterialBalanceType Enum* (importable from *idaes.core*). E.g.:

```
def default_material_balance_type_definition():
    return MaterialBalanceType.componentTotal
self.default_material_balance_type = default_material_balance_type_definition
```

default_energy_balance_type()

The IDAES Process Modeling Framework allows property packages to specify a default form for the energy balance equations to be used if the modeler does not specify a form. Whilst not strictly required, developers are strongly encouraged to define a default form for the energy balance equations.

To set the default energy balance type, the State Definition must implement a method which returns an *EnergyBalanceType Enum* (importable from *idaes.core*). For an example, see *default_material_balance_type* above.

define_port_members()

In some situations, it is desirable to pass additional information between unit operations in a model beyond just the state variables. In these circumstance, the developer may define a *define_port_members* method which describes the information to be passed in *Ports* connecting units. This method should return a *dict* with a form similar to that of *define_state_vars*. Note that developers must also ensure that any additional information passed in *Ports* does not result in an over-specified problem, generally by excluding certain constraints in *StateBlocks* where *config.defined_state* is *True*.

If this method is not defined, *Ports* will default to using the variables described in *define_state_vars* instead.

define_display_vars()

Developers may also define a *define_display_vars* method which is used by the IDAES *report* methods to determine what information should be displayed for each state. The *define_display_vars* method should return a *dict* containing the information to display with the keys being the display name for the information and value being the quantity to display (similar to the *define_state_Vars* method). If this method is not defined then the *define_state_vars* method is used by the *report* methods instead.

state_initialization(self)

The *state_initialization* method is called as part of the Generic Property Package Framework *initialize* method and is expected to set initial guesses for any auxiliary variables defined by the State Definition based on the current values of the state variables. Note that the state variables will have been provided with initial guesses for the current state of the material from the process models, and thus will likely not be at their pre-defined initial conditions.

self.do_not_initialize

The *do_not_initialize* component is a list containing a list of *Constraint* names which should remain deactivated during initialization of the StateBlock and only reactivated during the final step on initialization. Common examples of these are those constraints that are only written for outlet Blocks (i.e. those when *config.defined_state* is False), such as overall sum of mole fraction constraints.

Developing Phase Equilibrium Methods

Contents

- *Developing Phase Equilibrium Methods*
 - *phase_equil(self)*
 - *phase_equil_initialization(self)*

Handling phase equilibrium and phase transitions within an equation oriented framework can be challenging as it is necessary to ensure that all constraints and variables has feasible solution at all states. When dealing with disappearing phases and correlations that can become ill-defined or singular outside of the two phase envelope, it is necessary to either bound the problem to the two-phase region or reformulate the problem.

The IDAES Generic Property Package Framework provides support for reformulating the problem by defining an “equilibrium temperature” (*self.teq*) at which all phase equilibrium calculations are performed. Issues surrounding phase transitions can be avoided by providing a definition for the equilibrium temperature that satisfies the following constraints:

$$T_{\text{bubble}} \leq T_{\text{eq}} \leq T_{\text{dew}}$$

The Phase Equilibrium module allows users to provide a definition for the equilibrium temperature, along with any necessary instructions on how to initialize the components associated with this definition.

A Phase Equilibrium module consists of two methods , which are described below.

phase_equil(self)

The *phase_equil* method is responsible for defining the variables and constraints necessary for calculating the equilibrium temperature, and at a minimum must contain one constraint relating the equilibrium temperature (*self._teq*) to the system temperature (*self.temperature*).

phase_equil_initialization(self)

This method is called by the Generic Property Package Framework initialization routine and should initialize the constraints associated with the phase equilibrium definition.

Note that the Generic Property Package Framework beings by deactivating all constraints in the *StateBlock* so the first step in the *phase_equil_initialization* method should be to activate any constraints defined in *phase_equil*. Additionally, this method may calculate initial values for any supporting variables defined in *phase_equil* based on variables that have already been initialized (primarily *temperature* and bubble and dew points if used). Developers should be careful however to fully understand the initialization sequence of the Generic Property Package Framework to understand which variables may have been initialized at this point.

Introduction

Note: The generic property package framework is still under development. Whilst the current framework is functional, features are still being developed and added to increase functionality.

The generic property package framework builds upon the existing framework for implementing property packages within IDAES, and will not prevent the user of custom written property packages in the future. However, it is envisioned that the generic property package framework will provide a more streamlined interface for developing property packages in most circumstances, and it is hoped that most property packages will migrate to using the generic property framework in the future.

Property packages represent the core of any process model, and having a suitable property package is key to successfully modeling any process system. However, developing property packages is a significant challenge even for the most experienced modelers, as they involve complex, non-linear equations. The goal of the IDAES Generic Property Package Framework is to provide a flexible platform on which users can build custom property packages by calling upon libraries of modular sub-models to build up complex property calculations with the least effort possible.

The Generic Property Package Framework breaks down property packages into a number of components which can be assembled in a modular fashion. Users need only provide those components which they require for their system of interest, and components can be drawn from libraries of existing components or provided by the user as custom code. The components which make up a generic property package are as follows:

1. *Definition* of the component list and phases of interest, along with any phase equilibrium the user wishes to include.
2. A definition of the *variables* the user wishes to use to define the state of their material (state variables), along with any bounds on these.
3. An *equation of state* to describe each phase within the user's property package.
4. *Correlations* for the pure component properties of each component in the users system. Correlations are only required for those properties the user will use within their model.
5. *Methods* to calculate the bubble and dew points of mixtures.
6. A *formulation* to use for defining any phase equilibrium within the user's system.

The following section will describe how to define a property package using the Generic Property Package Framework along with the libraries of sub-models currently available. Finally, the [developers](#) section describes how to go about defining your own custom components to use when creating custom property packages.

Property Interrogator Tool

When preparing to model a process flowsheet, it is necessary to specify models for all the thermophysical and kinetic properties that will be required by the different unit operations to simulate the process. However, it is often difficult to know what properties will be required *a priori*. The IDAES Property Interrogator tool allows a user to define a general flowsheet structure and interrogate it for the full list of properties that will be required, thus informing them of what methods they will need to define in their property package(s).

Tool Usage

The IDAES Properties Interrogator tool consists of two classes; a *PropertiesInterrogatorBlock* and a *ReactionInterrogatorBlock*. These blocks are used in place of the normal *PhysicalParameterBlock* and *ReactionParameterBlock* whilst declaring a flowsheet, however rather than constructing a solvable flowsheet they record all calls for properties made whilst constructing the flowsheet. These Blocks then contain a number of methods for reporting the logged property calls for the user.

An example of how Property Interrogator tool is used is shown below:

```
import pyomo.environ as pyo # Pyomo environment
from idaes.core import FlowsheetBlock
from idaes.generic_models.unit_models import CSTR
from idaes.generic_models.properties.interrogator import PropertyInterrogatorBlock, \
    ReactionInterrogatorBlock

m = pyo.ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": True})

m.fs.params = PropertyInterrogatorBlock()
m.fs.rxn_params = ReactionInterrogatorBlock(
    default={"property_package": m.fs.params})

m.fs.R01 = CSTR(default={"property_package": m.fs.params,
                        "reaction_package": m.fs.rxn_params,
                        "has_heat_of_reaction": True})
```

Note: Flowsheets constructed using the Property Interrogator tools are not solvable flowsheets, and will result in errors if sent to a solver.

Output and Display Methods

Both the *PropertiesInterrogatorBlock* and *ReactionInterrogatorBlock* support the following methods for reporting the results of the flowsheet interrogation. The *PropertiesInterrogatorBlock* will contain a summary of all thermophysical properties expected of a *StateBlock* in the flowsheet, whilst the *ReactionInterrogatorBlock* will contain a summary of all reaction related properties required of a *ReactionBlock*.

- `list_required_properties()` - returns a list containing all properties called for by the flowsheet.
- `print_required_properties()` - prints a summary of the required properties

- `list_models_requiring_property(property)` - returns a list of unit models within the flowsheet that require the given property
- `print_models_requiring_property(property)` - prints the name of all unit models within the flowsheet that require the given property
- `list_properties_required_by_model(model)` - returns a list of all properties required by a given unit model in the flowsheet
- `print_properties_required_by_model(model)` - prints a summary of all properties required by a given unit model in the flowsheet

For more details on these methods, see the detailed class documentation below.

Additionally, the *PropertiesInterrogatorBlock* and *ReactionInterrogatorBlock* contain a *dict* named *required_properties* which stores the data regarding the properties required by the model. The keys of this *dict* are the names of all the properties required (as strings) and the values are a list of names for the unit models requiring the given property.

Class Documentation

class `idaes.generic_models.properties.interrogator.properties_interrogator.PropertyInterrogator`

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls `build()`.
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

default_arguments Default arguments to use with Property Package

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (PropertyInterrogatorBlock) New instance

class `idaes.generic_models.properties.interrogator.properties_interrogator.PropertyInterrogator`
Interrogator Parameter Block Class

This class contains the methods and attributes for recording and displaying the properties required by the flowsheet.

build()

Callable method for Block construction.

classmethod define_metadata (*obj*)

Set all the metadata for properties and units.

This method should be implemented by subclasses. In the implementation, they should set information into the object provided as an argument.

Parameters **pcm** (*PropertyClassMetadata*) – Add metadata to this object.

Returns None

list_models_requiring_property (*prop*)

Method to list all models in the flowsheet requiring the given property.

Parameters *prop* – the property of interest

Returns A list of unit model names which require *prop*

list_properties_required_by_model (*model*)

Method to list all thermophysical properties required by a given unit model.

Parameters *model* – the unit model of interest. Can be given as either a model component or the unit name as a string

Returns A list of thermophysical properties required by *model*

list_required_properties ()

Method to list all thermophysical properties required by the flowsheet.

Parameters None –

Returns A list of properties required

print_models_requiring_property (*prop*, *ostream=None*)

Method to print a summary of the models in the flowsheet requiring a given property.

Parameters

- *prop* – the property of interest.
- *ostream* – output stream to print to. If not provided will print to sys.stdout

Returns None

print_properties_required_by_model (*model*, *ostream=None*)

Method to print a summary of the thermophysical properties required by a given unit model.

Parameters

- *model* – the unit model of interest.
- *ostream* – output stream to print to. If not provided will print to sys.stdout

Returns None

print_required_properties (*ostream=None*)

Method to print a summary of the thermophysical properties required by the flowsheet.

Parameters *ostream* – output stream to print to. If not provided will print to sys.stdout

Returns None

class `idaes.generic_models.properties.interrogator.reactions_interrogator.ReactionInterrogator`

Parameters

- *rule* (*function*) – A rule function or None. Default rule calls build().
- *concrete* (*bool*) – If True, make this a toplevel model. **Default** - False.
- *ctype* (*str*) – Pyomo ctype of the block. **Default** - “Block”
- *default* (*dict*) – Default ProcessBlockData config

Keys

property_package Reference to associated PropertyPackageParameter object

default_arguments Default arguments to use with Property Package

- **initialize**(*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map**(*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (ReactionInterrogatorBlock) New instance

class `idaes.generic_models.properties.interrogator.reactions_interrogator.ReactionInterrogator`
Interrogator Parameter Block Class

This class contains the methods and attributes for recording and displaying the reaction properties required by the flowsheet.

build()

Callable method for Block construction.

classmethod **define_metadata**(*obj*)

Set all the metadata for properties and units.

This method should be implemented by subclasses. In the implementation, they should set information into the object provided as an argument.

Parameters **pcm**(*PropertyClassMetadata*) – Add metadata to this object.

Returns None

list_models_requiring_property(*prop*)

Method to list all models in the flowsheet requiring the given property.

Parameters **prop** – the property of interest

Returns A list of unit model names which require prop

list_properties_required_by_model(*model*)

Method to list all reaction properties required by a given unit model.

Parameters **model** – the unit model of interest. Can be given as either a model component or the unit name as a string

Returns A list of reaction properties required by model

list_required_properties()

Method to list all reaction properties required by the flowsheet.

Parameters None –

Returns A list of properties required

print_models_requiring_property(*prop, ostream=None*)

Method to print a summary of the models in the flowsheet requiring a given property.

Parameters

- **prop** – the property of interest.
- **ostream** – output stream to print to. If not provided will print to sys.stdout

Returns None

print_properties_required_by_model(*model, ostream=None*)

Method to print a summary of the reaction properties required by a given unit model.

Parameters

- **model** – the unit model of interest.
- **ostream** – output stream to print to. If not provided will print to sys.stdout

Returns None

print_required_properties (*ostream=None*)

Method to print a summary of the reaction properties required by the flowsheet.

Parameters **ostream** – output stream to print to. If not provided will print to sys.stdout

Returns None

Unit Model Library

Compressor

The Compressor model is a *PressureChanger*, where the configuration is set so that the “compressor” option can only be True, and the default “thermodynamic_assumption” is “isentropic.” See the *PressureChanger documentation* for details.

Example

The example below demonstrates the basic Compressor model usage:

```
import pyomo.environ as pyo
from idaes.core import FlowsheetBlock
from idaes.generic_models.unit_models import Compressor
from idaes.generic_models.properties import iapws95

m = pyo.ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": False})
m.fs.properties = iapws95.Iapws95ParameterBlock()
m.fs.unit = Compressor(default={"property_package": m.fs.properties})

m.fs.unit.inlet.flow_mol[0].fix(100)
m.fs.unit.inlet.enth_mol[0].fix(4000)
m.fs.unit.inlet.pressure[0].fix(101325)

m.fs.unit.deltaP.fix(50000)
m.fs.unit.eta_isentropic.fix(0.9)
```

Continuous Stirred Tank Reactor

The IDAES CSTR model represents a unit operation where a material stream undergoes some chemical reaction(s) in a well-mixed vessel.

Degrees of Freedom

CSTRs generally have one degree of freedom. Typically, the fixed variable is reactor volume.

Model Structure

The core CSTR unit model consists of a single `ControlVolume0D` (named `control_volume`) with one Inlet Port (named `inlet`) and one Outlet Port (named `outlet`).

Additional Constraints

CSTR units write the following additional Constraints beyond those written by the `ControlVolume` Block.

$$X_{t,r} = V_t \times r_{t,r}$$

where $X_{t,r}$ is the extent of reaction of reaction r at time t , V_t is the volume of the reacting material at time t (allows for varying reactor volume with time) and $r_{t,r}$ is the volumetric rate of reaction of reaction r at time t (from the outlet property package).

Variables

CSTR units add the following additional Variables beyond those created by the `ControlVolume` Block.

Vari- able	Name	Notes
V_t	vol- ume	If <code>has_holdup = True</code> this is a reference to <code>control_volume.volume</code> , otherwise a <code>Var</code> attached to the Unit Model
Q_t	heat	Only if <code>has_heat_transfer = True</code> , reference to <code>control_volume.heat</code>

CSTR Class

```
class idaes.generic_models.unit_models.cstr.CSTR(*args, **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or `None`. Default rule calls `build()`.
- **concrete** (*bool*) – If `True`, make this a toplevel model. **Default** - `False`.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default `ProcessBlockData` config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = `useDefault`.
Valid values: { **useDefault** - get flag from parent (default = `False`), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be `True` if `dynamic = True`, **default** - `False`. **Valid values:** { **useDefault** - get flag from parent (default = `False`), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - `MaterialBalanceType.useDefault`. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBal-**

anceType.componentTotal - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance.}

energy_balance_type Indicates what type of energy balance should be constructed, **default** - `EnergyBalanceType.useDefault`. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type **EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase.}

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase.}

has_heat_transfer Indicates whether terms for heat transfer should be constructed, **default** - `False`. **Valid values:** { **True** - include heat transfer terms, **False** - exclude heat transfer terms.}

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - `False`. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms.}

has_equilibrium_reactions Indicates whether terms for equilibrium controlled reactions should be constructed, **default** - `True`. **Valid values:** { **True** - include equilibrium reaction terms, **False** - exclude equilibrium reaction terms.}

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** - `False`. **Valid values:** { **True** - include phase equilibrium terms, **False** - exclude phase equilibrium terms.}

has_heat_of_reaction Indicates whether terms for heat of reaction terms should be constructed, **default** - `False`. **Valid values:** { **True** - include heat of reaction terms, **False** - exclude heat of reaction terms.}

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PhysicalParameterObject** - a `PhysicalParameterBlock` object.}

property_package_args A `ConfigBlock` with arguments to be passed to a property block(s) and used when constructing these, **default** - `None`. **Valid values:** { see property package for documentation.}

reaction_package Reaction parameter object used to define reaction calculations, **default** - `None`. **Valid values:** { **None** - no reaction package, **ReactionParameterBlock** - a `ReactionParameterBlock` object.}

reaction_package_args A `ConfigBlock` with arguments to be passed to a reaction block(s) and used when constructing these, **default** - `None`. **Valid values:** { see reaction package for documentation.}

- **initialize** (*dict*) – `ProcessBlockData` config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.

- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (CSTR) New instance

CSTRData Class

class `idaes.generic_models.unit_models.cstr.CSTRData` (*component*)

Standard CSTR Unit Model Class

build ()

Begin building model (pre-DAE transformation). :param None:

Returns None

Equilibrium Reactor

The IDAES Equilibrium reactor model represents a unit operation where a material stream undergoes some chemical reaction(s) to reach an equilibrium state. This model is for systems with reaction with equilibrium coefficients - for Gibbs energy minimization see Gibbs reactor documentation.

Degrees of Freedom

Equilibrium reactors generally have 1 degree of freedom.

Typical fixed variables are:

- reactor heat duty (`has_heat_transfer = True` only).

Model Structure

The core Equilibrium reactor unit model consists of a single `ControlVolume0D` (named `control_volume`) with one Inlet Port (named `inlet`) and one Outlet Port (named `outlet`).

Additional Constraints

Equilibrium reactors units write the following additional Constraints beyond those written by the Control Volume if rate controlled reactions are present.

$$r_{t,r} = 0$$

where $r_{t,r}$ is the rate of reaction for reaction r at time t . This enforces equilibrium in any reversible rate controlled reactions which are present. Any non-reversible reaction that may be present will proceed to completion.

Variables

Equilibrium reactor units add the following additional Variables beyond those created by the Control Volume.

Variable	Name	Notes
V_t	volume	If <code>has_holdup = True</code> this is a reference to <code>control_volume.volume</code> , otherwise a Var attached to the Unit Model
Q_t	heat	Only if <code>has_heat_transfer = True</code> , reference to <code>control_volume.heat</code>

EquilibriumReactor Class

```
class idaes.generic_models.unit_models.equilibrium_reactor.EquilibriumReactor(*args,
                                                                              **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = False. Equilibrium Reactors do not support dynamic behavior.

has_holdup Indicates whether holdup terms should be constructed or not. **default** - False. Equilibrium reactors do not have defined volume, thus this must be False.

material_balance_type Indicates what type of mass balance should be constructed, **default** - `MaterialBalanceType.useDefault`. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type **MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - `EnergyBalanceType.useDefault`. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type **EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_rate_reactions Indicates whether terms for rate controlled reactions should be constructed, along with constraints equating these to zero, **default** - True. **Valid values:** { **True** - include rate reaction terms, **False** - exclude rate reaction terms. }

has_equilibrium_reactions Indicates whether terms for equilibrium controlled reactions should be constructed, **default** - True. **Valid values:** { **True** - include equilibrium reaction terms, **False** - exclude equilibrium reaction terms. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** - True. **Valid values:** { **True** - include phase equilibrium term, **False** - exclude phase equilibrium terms. }

has_heat_transfer Indicates whether terms for heat transfer should be constructed, **default** - False. **Valid values:** { **True** - include heat transfer terms, **False** - exclude heat transfer terms. }

has_heat_of_reaction Indicates whether terms for heat of reaction terms should be constructed, **default** - False. **Valid values:** { **True** - include heat of reaction terms, **False** - exclude heat of reaction terms. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - False. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms. }

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PhysicalParameterObject** - a PhysicalParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

reaction_package Reaction parameter object used to define reaction calculations, **default** - None. **Valid values:** { **None** - no reaction package, **ReactionParameterBlock** - a ReactionParameterBlock object. }

reaction_package_args A ConfigBlock with arguments to be passed to a reaction block(s) and used when constructing these, **default** - None. **Valid values:** { see reaction package for documentation. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (EquilibriumReactor) New instance

EquilibriumReactorData Class

class `idaes.generic_models.unit_models.equilibrium_reactor.EquilibriumReactorData` (*component*)
Standard Equilibrium Reactor Unit Model Class

build ()
Begin building model.

Parameters None –

Returns None

Feed Block

Feed Blocks are used to represent sources of material in Flowsheets. Feed blocks do not calculate phase equilibrium of the feed stream, and the composition of the material in the outlet stream will be exactly as specified in the input. For applications where the users wishes the outlet stream to be in phase equilibrium, see the Feed_Flash unit model.

Degrees of Freedom

The degrees of freedom of Feed blocks depends on the property package being used and the number of state variables necessary to fully define the system. Users should refer to documentation on the property package they are using.

Model Structure

Feed Blocks consists of a single StateBlock (named properties), each with one Outlet Port (named outlet). Feed Blocks also contain References to the state variables defined within the StateBlock

Additional Constraints

Feed Blocks write no additional constraints to the model.

Variables

Feed blocks add no additional Variables.

Feed Class

```
class idaes.generic_models.unit_models.feed.Feed(*args, **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = False. Feed blocks are always steady-state.

has_holdup Feed blocks do not contain holdup, thus this must be False.

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PhysicalParameterObject** - a PhysicalParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (Feed) New instance

FeedData Class

class `idaes.generic_models.unit_models.feed.FeedData` (*component*)

Standard Feed Block Class

build ()

Begin building model.

Parameters None –

Returns None

initialize (*state_args={}*, *outlvl=0*, *solver='ipopt'*, *optarg={'tol': 1e-06}*)

This method calls the initialization method of the state block.

Keyword Arguments

- **state_args** – a dict of arguments to be passed to the property package(s) to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={'tol': 1e-6})
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')

Returns None

Feed Block with Flash

Feed Blocks are used to represent sources of material in Flowsheets. In some cases, users may have a situation where a feed stream may be in a multi-phase state, but may not know the full details of the equilibrium state. The IDAES Feed Block with Flash (FeedFlash) allows users to define a feed block where the outlet is in phase equilibrium based on calculations from the chosen property package and a sufficient set of state variables prior to being passed to the first unit operation. The phase equilibrium is performed assuming an isobaric and isothermal flash operation.

A Feed Block with Flash is only required in cases where the feed may be in phase equilibrium AND the chosen property package uses a state definition that includes phase separations. Some property packages support phase equilibrium, but use a state definition that involves only total flows - in these cases a flash calculation is performed at the inlet of every unit and thus it is not necessary to perform a flash calculation at the feed block.

Degrees of Freedom

The degrees of freedom of FeedFlash blocks depends on the property package being used and the number of state variables necessary to fully define the system. Users should refer to documentation on the property package they are using.

Model Structure

FeedFlash Blocks contain a single `ControlVolume0D` (named `control_volume`) with one Outlet Port (named `outlet`). FeedFlash Blocks also contain References to the state variables defined within the inlet StateBlock of the `ControlVolume` (representing the unflashed state of the feed).

FeedFlash Blocks do not write a set of energy balances within the Control Volume - instead a constraint is written which enforces an isothermal flash.

Additional Constraints

The FeedFlash Block writes one additional constraint to enforce isothermal behavior.

$$T_{in,t} = T_{out,t}$$

where $T_{in,t}$ and $T_{out,t}$ are the temperatures of the material before and after the flash operation.

Variables

FeedFlash blocks add no additional Variables.

FeedFlash Class

```
class idaes.generic_models.unit_models.feed_flash.FeedFlash(*args, **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls `build()`.
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Feed units do not support dynamic behavior.

has_holdup Feed units do not have defined volume, thus this must be False.

material_balance_type Indicates what type of mass balance should be constructed, **default** - `MaterialBalanceType.useDefault`. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

flash_type Indicates what type of flash operation should be used. **default** - `FlashType.isothermal`. **Valid values:** { **FlashType.isothermal** - specify temperature, **FlashType.isenthalpic** - specify enthalpy. }

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PhysicalParameterObject** - a `PhysicalParameterBlock` object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation.}

- **initialize**(*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map**(*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (FeedFlash) New instance

FeedFlashData Class

class `idaes.generic_models.unit_models.feed_flash.FeedFlashData` (*component*)
Standard Feed block with phase equilibrium

build()
Begin building model.

Parameters None –

Returns None

Flash Unit

The IDAES Flash model represents a unit operation where a single stream undergoes a flash separation into two phases. The Flash model supports mutile types of flash operations, including pressure changes and addition or removal of heat.

Degrees of Freedom

Flash units generally have 2 degrees of freedom.

Typical fixed variables are:

- heat duty or outlet temperature (see note),
- pressure change or outlet pressure.

Note: When setting the outlet temeptrature of a Flash unit, it is best to set `control_volume.properties_out[t].temperature`. Setting the temperature in one of the outlet streams directly results in a much harder problme to solve, and may be degenerate or unbounded in some cases.

Model Structure

The core Flash unit model consists of a single ControlVolume0DBlock (named `control_volume`) with one Inlet Port (named `inlet`) connected to a Separator unit model with two outlet Ports named ‘`vap_outlet`’ and ‘`liq_outlet`’. The Flash model utilizes the separator unit model in IDAES to split the outlets by phase flows to the liquid and vapor outlets respectively.

The Separator unit model supports both direct splitting of state variables and writting of full splitting constraints via the *ideal_separation* construction argument. Full details on the Separator unit model can be found in the documentation for that unit. To support direct splitting, the property package must use one of a specified set of state variables and support a certain set of property calacuations, as outlined in the table below.

State Variables	Required Properties
Material flow and composition	
flow_mol & mole_frac	flow_mol_phase & mole_frac_phase
flow_mol_phase & mole_frac_phase	flow_mol_phase & mole_frac_phase
flow_mol_comp	flow_mol_phase_comp
flow_mol_phase_comp	flow_mol_phase_comp
flow_mass & mass_frac	flow_mass_phase & mass_frac_phase
flow_mass_phase & mass_frac_phase	flow_mass_phase & mass_frac_phase
flow_mass_comp	flow_mass_phase_comp
flow_mass_phase_comp	flow_mass_phase_comp
Energy state	
temperature	temperature
enth_mol	enth_mol_phase
enth_mol_phase	enth_mol_phase
enth_mass	enth_mass_phase
enth_mass_phase	enth_mass_phase
Pressure state	
pressure	pressure

Construction Arguments

Flash units have the following construction arguments:

- property_package - property package to use when constructing Property Blocks (default = 'use_parent_value'). This is provided as a Property Parameter Block by the Flowsheet when creating the model. If a value is not provided, the Holdup Block will try to use the default property package if one is defined.
- property_package_args - set of arguments to be passed to the Property Blocks when they are created.

Additionally, Flash units have the following construction arguments which are passed to the Holdup Block for determining which terms to construct in the balance equations.

Argument	Default Value
dynamic	False
include_holdup	False
material_balance_type	MaterialBalanceType.componentPhase
energy_balance_type	EnergyBalanceType.enthalpyTotal
momentum_balance_type	MomentumBalanceType.pressureTotal
has_phase_equilibrium	True
has_heat_transfer	True
has_pressure_change	True

Finally, Flash units also have the following arguments which are passed to the Separator block for determining how to split to two-phase mixture.

Argument	Default Value
ideal_separation	True
energy_split_basis	EnergySplittingType.equal_temperature

Additional Constraints

Flash units write no additional Constraints beyond those written by the ControlVolume0DBlock and the Separator block.

Variables

Name	Notes
heat_duty	Reference to control_volume.heat
deltaP	Reference to control_volume.deltaP

Flash Class

```
class idaes.generic_models.unit_models.flash.Flash(*args, **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = False. Flash units do not support dynamic behavior.

has_holdup Indicates whether holdup terms should be constructed or not. **default** - False. Flash units do not have defined volume, thus this must be False.

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.useDefault. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - MomentumBalanceType.pressureTotal. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalance-**

Type.momentumTotal - single momentum balance for material, **MomentumBalance-Type.momentumPhase** - momentum balances for each phase.}

energy_split_basis Argument indicating basis to use for splitting energy this is not used for when `ideal_separation == True`. **default** - `EnergySplittingType.equal_temperature`. **Valid values:** { `EnergySplittingType.equal_temperature` - outlet temperatures equal inlet `EnergySplittingType.equal_molar_enthalpy` - outlet molar enthalpies equal inlet, `EnergySplittingType.enthalpy_split` - apply split fractions to enthalpy flows.}

ideal_separation Argument indicating whether ideal splitting should be used. Ideal splitting assumes perfect separation of material, and attempts to avoid duplication of StateBlocks by directly partitioning outlet flows to ports, **default** - `True`. **Valid values:** { `True` - use ideal splitting methods. Cannot be combined with `has_phase_equilibrium == True`, `False` - use explicit splitting equations with split fractions.}

has_heat_transfer Indicates whether terms for heat transfer should be constructed, **default** - `False`. **Valid values:** { `True` - include heat transfer terms, `False` - exclude heat transfer terms.}

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - `True`. **Valid values:** { `True` - include pressure change terms, `False` - exclude pressure change terms.}

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { `useDefault` - use default package from parent model or flowsheet, `PropertyParameterObject` - a `PropertyParameterBlock` object.}

property_package_args A `ConfigBlock` with arguments to be passed to a property block(s) and used when constructing these, **default** - `None`. **Valid values:** { see property package for documentation.}

- **initialize** (*dict*) – `ProcessBlockData` config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a `BlockData` element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the `BlockData` index exactly to the index in initialize.

Returns (Flash) New instance

FlashData Class

```
class idaes.generic_models.unit_models.flash.FlashData (component)
```

Standard Flash Unit Model Class

build ()

Begin building model (pre-DAE transformation).

Parameters `None` –

Returns `None`

Gibbs Reactor

The IDAES Gibbs reactor model represents a unit operation where a material stream undergoes some set of reactions such that the Gibbs energy of the resulting mixture is minimized. Gibbs reactors rely on conservation of individual elements within the system, and thus require element balances, and make use of Lagrange multipliers to find the minimum Gibbs energy state of the system.

Degrees of Freedom

Gibbs reactors generally have between 0 and 2 degrees of freedom, depending on construction arguments.

Typical fixed variables are:

- reactor heat duty (has_heat_transfer = True only).
- reactor pressure change (has_pressure_change = True only).

Model Structure

The core Gibbs reactor unit model consists of a single ControlVolume0DBlock (named control_volume) with one Inlet Port (named inlet) and one Outlet Port (named outlet).

Variables

Gibbs reactor units add the following additional Variables beyond those created by the Control Volume Block.

Variable Name	Symbol	Notes
lagrange_mult	$L_{t,e}$	Lagrange multipliers
heat_duty	Q_t	Only if has_heat_transfer = True, reference
deltaP	ΔP_t	Only if has_pressure_change = True, reference

Constraints

Gibbs reactor models write the following additional constraints to calculate the state that corresponds to the minimum Gibbs energy of the system.

gibbs_minimization(time, phase, component):

$$0 = g_{\text{partial},t,j} + \sum_e (L_{t,e} \times \alpha_{j,e})$$

where $g_{\text{partial},t,j}$ is the partial molar Gibbs energy of component j at time t , $L_{t,e}$ is the Lagrange multiplier for element e at time t and $\alpha_{j,e}$ is the number of moles of element e in one mole of component j . $g_{\text{partial},t,j}$ and $\alpha_{j,e}$ come from the outlet StateBlock.

GibbsReactor Class

```
class idaes.generic_models.unit_models.gibbs_reactor.GibbsReactor(*args,
                                                                    **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Gibbs reactors do not support dynamic models, thus this must be False.

has_holdup Gibbs reactors do not have defined volume, thus this must be False.

energy_balance_type Indicates what type of energy balance should be constructed, **default** - `EnergyBalanceType.useDefault`. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type **EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_heat_transfer Indicates whether terms for heat transfer should be constructed, **default** - False. **Valid values:** { **True** - include heat transfer terms, **False** - exclude heat transfer terms. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - False. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms. }

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a `PropertyParameterBlock` object. }

property_package_args A `ConfigBlock` with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

- **initialize** (*dict*) – `ProcessBlockData` config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (`GibbsReactor`) New instance

GibbsReactorData Class

class `idaes.generic_models.unit_models.gibbs_reactor.GibbsReactorData` (*component*)
Standard Gibbs Reactor Unit Model Class

This model assume all possible reactions reach equilibrium such that the system partial molar Gibbs free energy is minimized. Since some species mole flow rate might be very small, the natural log of the species molar flow rate is used. Instead of specifying the system Gibbs free energy as an objective function, the equations for zero partial derivatives of the grand function with Lagrangian multiple terms with respect to product species mole flow rates and the multiples are specified as constraints.

build ()

Begin building model (pre-DAE transformation).

Parameters None –

Returns None

Heater

The Heater model is a simple 0D model that adds or removes heat from a material stream.

Example

```
import pyomo.environ as pe # Pyomo environment
from idaes.core import FlowsheetBlock, StateBlock
from idaes.generic_models.unit_models import Heater
from idaes.generic_models.properties import iapws95

# Create an empty flowsheet and steam property parameter block.
model = pe.ConcreteModel()
model.fs = FlowsheetBlock(default={"dynamic": False})
model.fs.properties = iapws95.Iapws95ParameterBlock()

# Add a Heater model to the flowsheet.
model.fs.heater = Heater(default={"property_package": model.fs.properties})

# Setup the heater model by fixing the inputs and heat duty
model.fs.heater.inlet[:].enth_mol.fix(4000)
model.fs.heater.inlet[:].flow_mol.fix(100)
model.fs.heater.inlet[:].pressure.fix(101325)
model.fs.heater.heat_duty[:].fix(100*20000)

# Initialize the model.
model.fs.heater.initialize()
```

Degrees of Freedom

Aside from the inlet conditions, a heater model usually has one degree of freedom, which is the heat duty.

Model Structure

A heater model contains one `ControlVolume0DBlock` block.

Variables

The `heat_duty` variable is a reference to `control_volume.heat`.

Constraints

A heater model contains no additional constraints beyond what are contained in a `ControlVolume0DBlock` model.

Heater Class

class `idaes.generic_models.unit_models.heater.Heater(*args, **kwargs)`
Simple 0D heater/cooler model.

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.
Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.useDefault. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - MomentumBalanceType.pressureTotal. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = False. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - False. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms. }

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation.}

- **initialize**(*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map**(*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (Heater) New instance

HeaterData Class

class `idaes.generic_models.unit_models.heater.HeaterData` (*component*)

Simple 0D heater unit. Unit model to add or remove heat from a material.

build()

Building model

Parameters None –

Returns None

HeatExchanger (0D)

The HeatExchanger model can be imported from `idaes.generic_models.unit_models`, while additional rules and utility functions can be imported from `idaes.generic_models.unit_models.heat_exchanger`.

Example

The example below demonstrates how to initialize the HeatExchanger model, and override the default temperature difference calculation.

```
import pyomo.environ as pe # Pyomo environment
from idaes.core import FlowsheetBlock, StateBlock
from idaes.generic_models.unit_models import HeatExchanger
from idaes.generic_models.unit_models.heat_exchanger import delta_temperature_amtd_
↳ callback
from idaes.generic_models.properties import iapws95

# Create an empty flowsheet and steam property parameter block.
model = pe.ConcreteModel()
model.fs = FlowsheetBlock(default={"dynamic": False})
model.fs.properties = iapws95.Iapws95ParameterBlock()

# Add a Heater model to the flowsheet.
model.fs.heat_exchanger = HeatExchanger(default={
    "delta_temperature_callback": delta_temperature_amtd_callback,
    "shell": {"property_package": model.fs.properties},
    "tube": {"property_package": model.fs.properties}})

model.fs.heat_exchanger.area.fix(1000)
```

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```

model.fs.heat_exchanger.overall_heat_transfer_coefficient[0].fix(100)
model.fs.heat_exchanger.shell_inlet.flow_mol.fix(100)
model.fs.heat_exchanger.shell_inlet.pressure.fix(101325)
model.fs.heat_exchanger.shell_inlet.enth_mol.fix(4000)
model.fs.heat_exchanger.tube_inlet.flow_mol.fix(100)
model.fs.heat_exchanger.tube_inlet.pressure.fix(101325)
model.fs.heat_exchanger.tube_inlet.enth_mol.fix(3000)

# Initialize the model
model.fs.heat_exchanger.initialize()

```

Degrees of Freedom

Aside from the inlet conditions, a heat exchanger model usually has two degrees of freedom, which can be fixed for it to be fully specified. Things that are frequently fixed are two of:

- heat transfer area,
- heat transfer coefficient, or
- temperature approach.

The user may also provide constants to calculate the heat transfer coefficient.

Model Structure

The `HeatExchanger` model contains two `ControlVolume0DBlock` blocks. By default the hot side is named `shell` and the cold side is named `tube`. These names are configurable. The sign convention is that duty is positive for heat flowing from the hot side to the cold side. Aside from the sign convention there is no requirement that the hot side be hotter than the cold side.

The control volumes are configured the same as the `ControlVolume0DBlock` in the *Heater model*. The `HeatExchanger` model contains additional constraints that calculate the amount of heat transferred from the hot side to the cold side.

The `HeatExchanger` has two inlet ports and two outlet ports. By default these are `shell_inlet`, `tube_inlet`, `shell_outlet`, and `tube_outlet`. If the user supplies different hot and cold side names the inlet and outlets are named accordingly.

Variables

Variable	Symbol	Index Sets	Doc
heat_duty	Q	t	Heat transferred from hot side to the cold side
area	A	None	Heat transfer area
heat_transfer_coefficient	U	t	Heat transfer coefficient
delta_temperature	ΔT	t	Temperature difference, defaults to LMTD

Note: `delta_temperature` may be either a variable or expression depending on the callback used. If the specified cold side is hotter than the specified hot side this value will be negative.

Constraints

The default constants can be overridden by providing *alternative rules* for the heat transfer equation, temperature difference, and heat transfer coefficient. The section describes the default constraints.

Heat transfer from shell to tube:

$$Q = UA\Delta T$$

Temperature difference is an expression:

$$\Delta T = \frac{\Delta T_1 - \Delta T_2}{\log_e \left(\frac{\Delta T_1}{\Delta T_2} \right)}$$

The heat transfer coefficient is a variable with no associated constraints by default.

Class Documentation

Note: The `hot_side_config` and `cold_side_config` can also be supplied using the name of the hot and cold sides (shell and tube by default) as in *the example*.

```
class idaes.generic_models.unit_models.heat_exchanger.HeatExchanger (*args,
                                                                    **kwargs)
```

Simple 0D heat exchanger model.

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.
Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

hot_side_name Hot side name, sets control volume and inlet and outlet names

cold_side_name Cold side name, sets control volume and inlet and outlet names

hot_side_config A config block used to construct the hot side control volume. This config can be given by the hot side name instead of `hot_side_config`.

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalance-**

Type.elementTotal - use total element balances, **MaterialBalanceType.total** - use total material balance.}

energy_balance_type Indicates what type of energy balance should be constructed, **default** - `EnergyBalanceType.useDefault`. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type **EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = `False`. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - `False`. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms. }

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a `PropertyParameterBlock` object. }

property_package_args A `ConfigBlock` with arguments to be passed to a property block(s) and used when constructing these, **default** - `None`. **Valid values:** { see property package for documentation. }

cold_side_config A config block used to construct the cold side control volume. This config can be given by the cold side name instead of `cold_side_config`.

material_balance_type Indicates what type of mass balance should be constructed, **default** - `MaterialBalanceType.useDefault`. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type **MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - `EnergyBalanceType.useDefault`. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type **EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { `MomentumBalanceType.none` - exclude momentum balances, `MomentumBalanceType.pressureTotal` - single pressure balance for material, `MomentumBalanceType.pressurePhase` - pressure balances for each phase, `MomentumBalanceType.momentumTotal` - single momentum balance for material, `MomentumBalanceType.momentumPhase` - momentum balances for each phase. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = `False`. **Valid values:** { `True` - include phase equilibrium terms `False` - exclude phase equilibrium terms. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - `False`. **Valid values:** { `True` - include pressure change terms, `False` - exclude pressure change terms. }

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { `useDefault` - use default package from parent model or flowsheet, `PropertyParameterObject` - a `PropertyParameterBlock` object. }

property_package_args A `ConfigBlock` with arguments to be passed to a property block(s) and used when constructing these, **default** - `None`. **Valid values:** { see property package for documentation. }

delta_temperature_callback Callback for for temperature difference calculations

flow_pattern Heat exchanger flow pattern, **default** - `HeatExchangerFlowPattern.countercurrent`. **Valid values:** { `HeatExchangerFlowPattern.countercurrent` - countercurrent flow, `HeatExchangerFlowPattern.cocurrent` - cocurrent flow, `HeatExchangerFlowPattern.crossflow` - cross flow, factor times countercurrent temperature difference. }

- **initialize** (*dict*) – `ProcessBlockData` config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a `BlockData` element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the `BlockData` index exactly to the index in initialize.

Returns (`HeatExchanger`) New instance

class `idaes.generic_models.unit_models.heat_exchanger.HeatExchangerData` (*component*)
Simple 0D heat exchange unit. Unit model to transfer heat from one material to another.

build ()
Building model

Parameters `None` –

Returns `None`

initialize (*state_args_1=None, state_args_2=None, outlvl=0, solver='ipopt', optarg={'tol': 1e-06}, duty=1000*)
Heat exchanger initialization method.

Parameters

- **state_args_1** – a dict of arguments to be passed to the property initialization for side_1 (see documentation of the specific property package) (default = {}).
- **state_args_2** – a dict of arguments to be passed to the property initialization for side_2 (see documentation of the specific property package) (default = {}).

- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={ 'tol': 1e-6})
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')
- **duty** – an initial guess for the amount of heat transfered (default = 10000)

Returns None

set_scaling_factor_energy (*f*)

This function sets `scaling_factor_energy` for both `side_1` and `side_2`. This factor multiplies the energy balance and heat transfer equations in the heat exchanger. The value of this factor should be about 1/(expected heat duty).

Parameters *f* – Energy balance scaling factor

Callbacks

A selection of functions for constructing the `delta_temperature` variable or expression are provided in the `idaes.generic_models.unit_models.heat_exchanger` module. The user may also provide their own function. These callbacks should all take one argument (the `HeatExchanger` block). With the block argument, the function can add any additional variables, constraints, and expressions needed. The only requirement is that either a variable or expression called `delta_temperature` must be added to the block.

Defined Callbacks for the `delta_temperature_callback` Option

These callbacks provide expressions for the temperature difference used in the heat transfer equations.

`idaes.generic_models.unit_models.heat_exchanger.delta_temperature_lmt_d_callback` (*b*)

This is a callback for a temperature difference expression to calculate ΔT in the heat exchanger model using log-mean temperature difference (LMTD). It can be supplied to “delta_temperature_callback” HeatExchanger configuration option.

`idaes.generic_models.unit_models.heat_exchanger.delta_temperature_amtd_callback` (*b*)

This is a callback for a temperature difference expression to calculate ΔT in the heat exchanger model using arithmetic-mean temperature difference (AMTD). It can be supplied to “delta_temperature_callback” HeatExchanger configuration option.

`idaes.generic_models.unit_models.heat_exchanger.delta_temperature_underwood_callback` (*b*)

This is a callback for a temperature difference expression to calculate ΔT in the heat exchanger model using log-mean temperature difference (LMTD) approximation given by Underwood (1970). It can be supplied to “delta_temperature_callback” HeatExchanger configuration option. This uses a cube root function that works with negative numbers returning the real negative root. This should always evaluate successfully.

Heat Exchangers (1D)

Heat Exchanger models represents a unit operation with two material streams which exchange heat. The IDAES 1-D Heat Exchanger model is used for detailed modeling of heat exchanger units with variations in one spatial dimension. For a simpler representation of a heat exchanger unit see Heat Exchanger (0-D).

Degrees of Freedom

1-D Heat Exchangers generally have 7 degrees of freedom.

Typical fixed variables are:

- shell length and diameter,
- tube length and diameter,
- number of tubes,
- heat transfer coefficients (at all spatial points) for both shell and tube sides.

Model Structure

The core 1-D Heat Exchanger Model unit model consists of two `ControlVolume1DBlock` Blocks (named shell and tube), each with one Inlet Port (named shell_inlet and tube_inlet) and one Outlet Port (named shell_outlet and tube_outlet).

Construction Arguments

1-D Heat Exchanger units have construction arguments specific to the shell side, tube side and for the unit as a whole.

Arguments that are applicable to the heat exchanger unit are as follows:

- `flow_type` - indicates the flow arrangement within the unit to be modeled. Options are:
 - ‘co-current’ - (default) shell and tube both flow in the same direction (from $x=0$ to $x=1$)
 - ‘counter-current’ - shell and tube flow in opposite directions (shell from $x=0$ to $x=1$ and tube from $x=1$ to $x=0$).
- `finite_elements` - sets the number of finite elements to use when discretizing the spatial domains (default = 20). This is used for both shell and tube side domains.
- `collocation_points` - sets the number of collocation points to use when discretizing the spatial domains (default = 5, collocation methods only). This is used for both shell and tube side domains.
- **has_wall_conduction - option to enable a model for heat conduction across the tube wall:**
 - ‘none’ - 0D wall model
 - ‘1D’ - 1D heat conduction equation along the thickness of the tube wall
 - ‘2D’ - 2D heat conduction equation along the length and thickness of the tube wall

Arguments that are applicable to the shell side:

- `property_package` - property package to use when constructing shell side Property Blocks (default = ‘use_parent_value’). This is provided as a Physical Parameter Block by the Flowsheet when creating the model. If a value is not provided, the `ControlVolume` Block will try to use the default property package if one is defined.
- `property_package_args` - set of arguments to be passed to the shell side Property Blocks when they are created.
- `transformation_method` - argument to specify the DAE transformation method for the shell side; should be compatible with the Pyomo DAE TransformationFactory
- `transformation_scheme` - argument to specify the scheme to use for the selected DAE transformation method; should be compatible with the Pyomo DAE TransformationFactory

Arguments that are applicable to the tube side:

- `property_package` - property package to use when constructing tube side Property Blocks (default = ‘use_parent_value’). This is provided as a Property Parameter Block by the Flowsheet when creating the model. If a value is not provided, the `ControlVolume` Block will try to use the default property package if one is defined.

- `property_package_args` - set of arguments to be passed to the tube side Property Blocks when they are created.
- `transformation_method` - argument to specify the DAE transformation method for the tube side; should be compatible with the Pyomo DAE TransformationFactory
- `transformation_scheme` - argument to specify the scheme to use for the selected DAE transformation method; should be compatible with the Pyomo DAE TransformationFactory

Additionally, 1-D Heat Exchanger units have the following construction arguments which are passed to the `ControlVolume1DBlock` Block for determining which terms to construct in the balance equations for the shell and tube side.

Argument	Default Value
<code>dynamic</code>	<code>useDefault</code>
<code>has_holdup</code>	<code>False</code>
<code>material_balance_type</code>	<code>'componentTotal'</code>
<code>energy_balance_type</code>	<code>'enthalpyTotal'</code>
<code>momentum_balance_type</code>	<code>'pressureTotal'</code>
<code>has_phase_equilibrium</code>	<code>False</code>
<code>has_heat_transfer</code>	<code>True</code>
<code>has_pressure_change</code>	<code>False</code>

Additional Constraints

1-D Heat Exchanger models write the following additional Constraints to describe the heat transfer between the two sides of the heat exchanger. Firstly, the shell- and tube-side heat transfer is calculated as:

$$Q_{shell,t,x} = -N_{tubes} \times (\pi \times U_{shell,t,x} \times D_{tube,outer} \times (T_{shell,t,x} - T_{wall,t,x}))$$

where $Q_{shell,t,x}$ is the shell-side heat duty at point x and time t , N_{tubes} D_{tube} are the number of and diameter of the tubes in the heat exchanger, $U_{shell,t,x}$ is the shell-side heat transfer coefficient, and $T_{shell,t,x}$ and $T_{wall,t,x}$ are the shell-side and tube wall temperatures respectively.

$$Q_{tube,t,x} = N_{tubes} \times (\pi \times U_{tube,t,x} \times D_{tube,inner} \times (T_{wall,t,x} - T_{tube,t,x}))$$

where $Q_{tube,t,x}$ is the tube-side heat duty at point x and time t , $U_{tube,t,x}$ is the tube-side heat transfer coefficient and $T_{tube,t,x}$ is the tube-side temperature.

If a OD wall model is used for the tube wall conduction, the following constraint is implemented to connect the heat terms on the shell and tube side:

$$N_{tubes} \times Q_{tube,t,x} = -Q_{shell,t,x}$$

Finally, the following Constraints are written to describe the unit geometry:

$$4 \times A_{tube} = \pi \times D_{tube}^2$$

$$4 \times A_{shell} = \pi \times (D_{shell}^2 - N_{tubes} \times D_{tube}^2)$$

where A_{shell} and A_{tube} are the shell and tube areas respectively and D_{shell} and D_{tube} are the shell and tube diameters.

Variables

1-D Heat Exchanger units add the following additional Variables beyond those created by the `ControlVolume1DBlock` Block.

Variable	Name	Notes
L_{shell}	shell_length	Reference to shell.length
A_{shell}	shell_area	Reference to shell.area
D_{shell}	d_shell	
L_{tube}	tube_length	Reference to tube.length
A_{tube}	tube_area	Reference to tube.area
D_{tube}	d_tube	
N_{tubes}	N_tubes	
$T_{wall,t,x}$	temperature_wall	
$U_{shell,t,x}$	shell_heat_transfer_coefficient	
$U_{tube,t,x}$	tube_heat_transfer_coefficient	

HeatExchanger1dClass

```
class idaes.generic_models.unit_models.heat_exchanger_1D.HeatExchanger1D(*args,
                                                                    **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.
Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

shell_side shell side config arguments

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.
Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - `EnergyBalanceType.useDefault`. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type **EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - `False`. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms. }

has_phase_equilibrium Argument to enable phase equilibrium on the shell side. - `True` - include phase equilibrium term - `False` - do not include phase equilibrium term

property_package Property parameter object used to define property calculations (default = `'use_parent_value'`) - `'use_parent_value'` - get package from parent (default = `None`) - a `ParameterBlock` object

property_package_args A dict of arguments to be passed to the `PropertyBlockData` and used when constructing these (default = `'use_parent_value'`) - `'use_parent_value'` - get package from parent (default = `None`) - a dict (see property package for documentation)

transformation_method Discretization method to use for DAE transformation. See Pyomo documentation for supported transformations.

transformation_scheme Discretization scheme to use when transforming domain. See Pyomo documentation for supported schemes.

tube_side tube side config arguments

dynamic Indicates whether this model will be dynamic or not, **default** = `useDefault`. **Valid values:** { **useDefault** - get flag from parent (default = `False`), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be `True` if `dynamic = True`, **default** - `False`. **Valid values:** { **useDefault** - get flag from parent (default = `False`), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - `MaterialBalanceType.useDefault`. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type **MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - `EnergyBalanceType.useDefault`. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - `False`. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms. }

has_phase_equilibrium Argument to enable phase equilibrium on the shell side. - `True` - include phase equilibrium term - `False` - do not include phase equilibrium term

property_package Property parameter object used to define property calculations (default = `'use_parent_value'`) - `'use_parent_value'` - get package from parent (default = `None`) - a `ParameterBlock` object

property_package_args A dict of arguments to be passed to the `PropertyBlockData` and used when constructing these (default = `'use_parent_value'`) - `'use_parent_value'` - get package from parent (default = `None`) - a dict (see property package for documentation)

transformation_method Discretization method to use for DAE transformation. See Pyomo documentation for supported transformations.

transformation_scheme Discretization scheme to use when transforming domain. See Pyomo documentation for supported schemes.

finite_elements Number of finite elements to use when discretizing length domain (default=20)

collocation_points Number of collocation points to use per finite element when discretizing length domain (default=3)

flow_type Flow configuration of heat exchanger - `HeatExchangerFlowPattern.cocurrent`: shell and tube flows from 0 to 1 (default) - `HeatExchangerFlowPattern.countercurrent`: shell side flows from 0 to 1 tube side flows from 1 to 0

has_wall_conduction Argument to enable type of wall heat conduction model. - `WallConductionType.zero_dimensional` - 0D wall model (default), - `WallConductionType.one_dimensional` - 1D wall model along the thickness of the tube, - `WallConductionType.two_dimensional` - 2D wall model along the length and thickness of the tube

- **initialize** (*dict*) – `ProcessBlockData` config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.

- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (HeatExchanger1D) New instance

HeatExchanger1dDataClass

class `idaes.generic_models.unit_models.heat_exchanger_1D.HeatExchanger1DData` (*component*)
Standard Heat Exchanger 1D Unit Model Class.

build ()

Begin building model (pre-DAE transformation).

Parameters None –

Returns None

initialize (*shell_state_args=None, tube_state_args=None, outlvl=0, solver='ipopt', optarg={'tol': 1e-06}*)

Initialization routine for the unit (default solver ipopt).

Keyword Arguments

- **state_args** – a dict of arguments to be passed to the property package(s) to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={ 'tol': 1e-6})
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')

Returns None

Mixer

The IDAES Mixer unit model represents operations where multiple streams of material are combined into a single flow. The Mixer class can be used to create either a stand-alone mixer unit, or as part of a unit model where multiple streams need to be mixed.

Degrees of Freedom

Mixer units have zero degrees of freedom.

Model Structure

The IDAES Mixer unit model does not use ControlVolumes, and instead writes a set of material, energy and momentum balances to combine the inlet streams into a single mixed stream. Mixer models have a user-defined number of inlet Ports (by default named inlet_1, inlet_2, etc.) and one outlet Port (named outlet).

Mixed State Block

If a mixed state block is provided in the construction arguments, the Mixer model will use this as the StateBlock for the mixed stream in the resulting balance equations. This allows a Mixer unit to be used as part of a larger unit operation by linking multiple inlet streams to a single existing StateBlock.

Variables

Mixer units have the following variables (i indicates index by inlet):

Variable Name	Sym- bol	Notes
phase_equilibrium_generation	$X_{eq,t,r}$	Only if has_phase_equilibrium = True, Generation term for phase equilibrium
minimum_pressure	$P_{min,t,i}$	Only if momentum_mixing_type = MomemntumMixingType.minimize

Parameters

Mixer units have the following parameters:

Variable Name	Sym- bol	Notes
eps_pressure	ϵ	Only if momentum_mixing_type = MomemntumMixingType.minimize, smooth minimum parameter

Constraints

The constraints written by the Mixer model depend upon the construction arguments chosen.

If *material_mixing_type* is *extensive*:

- If *material_balance_type* is *componentPhase*:

material_mixing_equations(t, p, j):

$$0 = \sum_i F_{in,i,p,j} - F_{out,p,j} + \sum_r n_{r,p,j} \times X_{eq,t,r}$$

- If *material_balance_type* is *componentTotal*:

material_mixing_equations(t, j):

$$0 = \sum_p \left(\sum_i F_{in,i,p,j} - F_{out,p,j} + \sum_r n_{r,p,j} \times X_{eq,t,r} \right)$$

- If *material_balance_type* is *total*:

material_mixing_equations(t):

$$0 = \sum_p \sum_j \left(\sum_i F_{in,i,p,j} - F_{out,p,j} + \sum_r n_{r,p,j} \times X_{eq,t,r} \right)$$

where $n_{r,p,j}$ is the stoichiometric coefficient of component j in phase p in reaction r .

If 'energy_mixing_type' is *extensive*:

enthalpy_mixing_equations(t):

$$0 = \sum_i \sum_p H_{in,i,p} - \sum_p H_{out,p}$$

If 'momentum_mixing_type' is *minimize*, a series of smooth minimum operations are performed:

minimum_pressure_constraint(t, i):

For the first inlet:

$$P_{min,t,i} = P_{t,i}$$

Otherwise:

$$P_{min,t,i} = \text{smín}(P_{min,t,i-1}, P_{t,i}, \text{eps})$$

Here, $P_{t,i}$ is the pressure in inlet i at time t , $P_{min,t,i}$ is the minimum pressure in all inlets up to inlet i , and smín is the smooth minimum operator (see IDAES Utility Function documentation).

The minimum pressure in all inlets is then:

mixture_pressure(t):

$$P_{mix,t} = P_{min,t,i=last}$$

If *momentum_mixing_type* is *equality*, the pressure in all inlets and the outlet are equated.

Note: This may result in an over-specified problem if the user is not careful.

pressure_equality_constraints(t, i):

$$P_{mix,t} = P_{t,i}$$

Often the minimum inlet pressure constraint is useful for sequential modular type initialization, but the equal pressure constants are required for pressure-driven flow models. In these cases it may be convenient to use the minimum pressure constraint for some initialization steps, then deactivate it and use the equal pressure constraints. The *momentum_mixing_type* is *minimum_and_equality* this will create the constraints for both with the minimum pressure constraint being active.

The *mixture_pressure(t)* and *pressure_equality_constraints(t, i)* can be directly activated and deactivated, but only one set of constraints should be active at a time. The `use_minimum_inlet_pressure_constraint()` and `use_equal_pressure_constraint()` methods are also provided to switch between constant sets.

Mixer Class

```
class idaes.generic_models.unit_models.mixer.Mixer(*args, **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = False. Mixer blocks are always steady-state.

has_holdup Mixer blocks do not contain holdup, thus this must be False.

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

inlet_list A list containing names of inlets, **default** - None. **Valid values:** { **None** - use num_inlets argument, **list** - a list of names to use for inlets. }

num_inlets Argument indicating number (int) of inlets to construct, not used if inlet_list arg is provided, **default** - None. **Valid values:** { **None** - use inlet_list arg instead, or default to 2 if neither argument provided, **int** - number of inlets to create (will be named with sequential integers from 1 to num_inlets). }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type, **MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

has_phase_equilibrium Argument indicating whether phase equilibrium should be calculated for the resulting mixed stream, **default** - False. **Valid values:** { **True** - calculate phase equilibrium in mixed stream, **False** - do not calculate equilibrium in mixed stream. }

energy_mixing_type Argument indicating what method to use when mixing energy flows of incoming streams, **default** - MixingType.extensive. **Valid values:** { **MixingType.none** - do not include energy mixing equations, **MixingType.extensive** - mix total enthalpy flows of each phase. }

momentum_mixing_type Argument indicating what method to use when mixing momentum/ pressure of incoming streams, **default** - MomentumMixingType.minimize. **Valid values:** { **MomentumMixingType.none** - do not include momentum mixing equations, **MomentumMixingType.minimize** - mixed stream has pressure equal to the minimum pressure of the incoming streams (uses smoothMin operator), **MomentumMixingType.equality** - enforces equality of pressure in mixed and all incoming streams., **MomentumMixingType.minimize_and_equality** - add constraints for pressure equal to the minimum pressure of the inlets and constraints for equality of pressure in mixed and all incoming streams. When the model is initially built, the equality constraints are deactivated. This option is useful for switching between flow and pressure driven simulations. }

mixed_state_block An existing state block to use as the outlet stream from the Mixer block, **default** - None. **Valid values:** { **None** - create a new StateBlock for the mixed stream, **StateBlock** - a StateBlock to use as the destination for the mixed stream. }

construct_ports Argument indicating whether model should construct Port objects linked to all inlet states and the mixed state, **default** - True. **Valid values:** { **True** - construct Ports for all states, **False** - do not construct Ports. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.

- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (Mixer) New instance

MixerData Class

class `idaes.generic_models.unit_models.mixer.MixerData` (*component*)

This is a general purpose model for a Mixer block with the IDAES modeling framework. This block can be used either as a stand-alone Mixer unit operation, or as a sub-model within another unit operation.

This model creates a number of StateBlocks to represent the incoming streams, then writes a set of phase-component material balances, an overall enthalpy balance and a momentum balance (2 options) linked to a mixed-state StateBlock. The mixed-state StateBlock can either be specified by the user (allowing use as a sub-model), or created by the Mixer.

When being used as a sub-model, Mixer should only be used when a set of new StateBlocks are required for the streams to be mixed. It should not be used to mix streams from multiple ControlVolumes in a single unit model - in these cases the unit model developer should write their own mixing equations.

add_energy_mixing_equations (*inlet_blocks, mixed_block*)

Add energy mixing equations (total enthalpy balance).

add_inlet_state_blocks (*inlet_list*)

Construct StateBlocks for all inlet streams.

Parameters of strings to use as StateBlock names (*list*) –

Returns list of StateBlocks

add_material_mixing_equations (*inlet_blocks, mixed_block, mb_type*)

Add material mixing equations.

add_mixed_state_block ()

Constructs StateBlock to represent mixed stream.

Returns New StateBlock object

add_port_objects (*inlet_list, inlet_blocks, mixed_block*)

Adds Port objects if required.

Parameters

- **list of inlet StateBlock objects** (*a*) –
- **mixed state StateBlock object** (*a*) –

Returns None

add_pressure_equality_equations (*inlet_blocks, mixed_block*)

Add pressure equality equations. Note that this writes a number of constraints equal to the number of inlets, enforcing equality between all inlets and the mixed stream.

add_pressure_minimization_equations (*inlet_blocks, mixed_block*)

Add pressure minimization equations. This is done by sequential comparisons of each inlet to the minimum pressure so far, using the IDAES smooth minimum function.

build ()

General build method for MixerData. This method calls a number of sub-methods which automate the construction of expected attributes of unit models.

Inheriting models should call *super().build*.

Parameters None –

Returns None

create_inlet_list ()

Create list of inlet stream names based on config arguments.

Returns list of strings

get_mixed_state_block ()

Validates StateBlock provided in user arguments for mixed stream.

Returns The user-provided StateBlock or an Exception

initialize (outlvl=6, optarg={}, solver='ipopt', hold_state=False)

Initialization routine for mixer (default solver ipopt)

Keyword Arguments

- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={})
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')
- **hold_state** – flag indicating whether the initialization routine should unfix any state variables fixed during initialization, **default** - False. **Valid values:** **True** - states variables are not unfixed, and a dict of returned containing flags for which states were fixed during initialization, **False** - state variables are unfixed after initialization by calling the `release_state` method.

Returns If hold_states is True, returns a dict containing flags for which states were fixed during initialization.

model_check ()

This method executes the `model_check` methods on the associated state blocks (if they exist). This method is generally called by a unit model as part of the unit's `model_check` method.

Parameters None –

Returns None

release_state (flags, outlvl=0)

Method to release state variables fixed during initialization.

Keyword Arguments

- **flags** – dict containing information of which state variables were fixed during initialization, and should now be unfixed. This dict is returned by `initialize` if `hold_state = True`.
- **outlvl** – sets output level of logging

Returns None

use_equal_pressure_constraint ()

Deactivate the mixer pressure = minimum inlet pressure constraint and activate the mixer pressure and all inlet pressures are equal constraints. This should only be used when `momentum_mixing_type == MomentumMixingType.minimize_and_equality`.

use_minimum_inlet_pressure_constraint ()

Activate the mixer pressure = minimum inlet pressure constraint and deactivate the mixer pressure and all inlet pressures are equal constraints. This should only be used when `momentum_mixing_type == MomentumMixingType.minimize_and_equality`.

Plug Flow Reactor

The IDAES Plug Flow Reactor (PFR) model represents a unit operation where a material stream passes through a linear reactor vessel whilst undergoing some chemical reaction(s). This model requires modeling the system in one spatial dimension.

Degrees of Freedom

PFRs generally have at least 2 degrees of freedom.

Typical fixed variables are:

- 2 of reactor length, area and volume.

Model Structure

The core PFR unit model consists of a single `ControlVolume1DBlock` (named `control_volume`) with one Inlet Port (named `inlet`) and one Outlet Port (named `outlet`).

Variables

PFR units add the following additional Variables:

Variable	Name	Notes
L	length	Reference to <code>control_volume.length</code>
A	area	Reference to <code>control_volume.area</code>
V	volume	Reference to <code>control_volume.volume</code>
$Q_{t,x}$	heat	Only if <code>has_heat_transfer = True</code> , reference to <code>holdup.heat</code>
$\Delta P_{t,x}$	deltaP	Only if <code>has_pressure_change = True</code> , reference to <code>holdup.deltaP</code>

Constraints

PFR units write the following additional Constraints at all points in the spatial domain:

$$X_{t,x,r} = A \times r_{t,x,r}$$

where $X_{t,x,r}$ is the extent of reaction of reaction r at point x and time t , A is the cross-sectional area of the reactor and $r_{t,r}$ is the volumetric rate of reaction of reaction r at point x and time t (from the outlet `StateBlock`).

PFR Class

```
class idaes.generic_models.unit_models.plug_flow_reactor.PFR(*args, **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls `build()`.
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default `ProcessBlockData` config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.useDefault. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - MomentumBalanceType.pressureTotal. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_equilibrium_reactions Indicates whether terms for equilibrium controlled reactions should be constructed, **default** - True. **Valid values:** { **True** - include equilibrium reaction terms, **False** - exclude equilibrium reaction terms. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = False. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms. }

has_heat_of_reaction Indicates whether terms for heat of reaction terms should be constructed, **default** - False. **Valid values:** { **True** - include heat of reaction terms, **False** - exclude heat of reaction terms. }

has_heat_transfer Indicates whether terms for heat transfer should be constructed, **default** - False. **Valid values:** { **True** - include heat transfer terms, **False** - exclude heat transfer terms. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - False. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms. }

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation.}

reaction_package Reaction parameter object used to define reaction calculations, **default** - None. **Valid values:** { **None** - no reaction package, **ReactionParameterBlock** - a ReactionParameterBlock object.}

reaction_package_args A ConfigBlock with arguments to be passed to a reaction block(s) and used when constructing these, **default** - None. **Valid values:** { see reaction package for documentation.}

length_domain_set A list of values to be used when constructing the length domain of the reactor. Point must lie between 0.0 and 1.0, **default** - [0.0, 1.0]. **Valid values:** { a list of floats }

transformation_method Method to use to transform domain. Must be a method recognised by the Pyomo TransformationFactory, **default** - "dae.finite_difference".

transformation_scheme Scheme to use when transforming domain. See Pyomo documentation for supported schemes, **default** - "BACKWARD".

finite_elements Number of finite elements to use when transforming length domain, **default** - 20.

collocation_points Number of collocation points to use when transforming length domain, **default** - 3.

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the "default" argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (PFR) New instance

PFRData Class

class `idaes.generic_models.unit_models.plug_flow_reactor.PFRData` (*component*)
Standard Plug Flow Reactor Unit Model Class

build ()
Begin building model (pre-DAE transformation).

Parameters **None** –

Returns **None**

Pressure Changer

The IDAES Pressure Changer model represents a unit operation with a single stream of material which undergoes a change in pressure due to the application of a work. The Pressure Changer model contains support for a number of different thermodynamic assumptions regarding the working fluid.

Degrees of Freedom

Pressure Changer units generally have one or more degrees of freedom, depending on the thermodynamic assumption used.

Typical fixed variables are:

- outlet pressure, P_{ratio} or ΔP ,
- unit efficiency (isentropic or pump assumption).

Model Structure

The core Pressure Changer unit model consists of a single `ControlVolume0D` (named `control_volume`) with one Inlet Port (named `inlet`) and one Outlet Port (named `outlet`). Additionally, if an isentropic pressure changer is used, the unit model contains an additional `StateBlock` named `properties_isentropic` at the unit model level.

Variables

Pressure Changers contain the following Variables (not including those contained within the control volume Block):

Variable	Name	Notes
P_{ratio}	ratioP	
V_t	volume	Only if <code>has_rate_reactions = True</code> , reference to <code>control_volume.rate_reaction_extent</code>
$W_{mechanical,t}$	work_mechanical	Reference to <code>control_volume.work</code>
$W_{fluid,t}$	work_fluid	Pump assumption only
$\eta_{pump,t}$	efficiency_pump	Pump assumption only
$W_{isentropic,t}$	work_isentropic	Isentropic assumption only
$\eta_{isentropic,t}$	efficiency_isentropic	Isentropic assumption only

Isentropic Pressure Changers also have an additional Property Block named `properties_isentropic` (attached to the Unit Model).

Constraints

In addition to the Constraints written by the Control Volume block, Pressure Changer writes additional Constraints which depend on the thermodynamic assumption chosen. All Pressure Changers add the following Constraint to calculate the pressure ratio:

$$P_{ratio,t} \times P_{in,t} = P_{out,t}$$

Isothermal Assumption

The isothermal assumption writes one additional Constraint:

$$T_{out} = T_{in}$$

Adiabatic Assumption

The isothermal assumption writes one additional Constraint:

$$H_{out} = H_{in}$$

Isentropic Assumption

The isentropic assumption creates an additional set of Property Blocks (indexed by time) for the isentropic fluid calculations (named `properties_isentropic`). This requires a set of balance equations relating the inlet state to the isentropic conditions, which are shown below:

$$F_{in,t,p,j} = F_{isentropic,t,p,j}$$

$$s_{in,t} = s_{isentropic,t}$$

$$P_{in,t} \times P_{ratio,t} = P_{isentropic,t}$$

where $F_{t,p,j}$ is the flow of component j in phase p at time t and s is the specific entropy of the fluid at time t .

Next, the isentropic work is calculated as follows:

$$W_{isentropic,t} = \sum_p H_{isentropic,t,p} - \sum_p H_{in,t,p}$$

where $H_{t,p}$ is the total energy flow of phase p at time t . Finally, a constraint which relates the fluid work to the actual mechanical work via an efficiency term η .

If compressor is True, $W_{isentropic,t} = W_{mechanical,t} \times \eta_t$

If compressor is False, $W_{isentropic,t} \times \eta_t = W_{mechanical,t}$

Pump (Incompressible Fluid) Assumption

The incompressible fluid assumption writes two additional constraints. Firstly, a Constraint is written which relates fluid work to the pressure change of the fluid.

$$W_{fluid,t} = (P_{out,t} - P_{in,t}) \times F_{vol,t}$$

where $F_{vol,t}$ is the total volumetric flowrate of material at time t (from the outlet Property Block). Secondly, a constraint which relates the fluid work to the actual mechanical work via an efficiency term η .

If compressor is True, $W_{fluid,t} = W_{mechanical,t} \times \eta_t$

If compressor is False, $W_{fluid,t} \times \eta_t = W_{mechanical,t}$

PressureChanger Class

```
class idaes.generic_models.unit_models.pressure_changer.PressureChanger (*args,  
                                                                    **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls `build()`.
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.

- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.

Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.useDefault. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - MomentumBalanceType.pressureTotal. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = False. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms. }

compressor Indicates whether this unit should be considered a compressor (True (default), pressure increase) or an expander (False, pressure decrease).

thermodynamic_assumption Flag to set the thermodynamic assumption to use for the unit. - ThermodynamicAssumption.isothermal (default) - ThermodynamicAssumption.isentropic - ThermodynamicAssumption.pump - ThermodynamicAssumption.adiabatic

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

- **initialize**(*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map**(*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (PressureChanger) New instance

PressureChangerData Class

class `idaes.generic_models.unit_models.pressure_changer.PressureChangerData` (*component*)
Standard Compressor/Expander Unit Model Class

add_adiabatic()

Add constraints for adiabatic assumption.

Parameters **None** –

Returns **None**

add_isentropic()

Add constraints for isentropic assumption.

Parameters **None** –

Returns **None**

add_isothermal()

Add constraints for isothermal assumption.

Parameters **None** –

Returns **None**

add_pump()

Add constraints for the incompressible fluid assumption

Parameters **None** –

Returns **None**

build()

Parameters **None** –

Returns **None**

init_isentropic(*state_args, outlvl, solver, optarg*)

Initialization routine for unit (default solver ipopt)

Keyword Arguments

- **state_args** – a dict of arguments to be passed to the property package(s) to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={ ‘tol’: 1e-6})
- **solver** – str indicating which solver to use during initialization (default = ‘ipopt’)

Returns **None**

initialize (*state_args=None, routine=None, outlvl=0, solver='ipopt', optarg={'tol': 1e-06}*)

General wrapper for pressure changer initialization routines

Keyword Arguments

- **routine** – str stating which initialization routine to execute * None - use routine matching thermodynamic_assumption * 'isentropic' - use isentropic initialization routine * 'isothermal' - use isothermal initialization routine
- **state_args** – a dict of arguments to be passed to the property package(s) to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={'tol': 1e-6})
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')

Returns None

model_check ()

Check that pressure change matches with compressor argument (i.e. if compressor = True, pressure should increase or work should be positive)

Parameters None –

Returns None

Product Block

Product Blocks are used to represent sinks of material in Flowsheets. These can be used as a convenient way to mark the final destination of a material stream and to view the state of that material.

Degrees of Freedom

Product blocks generally have zero degrees of freedom.

Model Structure

Product Blocks consists of a single StateBlock (named properties), each with one Inlet Port (named inlet). Product Blocks also contain References to the state variables defined within the StateBlock

Additional Constraints

Product Blocks write no additional constraints to the model.

Variables

Product blocks add no additional Variables.

Product Class

```
class idaes.generic_models.unit_models.product.Product(*args, **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = False. Product blocks are always steady- state.

has_holdup Product blocks do not contain holdup, thus this must be False.

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PhysicalParameterObject** - a PhysicalParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (Product) New instance

ProductData Class

```
class idaes.generic_models.unit_models.product.ProductData(component)
```

Standard Product Block Class

build()

Begin building model.

Parameters None –

Returns None

initialize (*state_args={}*, *outlvl=0*, *solver='ipopt'*, *optarg={'tol': 1e-06}*)

This method calls the initialization method of the state block.

Keyword Arguments

- **state_args** – a dict of arguments to be passed to the property package(s) to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={ ‘tol’: 1e-6})
- **solver** – str indicating which solver to use during initialization (default = ‘ipopt’)

Returns None

Pump

The Pump model is a *PressureChanger*, where the configuration is set so that the “compressor” option can only be True, and the default “thermodynamic_assumption” is “pump.” See the *PressureChanger documentation* for details.

Example

The example below demonstrates the basic Pump model usage:

```
import pyomo.environ as pyo
from idaes.core import FlowsheetBlock
from idaes.generic_models.unit_models import Pump
from idaes.generic_models.properties import iapws95

m = pyo.ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": False})
m.fs.properties = iapws95.Iapws95ParameterBlock()
m.fs.unit = Pump(default={"property_package": m.fs.properties})

m.fs.unit.inlet.flow_mol[0].fix(100)
m.fs.unit.inlet.enth_mol[0].fix(2000)
m.fs.unit.inlet.pressure[0].fix(101325)

m.fs.unit.deltaP.fix(100000)
m.fs.unit.eta_pump.fix(0.8)
```

Separator

The IDAES Separator unit model represents operations where a single stream is split into multiple flows. The Separator model supports separation using split fractions, or by ideal separation of flows. The Separator class can be used to create either a stand-alone separator unit, or as part of a unit model where a flow needs to be separated.

Degrees of Freedom

Separator units have a number of degrees of freedom based on the separation type chosen.

- If *split_basis* = ‘phaseFlow’, degrees of freedom are generally $(no.outlets - 1) \times no.phases$
- If *split_basis* = ‘componentFlow’, degrees of freedom are generally $(no.outlets - 1) \times no.components$
- If *split_basis* = ‘phaseComponentFlow’, degrees of freedom are generally $(no.outlets - 1) \times no.phases \times no.components$
- If *split_basis* = ‘totalFlow’, degrees of freedom are generally $(no.outlets - 1) \times no.phases \times no.components$

Typical fixed variables are:

- split fractions.

Model Structure

The IDAES Separator unit model does not use ControlVolumes, and instead writes a set of material, energy and momentum balances to split the inlet stream into a number of outlet streams. Separator models have a single inlet Port (named inlet) and a user-defined number of outlet Ports (by default named outlet_1, outlet_2, etc.).

Mixed State Block

If a mixed state block is provided in the construction arguments, the Mixer model will use this as the StateBlock for the mixed stream in the resulting balance equations. This allows a Mixer unit to be used as part of a larger unit operation by linking to an existing StateBlock.

Ideal Separation

The IDAES Separator model supports ideal separations, where all of a given subset of the mixed stream is sent to a single outlet (i.e. split fractions are equal to zero or one). In these cases, no Constraints are necessary for performing the separation, as the mixed stream states can be directly partitioned to the outlets.

Ideal separations will not work for all choices of state variables, and thus will not work for all property packages. To use ideal separations, the user must provide a map of what part of the mixed flow should be partitioned to each outlet. The *ideal_split_map* should be a dict-like object with keys as tuples matching the *split_basis* argument and values indicating which outlet this subset should be partitioned to.

Variables

Separator units have the following variables (*o* indicates index by outlet):

Variable Name	Symbol	Notes
split_fraction	$\phi_{t,o,*}$	Indexing sets depend upon <i>split_basis</i>

Constraints

Separator units have the following Constraints, unless *ideal_separation* is True.

- If *material_balance_type* is *componentPhase*:

material_splitting_eqn(*t*, *o*, *p*, *j*):

$$F_{in,t,p,j} = \phi_{t,p,*} \times F_{t,o,p,j}$$

- If *material_balance_type* is *componentTotal*:

material_splitting_eqn(*t*, *o*, *j*):

$$\sum_p F_{in,t,p,j} = \sum_p \phi_{t,p,*} \times F_{t,o,p,j}$$

- If *material_balance_type* is *total*:

material_splitting_eqn(*t*, *o*):

$$\sum_p \sum_j F_{in,t,p,j} = \sum_p \sum_j \phi_{t,p,*} \times F_{t,o,p,j}$$

If *energy_split_basis* is *equal_temperature*:

temperature_equality_eqn(t, o):

$$T_{in,t} = T_{t,o}$$

If *energy_split_basis* is *equal_molar_enthalpy*:

molar_enthalpy_equality_eqn(t, o):

$$h_{in,t} = h_{t,o}$$

If *energy_split_basis* is *enthalpy_split*:

molar_enthalpy_splitting_eqn(t, o):

$$\sum_p h_{in,t,p} * sf_{t,o,p} = \sum_p h_{t,o,p}$$

pressure_equality_eqn(t, o):

$$P_{in,t} = P_{t,o}$$

Separator Class

class `idaes.generic_models.unit_models.separator.Separator(*args, **kwargs)`

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = False. Product blocks are always steady- state.

has_holdup Product blocks do not contain holdup, thus this must be False.

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

outlet_list A list containing names of outlets, **default** - None. **Valid values:** { **None** - use num_outlets argument, **list** - a list of names to use for outlets. }

num_outlets Argument indicating number (int) of outlets to construct, not used if outlet_list arg is provided, **default** - None. **Valid values:** { **None** - use outlet_list arg instead, or default to 2 if neither argument provided, **int** - number of outlets to create (will be named with sequential integers from 1 to num_outlets). }

split_basis Argument indicating basis to use for splitting mixed stream, **default** - SplittingType.totalFlow. **Valid values:** { **SplittingType.totalFlow** - split based on total flow (split fraction indexed only by time and outlet), **SplittingType.phaseFlow** - split

based on phase flows (split fraction indexed by time, outlet and phase), **SplittingType.componentFlow** - split based on component flows (split fraction indexed by time, outlet and components), **SplittingType.phaseComponentFlow** - split based on phase-component flows (split fraction indexed by both time, outlet, phase and components).}

material_balance_type Indicates what type of mass balance should be constructed, **default** - `MaterialBalanceType.useDefault`. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

has_phase_equilibrium Argument indicating whether phase equilibrium should be calculated for the resulting mixed stream, **default** - `False`. **Valid values:** { **True** - calculate phase equilibrium in mixed stream, **False** - do not calculate equilibrium in mixed stream. }

energy_split_basis Argument indicating basis to use for splitting energy this is not used for when `ideal_separation == True`. **default** - `EnergySplittingType.equal_temperature`. **Valid values:** { **EnergySplittingType.equal_temperature** - outlet temperatures equal inlet **EnergySplittingType.equal_molar_enthalpy** - outlet molar enthalpies equal inlet, **EnergySplittingType.enthalpy_split** - apply split fractions to enthalpy flows. Does not work with component or phase-component splitting. }

ideal_separation Argument indicating whether ideal splitting should be used. Ideal splitting assumes perfect separation of material, and attempts to avoid duplication of `StateBlocks` by directly partitioning outlet flows to ports, **default** - `False`. **Valid values:** { **True** - use ideal splitting methods. Cannot be combined with `has_phase_equilibrium = True`, **False** - use explicit splitting equations with split fractions. }

ideal_split_map Dictionary containing information on how extensive variables should be partitioned when using ideal splitting (`ideal_separation = True`). **default** - `None`. **Valid values:** { **dict** with keys of indexing set members and values indicating which outlet this combination of keys should be partitioned to. E.g. {("Vap", "H2"): "outlet_1"} }

mixed_state_block An existing state block to use as the source stream from the Separator block, **default** - `None`. **Valid values:** { **None** - create a new `StateBlock` for the mixed stream, **StateBlock** - a `StateBlock` to use as the source for the mixed stream. }

construct_ports Argument indicating whether model should construct Port objects linked the mixed state and all outlet states, **default** - `True`. **Valid values:** { **True** - construct Ports for all states, **False** - do not construct Ports. }

- **initialize** (*dict*) – `ProcessBlockData` config for individual elements. Keys are `BlockData` indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a `BlockData` element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the `BlockData` index exactly to the index in initialize.

Returns (Separator) New instance

SeparatorData Class

class `idaes.generic_models.unit_models.separator.SeparatorData` (*component*)

This is a general purpose model for a Separator block with the IDAES modeling framework. This block can be used either as a stand-alone Separator unit operation, or as a sub-model within another unit operation.

This model creates a number of StateBlocks to represent the outgoing streams, then writes a set of phase-component material balances, an overall enthalpy balance (2 options), and a momentum balance (2 options) linked to a mixed-state StateBlock. The mixed-state StateBlock can either be specified by the user (allowing use as a sub-model), or created by the Separator.

When being used as a sub-model, Separator should only be used when a set of new StateBlocks are required for the streams to be separated. It should not be used to separate streams to go to multiple ControlVolumes in a single unit model - in these cases the unit model developer should write their own splitting equations.

add_energy_splitting_constraints (*mixed_block*)

Creates constraints for splitting the energy flows - done by equating temperatures in outlets.

add_inlet_port_objects (*mixed_block*)

Adds inlet Port object if required.

Parameters *mixed state StateBlock object* (*a*) –

Returns None

add_material_splitting_constraints (*mixed_block*)

Creates constraints for splitting the material flows

add_mixed_state_block ()

Constructs StateBlock to represent mixed stream.

Returns New StateBlock object

add_momentum_splitting_constraints (*mixed_block*)

Creates constraints for splitting the momentum flows - done by equating pressures in outlets.

add_outlet_port_objects (*outlet_list*, *outlet_blocks*)

Adds outlet Port objects if required.

Parameters *list of outlet StateBlock objects* (*a*) –

Returns None

add_outlet_state_blocks (*outlet_list*)

Construct StateBlocks for all outlet streams.

Parameters *of strings to use as StateBlock names* (*list*) –

Returns list of StateBlocks

add_split_fractions (*outlet_list*)

Creates outlet Port objects and tries to partition mixed stream flows between these

Parameters

- *representing the mixed flow to be split* (*StateBlock*) –
- *list of names for outlets* (*a*) –

Returns None

build ()

General build method for SeparatorData. This method calls a number of sub-methods which automate the construction of expected attributes of unit models.

Inheriting models should call *super().build*.

Parameters None –

Returns None

create_outlet_list ()

Create list of outlet stream names based on config arguments.

Returns list of strings

get_mixed_state_block ()

Validates StateBlock provided in user arguments for mixed stream.

Returns The user-provided StateBlock or an Exception

initialize (outlvl=0, optarg={}, solver='ipopt', hold_state=False)

Initialization routine for separator (default solver ipopt)

Keyword Arguments

- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default=None)
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')
- **hold_state** – flag indicating whether the initialization routine should unfix any state variables fixed during initialization, **default** - False. **Valid values:** **True** - states variables are not unfixed, and a dict of returned containing flags for which states were fixed during initialization, **False** - state variables are unfixed after initialization by calling the *release_state* method.

Returns If hold_states is True, returns a dict containing flags for which states were fixed during initialization.

model_check ()

This method executes the *model_check* methods on the associated state blocks (if they exist). This method is generally called by a unit model as part of the unit's *model_check* method.

Parameters None –

Returns None

partition_outlet_flows (mb, outlet_list)

Creates outlet Port objects and tries to partition mixed stream flows between these

Parameters

- **representing the mixed flow to be split** (StateBlock) –
- **list of names for outlets** (a) –

Returns None

release_state (flags, outlvl=0)

Method to release state variables fixed during initialization.

Keyword Arguments

- **flags** – dict containing information of which state variables were fixed during initialization, and should now be unfixed. This dict is returned by *initialize* if *hold_state* = True.
- **outlvl** – sets output level of logging

Returns None

StateJunction Block

The IDAES StateJunction block represents a pass-through unit or simple pipe with no holdup. The primary use for this unit is in conceptual design applications for linking Arcs to/from different process alternatives.

Degrees of Freedom

StateJunctions have no degrees of freedom.

Model Structure

A StateJunction consists of a single StateBlock with two Ports (inlet and outlet), where the state variables in the state block are simultaneously connected to both Ports.

Additional Constraints

StateJunctions write no additional constraints beyond those in the StateBlock.

Variables

StateJunctions have no additional variables.

StateJunction Class

```
class idaes.generic_models.unit_models.statejunction.StateJunction(*args,
                                                                    **kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

- dynamic** Indicates whether this unit will be dynamic or not, **default** = False.
- has_holdup** Indicates whether holdup terms should be constructed or not. **default** - False. StateJunctions do not have defined volume, thus this must be False.
- property_package** Property parameter object used to define property state block, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PhysicalParameterObject** - a PhysicalParameterBlock object. }
- property_package_args** A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }
- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.

- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (StateJunction) New instance

StateJunctionData Class

class `idaes.generic_models.unit_models.statejunction.StateJunctionData` (*component*)
Standard StateJunction Unit Model Class

build ()

Begin building model. :param None:

Returns None

initialize (*state_args={}*, *outlvl=0*, *solver='ipopt'*, *optarg={'tol': 1e-06}*)

This method initializes the StateJunction block by calling the initialize method on the property block.

Keyword Arguments

- **state_args** – a dict of arguments to be passed to the property package(s) to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={'tol': 1e-6})
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')

Returns None

Stoichiometric (Yield) Reactor

The IDAES Stoichiometric reactor model represents a unit operation where a single material stream undergoes some chemical reaction(s) subject to a set of extent or yield specifications.

Degrees of Freedom

Stoichiometric reactors generally have degrees of freedom equal to the number of reactions + 1.

Typical fixed variables are:

- reaction extents or yields (1 per reaction),
- reactor heat duty (has_heat_transfer = True only).

Model Structure

The core Stoichiometric reactor unit model consists of a single ControlVolume0DBlock (named control_volume) with one Inlet Port (named inlet) and one Outlet Port (named outlet).

Variables

Stoichiometric reactors units add the following variables:

Variable	Name	Notes
Q_t	heat	Only if has_heat_transfer = True, reference to control_volume.heat
ΔP_t	pressure change	Only if has_pressure_change = True, reference to control_volume.deltaP

Constraints

Stoichiometric reactor units write no additional Constraints beyond those written by the control_volume Block.

StoichiometricReactor Class

```
class idaes.generic_models.unit_models.stoichiometric_reactor.StoichiometricReactor(*args,
**kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.
Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.useDefault. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { **`MomentumBalanceType.none`** - exclude momentum balances, **`MomentumBalanceType.pressureTotal`** - single pressure balance for material, **`MomentumBalanceType.pressurePhase`** - pressure balances for each phase, **`MomentumBalanceType.momentumTotal`** - single momentum balance for material, **`MomentumBalanceType.momentumPhase`** - momentum balances for each phase. }

has_heat_of_reaction Indicates whether terms for heat of reaction terms should be constructed, **default** - `False`. **Valid values:** { **`True`** - include heat of reaction terms, **`False`** - exclude heat of reaction terms. }

has_heat_transfer Indicates whether terms for heat transfer should be constructed, **default** - `False`. **Valid values:** { **`True`** - include heat transfer terms, **`False`** - exclude heat transfer terms. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - `False`. **Valid values:** { **`True`** - include pressure change terms, **`False`** - exclude pressure change terms. }

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { **`useDefault`** - use default package from parent model or flowsheet, **`PropertyParameterObject`** - a `PropertyParameterBlock` object. }

property_package_args A `ConfigBlock` with arguments to be passed to a property block(s) and used when constructing these, **default** - `None`. **Valid values:** { see property package for documentation. }

reaction_package Reaction parameter object used to define reaction calculations, **default** - `None`. **Valid values:** { **`None`** - no reaction package, **`ReactionParameterBlock`** - a `ReactionParameterBlock` object. }

reaction_package_args A `ConfigBlock` with arguments to be passed to a reaction block(s) and used when constructing these, **default** - `None`. **Valid values:** { see reaction package for documentation. }

- **`initialize(dict)`** – `ProcessBlockData` config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **`idx_map(function)`** – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (`StoichiometricReactor`) New instance

StoichiometricReactorData Class

class `idaes.generic_models.unit_models.stoichiometric_reactor.StoichiometricReactorData` (`com`)
Standard Stoichiometric Reactor Unit Model Class This model assumes that all given reactions are irreversible, and that each reaction has a fixed `rate_reaction` extent which has to be specified by the user.

build()

Begin building model (pre-DAE transformation). :param `None`:

Returns `None`

Translator Block

Translator blocks are used in complex flowsheets where the user desires to use different property packages for different parts of the flowsheet. In order to link two streams using different property packages, a translator block is required.

The core translator block provides a general framework for constructing Translator Blocks, however users need to add constraints to map the incoming states to the outgoing states as required by their specific application.

Degrees of Freedom

The degrees of freedom of Translator blocks depends on the property packages being used, and the user should write a sufficient number of constraints mapping inlet states to outlet states to satisfy these degrees of freedom.

Model Structure

The core Translator Block consists of two State Blocks, names `properties_in` and `properties_out`, which are linked to two Ports names `inlet` and `outlet` respectively.

Additional Constraints

The core Translator Block writes no additional constraints. Users should add constraints to their instances as required.

Variables

Translator blocks add no additional Variables.

Translator Class

```
class idaes.generic_models.unit_models.translator.Translator(*args,**kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls `build()`.
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Translator blocks are always steady-state.

has_holdup Translator blocks do not contain holdup.

outlet_state_defined Indicates whether unit model will fully define outlet state. If False, the outlet property package will enforce constraints such as sum of mole fractions and phase equilibrium. **default** - True. **Valid values:** { **True** - outlet state will be fully defined, **False** - outlet property package should enforce summation and equilibrium constraints. }

has_phase_equilibrium Indicates whether outlet property package should enforce phase equilibrium constraints. **default** - False. **Valid values:** { **True** - outlet property package should calculate phase equilibrium, **False** - outlet property package should not calculate phase equilibrium. }

inlet_property_package Property parameter object used to define property calculations for the incoming stream, **default** - None. **Valid values:** { **PhysicalParameterObject** - a `PhysicalParameterBlock` object. }

inlet_property_package_args A `ConfigBlock` with arguments to be passed to the property block associated with the incoming stream, **default** - None. **Valid values:** { see property package for documentation. }

outlet_property_package Property parameter object used to define property calculations for the outgoing stream, **default** - None. **Valid values:** { **PhysicalParameterObject** - a `PhysicalParameterBlock` object. }

outlet_property_package_args A `ConfigBlock` with arguments to be passed to the property block associated with the outgoing stream, **default** - None. **Valid values:** { see property package for documentation. }

- **initialize** (*dict*) – `ProcessBlockData` config for individual elements. Keys are `BlockData` indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a `BlockData` element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the `BlockData` index exactly to the index in initialize.

Returns (Translator) New instance

TranslatorData Class

class `idaes.generic_models.unit_models.translator.TranslatorData` (*component*)
Standard Translator Block Class

build ()

Begin building model.

Parameters None –

Returns None

initialize (*state_args_in={}*, *state_args_out={}*, *outlvl=0*, *solver='ipopt'*, *optarg={'tol': 1e-06}*)

This method calls the initialization method of the state blocks.

Keyword Arguments

- **state_args_in** – a dict of arguments to be passed to the inlet property package (to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **state_args_out** – a dict of arguments to be passed to the outlet property package (to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialization routine
- **optarg** – solver options dictionary object (default={ 'tol': 1e-6})
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')

Returns None

Turbine

The Turbine model is a *PressureChanger*, where the configuration is set so that the “compressor” option can only be False, and the default “thermodynamic_assumption” is “isentropic.” See the *PressureChanger documentation* for details.

Example

The example below demonstrates the basic Turbine model usage:

```
import pyomo.environ as pyo
from idaes.core import FlowsheetBlock
from idaes.generic_models.unit_models import Turbine
from idaes.generic_models.properties import iapws95

m = pyo.ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": False})
m.fs.properties = iapws95.Iapws95ParameterBlock()
m.fs.unit = Turbine(default={"property_package": m.fs.properties})

m.fs.unit.inlet.flow_mol[0].fix(1000)
m.fs.unit.inlet.enthalpy[0].fix(iapws95.htpx(T=800, P=1e7))
m.fs.unit.inlet.pressure[0].fix(1e7)
m.fs.unit.deltaP.fix(-2e6)
m.fs.unit.eta_isentropic.fix(0.9)
```

Control Model Library

This section contains documentation for core IDAES control models.

Contents

Proportional-Integral-Derivative (PID) Controller

The IDAES framework contains a basic PID control implementation, which is described in this section.

Example

The following code demonstrated the creation of a PIDBlock, but for simplicity, it does not create a dynamic process model. A full example of a dynamic process with PID control is being prepared for the IDAES examples repository and will be referenced here once completed.

The valve opening is the controlled output variable and pressure “1” is the measured variable. The controller output for the valve opening is restricted to be between 0 and 1. The measured and output variables should be indexed only by time. Fortunately there is no need to create new variables if the variables are in a property block or not indexed only by time. Pyomo’s Reference objects can be used to create references to existing variables with the proper indexing as shown in the example.

The `calculate_initial_integral` option calculates the integral error in the first time step to match the initial controller output. This keeps the controller output from immediately jumping to a new value. Unless the initial integral error is known, this option should usually be True.

The controller should be added after the DAE expansion is done. There are several variables in the controller that are usually meant to be fixed; as shown in the example, they are `gain`, `time_i`, `time_d`, and `setpoint`. For more information about the variables, expressions, and parameters in the `PIDBlock`, model see [Variables and Expressions](#).

```
from idaes.generic_models.control import PIDBlock, PIDForm
from idaes.core import FlowsheetBlock
import pyomo.environ as pyo

m = pyo.ConcreteModel(name="PID Example")
m.fs = FlowsheetBlock(default={"dynamic":True, "time_set":[0,10]})

m.fs.valve_opening = pyo.Var(m.fs.time, doc="Valve opening")
m.fs.pressure = pyo.Var(m.fs.time, [1,2], doc="Pressure in unit 1 and 2")

pyo.TransformationFactory('dae.finite_difference').apply_to(
    m.fs,
    nfe=10,
    wrt=m.fs.time,
    scheme='BACKWARD',
)

m.fs.measured_variable = pyo.Reference(m.fs.pressure[:,1])

m.fs.ctrl = PIDBlock(
    default={
        "pv":m.fs.measured_variable,
        "output":m.fs.valve_opening,
        "upper":1.0,
        "lower":0.0,
        "calculate_initial_integral":True,
        "pid_form":PIDForm.velocity,
    }
)

m.fs.ctrl.gain.fix(1e-6)
m.fs.ctrl.time_i.fix(0.1)
m.fs.ctrl.time_d.fix(0.1)
m.fs.ctrl.setpoint.fix(3e5)
```

Controller Windup

The current PID controller model has no integral windup prevention. This will be added to the model in the near future.

Class Documentation

class `idaes.generic_models.control.pid_controller.PIDBlock` (*args, **kwargs)
This is a PID controller block. The PID Controller block must be added after the DAE transformation.

Args: rule (function): A rule function or None. Default rule calls `build()`. concrete (bool): If True, make this a toplevel model. **Default** - False. ctype (str): Pyomo ctype of the block. **Default** - "Block" default (dict): Default `ProcessBlockData` config

Keys

pv A Pyomo Var, Expression, or Reference for the measured process variable. Should be indexed by time.

output A Pyomo Var, Expression, or Reference for the controlled process variable. Should be indexed by time.

upper The upper limit for the controller output, default=1

lower The lower limit for the controller output, default=0

calculate_initial_integral Calculate the initial integral term value if true, otherwise provide a variable `err_i0`, which can be fixed, default=True

pid_form Velocity or standard form

initialize (dict): ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.

idx_map (function): Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns: (PIDBlock) New instance

```
class idaes.generic_models.control.pid_controller.PIDBlockData (component)
```

```
    build()
```

Build the PID block

Variables and Expressions

Symbol	Name in Model	Description
$v_{sp}(t)$	setpoint[t]	Setpoint variable (usually fixed)
$v_{mv}(t)$	pv[t]	Measured process variable reference
$u(t)$	output[t]	Controller output variable reference
$K_p(t)$	gain[t]	Controller gain (usually fixed)
$T_i(t)$	time_i[t]	Integral time (usually fixed)
$T_d(t)$	time_d[t]	Derivative time (usually fixed)
$e(t)$	err[t]	Error expression (setpoint - pv)
–	err_d[t]	Derivative error expression
–	err_i[t]	Integral error expression (standard form)
–	err_d0	Initial derivative error value (fixed)
$e_{integral}(0)$	err_i0	Initial integral error value (fixed)
–	err_i_end	Last initial integral error expression
–	limits["h"]	Upper limit of output parameter
–	limits["l"]	Lower limit of output parameter
–	smooth_eps	Smooth min/max parameter

Formulation

There are two forms of the PID controller equation. The standard formulation can result in equations with very large summations. In the velocity form of the equation the controller output can be calculated based only on the previous state.

The two forms of the equations are equivalent, but the choice of form will affect robustness and solution time. It is not necessarily clear that the velocity form of the equation is always more numerically favorable, however it would usually be the default choice. Both forms are provided in case the standard form works better in some situations.

Standard Formulation

The PID controller equations are given by the following equations

$$e(t) = v_{sp}(t) - v_{mv}(t)$$

$$u(t) = K_p \left[e(t) + \frac{1}{T_i} \int_0^t e(s) ds + T_d \frac{de(t)}{dt} \right]$$

The PID equation now must be discretized.

$$u(t_i) = K_p \left[e(t_i) + \frac{e_{integral}(0)}{T_i} + \frac{1}{T_i} \sum_{j=0}^{i-1} \Delta t_j \frac{e(t_j) + e(t_{j+1})}{2} + T_d \frac{e(t_i) - e(t_{i-1})}{\Delta t_{i-1}} \right]$$

Velocity Formulation

The velocity formulation of the PID equation may also be useful. The way the equations are written in the PID model, the integral term is a summation expression and as time increases the integral term will build up an increasing number of terms potentially becoming very large. This potentially has two affects, increasing round off error and computation time. The velocity formulation allows the controller output to be calculated based on the previous output.

First the usual PID controller equation can be rearranged to solve for the integral error.

$$\frac{1}{T_i} \int_0^t e(s) ds = \frac{u(t)}{K_p} - e(t) - T_d \frac{de(t)}{dt}$$

The PID equation for some time $(t + \Delta t)$ is

$$u(t + \Delta t) = K_p \left[e(t + \Delta t) + \frac{1}{T_i} \int_0^{t+\Delta t} e(s) ds + T_d \frac{de(t + \Delta t)}{dt} \right]$$

$$u(t + \Delta t) = K_p \left[e(t + \Delta t) + \frac{1}{T_i} \int_t^{t+\Delta t} e(s) ds + \frac{1}{T_i} \int_0^t e(s) ds + T_d \frac{de(t + \Delta t)}{dt} \right]$$

$$u(t + \Delta t) = u(t) + K_p \left[e(t + \Delta t) - e(t) + \frac{1}{T_i} \int_t^{t+\Delta t} e(s) ds + T_d \left(\frac{de(t + \Delta t)}{dt} - \frac{de(t)}{dt} \right) \right]$$

Now we can discretize the equation using the trapezoid rule for the integral.

$$u(t + \Delta t) = u(t) + K_p \left[e(t + \Delta t) - e(t) + \frac{\Delta t}{T_i} \left(\frac{e(t + \Delta t) + e(t)}{2} \right) + T_d \left(\frac{de(t + \Delta t)}{dt} - \frac{de(t)}{dt} \right) \right]$$

Since the derivative error term will require the error at the previous time step to calculate, this form will still result in a large summation being formed since in the model there is no derivative error variable. To avoid this problem, the derivative error term can equivalently be replaced with the derivative of the negative measured process variable.

$$u(t + \Delta t) = u(t) + K_p \left[e(t + \Delta t) - e(t) + \frac{\Delta t}{T_i} \left(\frac{e(t + \Delta t) + e(t)}{2} \right) + T_d \left(\frac{dv_{mv}(t + \Delta t)}{dt} - \frac{dv_{mv}(t)}{dt} \right) \right]$$

Now the velocity form of the PID controller equation can be calculated at each time point from just the state at the previous time point.

Substitution

In both the proportional and integral terms, error can be replaced with the negative measured process variable yielding equivalent results. This substitution is provided by the PID class and is done by default.

Output Limits

Smooth min and smooth max expressions are used to keep the controller output between a minimum and maximum value.

Power Generation Model Library

The IDAES Process Modeling Framework contains a library of models specifically developed for modeling power generation systems. These models all built off of the core IDAES modeling framework and model libraries.

Power Generation Unit Models

Feedwater Heater (0D)

The FWH0D model is a 0D feedwater heater model suitable for steady state modeling. It is intended to be used primarily used with the *IAPWS95* property package. The feedwater heater is split into three sections the condensing section is required while the desuperheating and drain cooling sections are optional. There is also an optional mixer for adding a drain stream from another feedwater heater to the condensing section. The figure below shows the layout of the feedwater heater. All but the condensing section are optional.

Fig. 1: Feedwater Heater

Example

The example below shows how to setup a feedwater heater with all three sections. The feedwater flow rate, steam conditions, heat transfer coefficients and areas are not necessarily realistic.

```
import pyomo.environ as pyo
from idaes.core import FlowsheetBlock
from idaes.generic_models.unit_models.heat_exchanger import (delta_temperature_
↳underwood_callback,
    delta_temperature_lmtd_callback)
from idaes.generic_models.properties import iapws95
from idaes.power_generation.unit_models import FWH0D

def make_fwh_model():
    model = pyo.ConcreteModel()
    model.fs = FlowsheetBlock(default={
        "dynamic": False,
        "default_property_package": iapws95.Iapws95ParameterBlock() })
    model.fs.properties = model.fs.config.default_property_package
    model.fs.fwh = FWH0D(default={
        "has_desuperheat": True,
        "has_drain_cooling": True,
```

(continues on next page)

(continued from previous page)

```

    "has_drain_mixer":True,
    "property_package":model.fs.properties})

model.fs.fwh.desuperheat.inlet_1.flow_mol.fix(100)
model.fs.fwh.desuperheat.inlet_1.flow_mol.unfix()
model.fs.fwh.desuperheat.inlet_1.pressure.fix(201325)
model.fs.fwh.desuperheat.inlet_1.enth_mol.fix(60000)
model.fs.fwh.drain_mix.drain.flow_mol.fix(1)
model.fs.fwh.drain_mix.drain.pressure.fix(201325)
model.fs.fwh.drain_mix.drain.enth_mol.fix(20000)
model.fs.fwh.cooling.inlet_2.flow_mol.fix(400)
model.fs.fwh.cooling.inlet_2.pressure.fix(101325)
model.fs.fwh.cooling.inlet_2.enth_mol.fix(3000)
model.fs.fwh.condense.area.fix(1000)
model.fs.fwh.condense.overall_heat_transfer_coefficient.fix(100)
model.fs.fwh.desuperheat.area.fix(1000)
model.fs.fwh.desuperheat.overall_heat_transfer_coefficient.fix(10)
model.fs.fwh.cooling.area.fix(1000)
model.fs.fwh.cooling.overall_heat_transfer_coefficient.fix(10)

model.fs.fwh.initialize()
return(model)

# create a feedwater heater model with all optional units and initialize
model = make_fwh_model()

```

Model Structure

The condensing section uses the *FWHCondensing0D* model to calculate a steam flow rate such that all steam is condensed in the condensing section. This allows turbine steam extraction rates to be calculated. The other sections are regular *HeatExchanger* models. The table below shows the unit models which make up the feedwater heater, and the option to include or exclude them.

Unit	Option	Doc
condense	–	Condensing section (<i>FWHCondensing0D</i>)
desuperheat	has_desuperheat	Desuperheating section (<i>HeatExchanger</i>)
cooling	has_drain_cooling	Drain cooling section (<i>HeatExchanger</i>)
drain_mix	has_drain_mixer	Mixer for steam and other FWH drain (<i>Mixer</i>)

Degrees of Freedom

The area and overall_heat_transfer_coefficient should be fixed or constraints should be provided to calculate overall_heat_transfer_coefficient. If the inlets are also fixed except for the inlet steam flow rate (inlet_1.flow_mol), the model will have 0 degrees of freedom.

See FWH0D and FWH0DData for full Python class details.

Feedwater Heater (Condensing Section 0D)

The condensing feedwater heater is the same as the *HeatExchanger* model with one additional constraint to calculate the inlet flow rate such that all the entering steam is condensed. This model is suitable for steady state modeling, and

is intended to be used with the [IAWPS95](#) property package. For dynamic modeling, the 1D feedwater heater models should be used (not yet publicly available).

Degrees of Freedom

Usually `area` and `overall_heat_transfer_coefficient` are fixed or constraints are provided to calculate `overall_heat_transfer_coefficient`. If the inlets are also fixed except for the inlet steam flow rate (`inlet_1.flow_mol`), the model will have 0 degrees of freedom.

Variables

The variables are the same as [HeatExchanger](#).

Constraints

In addition to the [HeatExchanger](#) constraints, there is one additional constraint to calculate the inlet steam flow such that all steam condenses. The constraint is called `extraction_rate_constraint`, and is defined below.

$$h_{steam,out} = h_{sat,liquid}(P)$$

Where h is molar enthalpy, and the saturated liquid enthalpy is a function of pressure.

FWHCondensing0D Class

```
class idaes.power_generation.unit_models.feedwater_heater_0D.FWHCondensing0D(*args,  
                                                                           **kwargs)
```

Feedwater Heater Condensing Section The feedwater heater condensing section model is a normal 0D heat exchanger model with an added constraint to calculate the steam flow such that the outlet of shell is a saturated liquid.

Args: rule (function): A rule function or None. Default rule calls build(). concrete (bool): If True, make this a toplevel model. **Default** - False. ctype (str): Pyomo ctype of the block. **Default** - "Block" default (dict): Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.

Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

hot_side_name Hot side name, sets control volume and inlet and outlet names

cold_side_name Cold side name, sets control volume and inlet and outlet names

hot_side_config A config block used to construct the hot side control volume. This config can be given by the hot side name instead of hot_side_config.

material_balance_type Indicates what type of mass balance should be constructed, **default** - `MaterialBalanceType.useDefault`. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - `EnergyBalanceType.useDefault`. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = `False`. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - `False`. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms. }

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a `PropertyParameterBlock` object. }

property_package_args A `ConfigBlock` with arguments to be passed to a property block(s) and used when constructing these, **default** - `None`. **Valid values:** { see property package for documentation. }

cold_side_config A config block used to construct the cold side control volume. This config can be given by the cold side name instead of `cold_side_config`.

material_balance_type Indicates what type of mass balance should be constructed, **default** - `MaterialBalanceType.useDefault`. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - `EnergyBalanceType.useDefault`. **Valid values:** { **Ener-**

gyBalanceType.useDefault - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase.}

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - **MomentumBalanceType.pressureTotal**. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase.}

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = **False**. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms.}

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - **False**. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms.}

property_package Property parameter object used to define property calculations, **default** - **useDefault**. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a **PropertyParameterBlock** object.}

property_package_args A **ConfigBlock** with arguments to be passed to a property block(s) and used when constructing these, **default** - **None**. **Valid values:** { see property package for documentation.}

delta_temperature_callback Callback for for temperature difference calculations

flow_pattern Heat exchanger flow pattern, **default** - **HeatExchangerFlowPattern.countercurrent**. **Valid values:** { **HeatExchangerFlowPattern.countercurrent** - countercurrent flow, **HeatExchangerFlowPattern.cocurrent** - cocurrent flow, **HeatExchangerFlowPattern.crossflow** - cross flow, factor times countercurrent temperature difference.}

initialize (dict): ProcessBlockData config for individual elements. Keys are **BlockData** indexes and values are dictionaries described under the “default” argument above.

idx_map (function): Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the **BlockData** index exactly to the index in initialize.

Returns: (FWHCondensing0D) New instance

FWHCondensing0DData Class

```
class idaes.power_generation.unit_models.feedwater_heater_0D.FWHCondensing0DData (component)
```

```
    build()
        Building model
```

Parameters None –

Returns None

initialize (*args, **kwargs)

Use the regular heat exchanger initialization, with the extraction rate constraint deactivated; then it activates the constraint and calculates a steam inlet flow rate.

Turbine (Inlet Stage)

This is a steam power generation turbine model for the inlet stage. The turbine inlet model is based on:

Liese, (2014). “Modeling of a Steam Turbine Including Partial Arc Admission for Use in a Process Simulation Software Environment.” Journal of Engineering for Gas Turbines and Power. v136.

Example

```
from pyomo.environ import ConcreteModel, SolverFactory, TransformationFactory
from idaes.core import FlowsheetBlock
from idaes.power_generation.unit_models import TurbineInletStage
from idaes.generic_models.properties import iapws95

m = ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": False})
m.fs.properties = iapws95.Iapws95ParameterBlock()
m.fs.turb = TurbineInletStage(default={"property_package": m.fs.properties})
hin = iapws95.htpx(T=880, P=2.4233e7)
# set inlet
m.fs.turb.inlet[:].enth_mol.fix(hin)
m.fs.turb.inlet[:].flow_mol.fix(26000/4.0)
m.fs.turb.inlet[:].pressure.fix(2.4233e7)
m.fs.turb.eff_nozzle.fix(0.95)
m.fs.turb.blade_reaction.fix(0.9)
m.fs.turb.flow_coeff.fix(1.053/3600.0)
m.fs.turb.blade_velocity.fix(110.0)
m.fs.turb.eta_mech.fix(0.98)

m.fs.turb.initialize()
```

Degrees of Freedom

Usually the inlet stream, or the inlet stream minus flow rate plus discharge pressure are fixed. There are also a few variables which are turbine parameters and are usually fixed. See the variables section for more information.

Model Structure

The turbine inlet stage model contains one *ControlVolume0DBlock* block called `control_volume` and inherits the *PressureChanger model* using the isentropic option.

Variables

The variables below are defined in the TurbineInletStage model. Additional variables are inherited from the *PressureChanger model*.

Variable	Sym- bol	Index Sets	Doc
blade_reaction	R	None	Blade reaction
eff_nozzle	η_{nozzle}	None	Nozzle efficiency
efficiency_mech	η_{mech}	None	Mechanical Efficiency (accounts for losses in bearings. . .)
flow_coeff	C_{flow}	None	Turbine stage flow coefficient [kg*C ^{0.5} /Pa/s]
blade_velocity	V_{rbl}	None	Turbine blade velocity (should be constant while running) [m/s]
delta_enth_isentropic	Δh_{isen}	time	Isentropic enthalpy change through stage [J/mol]

The table below shows important variables inherited from the pressure changer model.

Variable	Symbol	Index Sets	Doc
efficiency_isentropic	η_{isen}	time	Isentropic efficiency
deltaP	ΔP	time	Pressure change ($P_{out} - P_{in}$) [Pa]
ratioP	P_{ratio}	time	Ratio of discharge pressure to inlet pressure $\left(\frac{P_{out}}{P_{in}}\right)$

Expressions

Variable	Sym- bol	Index Sets	Doc
power_thermo	\dot{w}_{thermo}	time	Turbine stage power output not including mechanical loss [W]
power_shaft	\dot{w}_{shaft}	time	Turbine stage power output including mechanical loss (bearings. . .) [W]
steam_entering_velocity	V_0	time	Steam velocity entering stage [m/s]

The expression defined below provides a calculation for steam velocity entering the stage, which is used in the efficiency calculation.

$$V_0 = 1.414 \sqrt{\frac{-(1 - R)\Delta h_{isen}}{WT_{in}\eta_{nozzel}}}$$

Constraints

In addition to the constraints inherited from the *PressureChanger model* with the isentropic options, this model contains two more constraints, one to estimate efficiency and one pressure-flow relation. From the isentropic pressure changer model, these constraints eliminate the need to specify efficiency and either inlet flow or outlet pressure.

The isentropic efficiency is given by:

$$\eta_{isen} = 2 \frac{V_{rbl}}{V_0} \left[\left(\sqrt{1 - R} - \frac{V_{rbl}}{V_0} \right) + \sqrt{\left(\sqrt{1 - R} - \frac{V_{rbl}}{V_0} \right)^2 + R} \right]$$

The pressure-flow relation is given by:

$$\dot{m} = C_{flow} \frac{P_{in}}{\sqrt{T_{in} - 273.15}} \sqrt{\frac{\gamma}{\gamma - 1} \left[\left(\frac{P_{out}}{P_{in}} \right)^{\frac{2}{\gamma}} - \left(\frac{P_{out}}{P_{in}} \right)^{\frac{\gamma+1}{\gamma}} \right]}$$

Initialization

The initialization method for this model will save the current state of the model before commencing initialization and reloads it afterwards. The state of the model will be the same after initialization, only the initial guesses for unfixed variables will be changed. To initialize this model, provide a starting value for the inlet port variables. Then provide a guess for one of: discharge pressure, `deltaP`, or `ratioP`.

The model should initialize readily, but it is possible to provide a flow coefficient that is incompatible with the given flow rate resulting in an infeasible problem.

TurbineInletStage Class

```
class idaes.power_generation.unit_models.turbine_inlet.TurbineInletStage (*args,  
                                                                    **kwargs)
```

Inlet stage steam turbine model

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.

Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.useDefault. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - `MomentumBalanceType.pressureTotal`. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = `False`. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms. }

compressor Indicates whether this unit should be considered a compressor (`True` (default), pressure increase) or an expander (`False`, pressure decrease).

thermodynamic_assumption Flag to set the thermodynamic assumption to use for the unit. - `ThermodynamicAssumption.isothermal` (default) - `ThermodynamicAssumption.isentropic` - `ThermodynamicAssumption.pump` - `ThermodynamicAssumption.adiabatic`

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a `PropertyParameterBlock` object. }

property_package_args A `ConfigBlock` with arguments to be passed to a property block(s) and used when constructing these, **default** - `None`. **Valid values:** { see property package for documentation. }

- **initialize** (*dict*) – `ProcessBlockData` config for individual elements. Keys are `BlockData` indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a `BlockData` element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the `BlockData` index exactly to the index in initialize.

Returns (`TurbineInletStage`) New instance

TurbineInletStageData Class

```
class idaes.power_generation.unit_models.turbine_inlet.TurbineInletStageData (component)
```

build ()

Parameters `None` –

Returns `None`

initialize (*state_args*={}, *outlvl*=0, *solver*='ipopt', *optarg*={'max_iter': 30, 'tol': 1e-06})

Initialize the inlet turbine stage model. This deactivates the specialized constraints, then does the isentropic turbine initialization, then reactivates the constraints and solves.

Parameters

- **state_args** (*dict*) – Initial state for property initialization
- **outlvl** (*int*) – Amount of output (0 to 3) 0 is lowest
- **solver** (*str*) – Solver to use for initialization
- **optarg** (*dict*) – Solver arguments dictionary

Turbine (Outlet Stage)

This is a steam power generation turbine model for the outlet stage. The turbine outlet model is based on:

Liese, (2014). “Modeling of a Steam Turbine Including Partial Arc Admission for Use in a Process Simulation Software Environment.” Journal of Engineering for Gas Turbines and Power. v136.

Example

```
from pyomo.environ import ConcreteModel, SolverFactory
from idaes.core import FlowsheetBlock
from idaes.power_generation.unit_models import TurbineOutletStage
from idaes.generic_models.properties import iapws95

m = ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": False})
m.fs.properties = iapws95.Iapws95ParameterBlock()
m.fs.turb = TurbineOutletStage(default={"property_package": m.fs.properties})
# set inlet
m.fs.turb.inlet[:].enth_mol.fix(47115)
m.fs.turb.inlet[:].flow_mol.fix(15000)
m.fs.turb.inlet[:].pressure.fix(8e4)

m.fs.turb.initialize()
```

Degrees of Freedom

Usually the inlet stream, or the inlet stream minus flow rate plus discharge pressure are fixed. There are also a few variables which are turbine parameters and are usually fixed. See the variables section for more information.

Model Structure

The turbine outlet stage model contains one *ControlVolume0DBlock* block called control_volume and inherits the *PressureChanger* model using the isentropic option.

Variables

The variables below are defined in the TurbineInletStage model. Additional variables are inherited from the *PressureChanger* model.

Variable	Symbol	Index Sets	Doc
eff_dry	η_{dry}	None	Turbine efficiency when no liquid is present.
efficiency_mech	η_{mech}	None	Mechanical Efficiency (accounts for losses in bearings...)
flow_coeff	C_{flow}	None	Turbine stage flow coefficient [kg*C ^{0.5} /Pa/s]
design_exhaust_flow_vol	$V_{des,exhaust}$	None	Design volumetric flow out of stage [m ³ /s]

The table below shows important variables inherited from the pressure changer model.

Variable	Symbol	Index Sets	Doc
efficiency_isentropic	η_{isen}	time	Isentropic efficiency
deltaP	ΔP	time	Pressure change ($P_{out} - P_{in}$) [Pa]
ratioP	P_{ratio}	time	Ratio of discharge pressure to inlet pressure $\left(\frac{P_{out}}{P_{in}}\right)$

Expressions

Variable	Sym- bol	Index Sets	Doc
power_thermo	\dot{w}_{thermo}	time	Turbine stage power output not including mechanical loss [W]
power_shaft	\dot{w}_{shaft}	time	Turbine stage power output including mechanical loss (bearings...) [W]
tel	TEL	time	Total exhaust loss [J/mol]

The expression defined below provides a total exhaust loss.

$$TEL = 1 \times 10^6 * (-0.0035f^5 + 0.022f^4 - 0.0542f^3 + 0.0638f^2 - 0.0328f + 0.0064)$$

Where f is the total volumetric flow of the exhaust divided by the design flow.

Constraints

In addition to the constraints inherited from the *PressureChanger model* with the isentropic options, this model contains two more constraints, one to estimate efficiency and one pressure-flow relation. From the isentropic pressure changer model, these constraints eliminate the need to specify efficiency and either inlet flow or outlet pressure.

The isentropic efficiency is given by:

$$\eta_{isen} = \eta_{dry}x(1 - 0.65(1 - x)) * \left(1 + \frac{TEL}{\Delta h_{isen}}\right)$$

Where x is the steam quality (vapor fraction).

The pressure-flow relation is given by the Stodola Equation:

$$\dot{m}\sqrt{T_{in} - 273.15} = C_{flow}P_{in}\sqrt{1 - Pr^2}$$

Initialization

The initialization method for this model will save the current state of the model before commencing initialization and reloads it afterwards. The state of the model will be the same after initialization, only the initial guesses for unfixed variables will be changed. To initialize this model, provide a starting value for the inlet port variables. Then provide a guess for one of: discharge pressure, deltaP, or ratioP.

The model should initialize readily, but it is possible to provide a flow coefficient that is incompatible with the given flow rate resulting in an infeasible problem.

TurbineOutletStage Class

```
class idaes.power_generation.unit_models.turbine_outlet.TurbineOutletStage (*args,  
                                                                           **kwargs)
```

Outlet stage steam turbine model

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.
Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.useDefault. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - MomentumBalanceType.pressureTotal. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = False. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms. }

compressor Indicates whether this unit should be considered a compressor (True (default), pressure increase) or an expander (False, pressure decrease).

thermodynamic_assumption Flag to set the thermodynamic assumption to use for the unit. - ThermodynamicAssumption.isothermal (default) - ThermodynamicAs-

sumption.isentropic - ThermodynamicAssumption.pump - ThermodynamicAssumption.adiabatic

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object. }

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (TurbineOutletStage) New instance

TurbineOutletStageData Class

```
class idaes.power_generation.unit_models.turbine_outlet.TurbineOutletStageData (component)
```

build()

Parameters None –

Returns None

initialize (*state_args*={}, *outlvl*=0, *solver*='ipopt', *optarg*={'max_iter': 30, 'tol': 1e-06})

Initialize the outlet turbine stage model. This deactivates the specialized constraints, then does the isentropic turbine initialization, then reactivates the constraints and solves.

Parameters

- **state_args** (*dict*) – Initial state for property initialization
- **outlvl** – sets output level of initialization routine
- **solver** (*str*) – Solver to use for initialization
- **optarg** (*dict*) – Solver arguments dictionary

Turbine (Stage)

This is a steam power generation turbine model for the stages between the inlet and outlet. This model inherits the *PressureChanger model* with the isentropic options. The initialization scheme is the same as the *TurbineInletStage model*.

Example

```
from pyomo.environ import ConcreteModel, SolverFactory

from idaes.core import FlowsheetBlock
from idaes.power_generation.unit_models import TurbineStage
```

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```

from idaes.generic_models.properties import iapws95

m = ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": False})
m.fs.properties = iapws95.Iapws95ParameterBlock()
m.fs.turb = TurbineStage(default={"property_package": m.fs.properties})
# set inlet
m.fs.turb.inlet[:].enth_mol.fix(70000)
m.fs.turb.inlet[:].flow_mol.fix(15000)
m.fs.turb.inlet[:].pressure.fix(8e6)
m.fs.turb.efficiency_isentropic[:].fix(0.8)
m.fs.turb.ratioP[:].fix(0.7)
m.fs.turb.initialize()

```

Variables

This model adds a variable to the base `PressureChanger` model to account for mechanical efficiency .

Variable	Symbol	Index Sets	Doc
efficiency_mech	η_{mech}	None	Mechanical Efficiency (accounts for losses in bearings...)

The table below shows important variables inherited from the pressure changer model.

Variable	Symbol	Index Sets	Doc
efficiency_isentropic	η_{isen}	time	Isentropic efficiency
deltaP	ΔP	time	Pressure change ($P_{out} - P_{in}$) [Pa]
ratioP	P_{ratio}	time	Ratio of discharge pressure to inlet pressure $\left(\frac{P_{out}}{P_{in}}\right)$

$\eta_{isentropic,t}$ efficiency_isentropic Isentropic assumption only

Expressions

This model provides two expressions that are not available in the pressure changer model.

Variable	Sym- bol	Index Sets	Doc
power_thermo	\dot{w}_{thermo}	time	Turbine stage power output not including mechanical loss [W]
power_shaft	\dot{w}_{shaft}	time	Turbine stage power output including mechanical loss (bearings...) [W]

Constraints

There are no additional constraints.

Initialization

This just calls the initialization routine from `PressureChanger`, but it is wrapped in a function to ensure the state after initialization is the same as before initialization. The arguments to the initialization method are the same as `PressureChanger`.

TurbineStage Class

```
class idaes.power_generation.unit_models.turbine_stage.TurbineStage(*args,
                                                                    **kwargs)
```

Basic steam turbine model

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.
Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.useDefault. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - MomentumBalanceType.pressureTotal. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = False. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms.}

compressor Indicates whether this unit should be considered a compressor (True (default), pressure increase) or an expander (False, pressure decrease).

thermodynamic_assumption Flag to set the thermodynamic assumption to use for the unit. - ThermodynamicAssumption.isothermal (default) - ThermodynamicAssumption.isentropic - ThermodynamicAssumption.pump - ThermodynamicAssumption.adiabatic

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object.}

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation.}

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (TurbineStage) New instance

TurbineStageData Class

```
class idaes.power_generation.unit_models.turbine_stage.TurbineStageData (component)
```

build()

Parameters None –

Returns None

initialize (*state_args={}*, *outlvl=0*, *solver='ipopt'*, *optarg={'max_iter': 30, 'tol': 1e-06}*)

Initialize the turbine stage model. This deactivates the specialized constraints, then does the isentropic turbine initialization, then reactivates the constraints and solves.

Parameters

- **state_args** (*dict*) – Initial state for property initialization
- **outlvl** – sets output level of initialization routine
- **solver** (*str*) – Solver to use for initialization
- **optarg** (*dict*) – Solver arguments dictionary

Turbine (Multistage)

This is a composite model for a power plant turbine with high, intermediate and low pressure sections. This model contains an inlet stage with throttle valves for partial arc admission and optional splitters for steam extraction.

The figure below shows the layout of the multistage turbine model. Optional splitters provide for steam extraction. The splitters can have two or more outlets (one being the main steam outlet). The streams that connect one stage to the next can also be omitted. This allows for connecting additional unit models (usually reheaters) between stages.

Fig. 2: MultiStage Turbine Model

Example

This example sets up a turbine multistage turbine model similar to what could be found in a power plant steam cycle. There are 7 high-pressure stages, 14 intermediate-pressure stages, and 11 low-pressure stages. Steam extractions are provided after stages hp4, hp7, ip5, ip14, lp4, lp7, lp9, lp11. The extraction at ip14 uses a splitter with three outlets, one for the main steam, one for the boiler feed pump, and one for a feedwater heater. There is a disconnection between the HP and IP sections so that steam can be sent to a reheater. In this example, a heater block is a stand-in for a reheater model.

```
from pyomo.environ import (ConcreteModel, SolverFactory, TransformationFactory,
                           Constraint, value)
from pyomo.network import Arc

from idaes.core import FlowsheetBlock
from idaes.unit_models import Heater
from idaes.power_generation.unit_models import (
    TurbineMultistage, TurbineStage, TurbineInletStage, TurbineOutletStage)
from idaes.generic_models.properties import iapws95

solver = SolverFactory('ipopt')
solver.options = {'tol': 1e-6}

m = ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": False})
m.fs.properties = iapws95.Iapws95ParameterBlock()
m.fs.turb = TurbineMultistage(default={
    "property_package": m.fs.properties,
    "num_hp": 7,
    "num_ip": 14,
    "num_lp": 11,
    "hp_split_locations": [4,7],
    "ip_split_locations": [5, 14],
    "lp_split_locations": [4,7,9,11],
    "hp_disconnect": [7], # 7 is last stage in hp so disconnect hp from ip
    "ip_split_num_outlets": {14:3}})
# Add reheater (for example using a simple heater block)
m.fs.reheat = Heater(default={"property_package": m.fs.properties})
# Add Arcs (streams) to connect the HP and IP sections through reheater
m.fs.hp_to_reheat = Arc(source=m.fs.turb.hp_split[7].outlet_1,
                        destination=m.fs.reheat.inlet)
m.fs.reheat_to_ip = Arc(source=m.fs.reheat.outlet,
                        destination=m.fs.turb.ip_stages[1].inlet)
# Set the turbine inlet conditions and an initial flow guess
p = 2.4233e7
hin = iapws95.htpx(T=880, P=p)
m.fs.turb.inlet_split.inlet.enth_mol[0].fix(hin)
m.fs.turb.inlet_split.inlet.flow_mol[0].fix(26000)
m.fs.turb.inlet_split.inlet.pressure[0].fix(p)
```

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```

# Set the inlet of the ip section for initialization, since it is disconnected
p = 7.802e+06
hin = iapws95.htpx(T=880, P=p)
m.fs.turb.ip_stages[1].inlet.enth_mol[0].value = hin
m.fs.turb.ip_stages[1].inlet.flow_mol[0].value = 25220.0
m.fs.turb.ip_stages[1].inlet.pressure[0].value = p
# Set the efficiency and pressure ratios of stages other than inlet and outlet
for i, s in turb.hp_stages.items():
    s.ratioP[:] = 0.88
    s.efficiency_isentropic[:] = 0.9
for i, s in turb.ip_stages.items():
    s.ratioP[:] = 0.85
    s.efficiency_isentropic[:] = 0.9
for i, s in turb.lp_stages.items():
    s.ratioP[:] = 0.82
    s.efficiency_isentropic[:] = 0.9
# Usually these fractions would be determined by the boiler feed water heater
# network. Since this example doesn't include them, just fix split fractions
turb.hp_split[4].split_fraction[0,"outlet_2"].fix(0.03)
turb.hp_split[7].split_fraction[0,"outlet_2"].fix(0.03)
turb.ip_split[5].split_fraction[0,"outlet_2"].fix(0.04)
turb.ip_split[14].split_fraction[0,"outlet_2"].fix(0.04)
turb.ip_split[14].split_fraction[0,"outlet_3"].fix(0.15)
turb.lp_split[4].split_fraction[0,"outlet_2"].fix(0.04)
turb.lp_split[7].split_fraction[0,"outlet_2"].fix(0.04)
turb.lp_split[9].split_fraction[0,"outlet_2"].fix(0.04)
turb.lp_split[11].split_fraction[0,"outlet_2"].fix(0.04)
# unfix inlet flow for pressure driven simulation
turb.inlet_split.inlet.flow_mol.unfix()
# Set the inlet steam mixer to use the constraints that the pressures of all
# inlet streams are equal
turb.inlet_mix.use_equal_pressure_constraint()
# Initialize turbine
turb.initialize(outlvl=1)
# Copy conditions out of turbine to initialize the reheater
for t in m.fs.time:
    m.fs.reheat.inlet.flow_mol[t].value = \
        value(turb.hp_split[7].outlet_1_state[t].flow_mol)
    m.fs.reheat.inlet.enth_mol[t].value = \
        value(turb.hp_split[7].outlet_1_state[t].enth_mol)
    m.fs.reheat.inlet.pressure[t].value = \
        value(turb.hp_split[7].outlet_1_state[t].pressure)
# initialize the reheater
m.fs.reheat.initialize(outlvl=4)
# Add constraint to the reheater to result in 880K outlet temperature
def reheater_T_rule(b, t):
    return m.fs.reheat.control_volume.properties_out[t].temperature == 880
m.fs.reheat.temperature_out_equation = Constraint(m.fs.reheat.time_ref,
    rule=reheater_T_rule)
# Expand the Arcs connecting the turbine to the reheater
TransformationFactory("network.expand_arcs").apply_to(m)
# Fix the outlet pressure (usually determined by condenser)
m.fs.turb.outlet_stage.control_volume.properties_out[0].pressure.fix()

# Solve the pressure driven flow model with reheater
solver.solve(m, tee=True)

```

Unit Models

The multistage turbine model contains the models in the table below. The splitters for steam extraction are not present if a turbine section contains no steam extractions.

Unit	Index Sets	Doc
inlet_split	None	Splitter to split the main steam feed into steams for each arc (<i>Separator</i>)
throttle_valve	Admission Arcs	Throttle valves for each admission arc (<i>SteamValve</i>)
inlet_stage	Admission Arcs	Parallel inlet turbine stages that represent admission arcs (<i>TurbineInlet</i>)
inlet_mix	None	Mixer to combine the streams from each arc back to one stream (<i>Mixer</i>)
hp_stages	HP stages	Turbine stages in the high-pressure section (<i>TurbineStage</i>)
ip_stages	IP stages	Turbine stages in the intermediate-pressure section (<i>TurbineStage</i>)
lp_stages	LP stages	Turbine stages in the low-pressure section (<i>TurbineStage</i>)
hp_splits	subset of HP stages	Extraction splitters in the high-pressure section (<i>Separator</i>)
ip_splits	subset of IP stages	Extraction splitters in the high-pressure section (<i>Separator</i>)
lp_splits	subset of LP stages	Extraction splitters in the high-pressure section (<i>Separator</i>)
outlet_stage	None	The final stage in the turbine, which calculates exhaust losses (<i>Turbine-Outlet</i>)

Initialization

The initialization approach is to sequentially initialize each sub-unit using the outlet of the previous model. Before initializing the model, the inlet of the turbine, and any stage that is disconnected should be given a reasonable guess. The efficiency and pressure ration of the stages in the HP, IP and LP sections should be specified. For the inlet and outlet stages the flow coefficient should be specified. Valve coefficients should also be specified. A reasonable guess for split fractions should also be given for any extraction splitters present. The most likely cause of initialization failure is flow coefficients in inlet stage, outlet stage, or valves that do not pair well with the specified flow rates.

TurbineMultistage Class

```
class idaes.power_generation.unit_models.turbine_multistage.TurbineMultistage(*args,
                                                                    **kwargs)
```

Multistage steam turbine with optional reheat and extraction

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether the model is dynamic.

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **True** - construct holdup terms, **False** - do not construct holdup terms }

has_phase_equilibrium Argument indicating whether phase equilibrium should be calculated for the resulting mixed stream, **default** - False. **Valid values:** { **True** - calculate phase equilibrium in mixed stream, **False** - do not calculate equilibrium in mixed stream. }

material_balance_type Indicates what type of mass balance should be constructed, **default** - `MaterialBalanceType.componentTotal`. **Valid values:** { **MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

property_package Property parameter object used to define property calculations, **default** - `useDefault`. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a `PropertyParameterBlock` object. }

property_package_args A `ConfigBlock` with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

num_parallel_inlet_stages Number of parallel inlet stages to simulate partial arc admission. Default=4

num_hp Number of high pressure stages not including inlet stage

num_ip Number of intermediate pressure stages

num_lp Number of low pressure stages not including outlet stage

hp_split_locations A list of index locations of splitters in the HP section. The indexes indicate after which stage to include splitters. 0 is between the inlet stage and the first regular HP stage.

ip_split_locations A list of index locations of splitters in the IP section. The indexes indicate after which stage to include splitters.

lp_split_locations A list of index locations of splitters in the LP section. The indexes indicate after which stage to include splitters.

hp_disconnect HP Turbine stages to not connect to next with an arc. This is usually used to insert additional units between stages on a flowsheet, such as a reheater

ip_disconnect IP Turbine stages to not connect to next with an arc. This is usually used to insert additional units between stages on a flowsheet, such as a reheater

lp_disconnect LP Turbine stages to not connect to next with an arc. This is usually used to insert additional units between stages on a flowsheet, such as a reheater

hp_split_num_outlets Dict, hp split index: number of splitter outlets, if not 2

ip_split_num_outlets Dict, ip split index: number of splitter outlets, if not 2

lp_split_num_outlets Dict, lp split index: number of splitter outlets, if not 2

- **initialize** (*dict*) – `ProcessBlockData` config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (`TurbineMultistage`) New instance

TurbineMultistageData Class

class `idaes.power_generation.unit_models.turbine_multistage.TurbineMultistageData` (*component*)

build()

General build method for UnitModelBlockData. This method calls a number of sub-methods which automate the construction of expected attributes of unit models.

Inheriting models should call *super().build*.

Parameters **None** –

Returns **None**

initialize (*outlvl=0, solver='ipopt', optarg={'max_iter': 35, 'tol': 1e-06}, copy_disconnected_flow=True*)
Initialize

throttle_cv_fix (*value*)

Fix the throttle valve coefficients. These are generally the same for each of the parallel stages so this provides a convenient way to set them.

Parameters **value** – The value to fix the turbine inlet flow coefficients at

turbine_inlet_cf_fix (*value*)

Fix the inlet turbine stage flow coefficient. These are generally the same for each of the parallel stages so this provides a convenient way to set them.

Parameters **value** – The value to fix the turbine inlet flow coefficients at

turbine_outlet_cf_fix (*value*)

Fix the inlet turbine stage flow coefficient. These are generally the same for each of the parallel stages so this provides a convenient way to set them.

Parameters **value** – The value to fix the turbine inlet flow coefficients at

Steam/Water Valve

This is a steam power generation turbine model for the stages between the inlet and outlet. This model inherits the *PressureChanger model* with the adiabatic options. Beyond the base pressure changer model this provides a pressure flow relation as a function of the valve opening fraction.

Example

```
from pyomo.environ import ConcreteModel, SolverFactory, TransformationFactory

from idaes.core import FlowsheetBlock
from idaes.power_generation.unit_models import SteamValve
from idaes.generic_models.properties import iapws95
from idaes.ui.report import degrees_of_freedom, active_equalities

solver = SolverFactory('ipopt')
solver.options = {'tol': 1e-6}

m = ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": False})
```

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```

m.fs.properties = iapws95.Iapws95ParameterBlock()
m.fs.valve = SteamValve(default={"property_package": m.fs.properties})

hin = iapws95.htpx(T=880, P=2.4233e7)
# set inlet
m.fs.valve.inlet.enth_mol[0].fix(hin)
m.fs.valve.inlet.flow_mol[0].fix(26000/4.0)
m.fs.valve.inlet.pressure[0].fix(2.5e7)
m.fs.valve.Cv.fix(0.01)
m.fs.valve.valve_opening.fix(0.5)
m.fs.valve.initialize(outlvl=1)

```

Parameters

Expression	Symbol	Index Sets	Doc
flow_scale	s_f	None	Factor for scaling the pressure-flow equation, should be same magnitude as expected flow rate

Variables

This model adds a variable to account for mechanical efficiency to the base PressureChanger model.

Variable	Symbol	Index Sets	Doc
Cv	C_v	None	Valve coefficient for liquid [mol/s/Pa ^{0.5}] for vapor [mol/s/Pa]
valve_opening	x	time	The fraction that the valve is open from 0 to 1

Expressions

Currently this model provides two additional expressions, with are not available in the pressure changer model.

Expression	Symbol	Index Sets	Doc
valve_function	$f(x)$	time	This is a valve function that describes how the fraction open affects flow.

Constraints

The pressure flow relation is added to the inherited constraints from the *PressureChanger model*.

If the phase option is set to "Liq" the following equation describes the pressure-flow relation.

$$\frac{1}{s_f^2} F^2 = \frac{1}{s_f^2} C_v^2 (P_{in} - P_{out}) f(x)^2$$

If the phase option is set to "Vap" the following equation describes the pressure-flow relation.

$$\frac{1}{s_f^2} F^2 = \frac{1}{s_f^2} C_v^2 (P_{in}^2 - P_{out}^2) f(x)^2$$

Initialization

This just calls the initialization routine from PressureChanger, but it is wrapped in a function to ensure the state after initialization is the same as before initialization. The arguments to the initialization method are the same as PressureChanger.

SteamValve Class

```
class idaes.power_generation.unit_models.valve_steam.SteamValve(*args,
                                                                **kwargs)
```

Basic steam valve models

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls build().
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”
- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault.
Valid values: { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - construct holdup terms, **False** - do not construct holdup terms }

material_balance_type Indicates what type of mass balance should be constructed, **default** - MaterialBalanceType.useDefault. **Valid values:** { **MaterialBalanceType.useDefault** - refer to property package for default balance type ****MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.useDefault. **Valid values:** { **EnergyBalanceType.useDefault** - refer to property package for default balance type ****EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - MomentumBalanceType.pressureTotal. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_phase_equilibrium Indicates whether terms for phase equilibrium should be constructed, **default** = False. **Valid values:** { **True** - include phase equilibrium terms **False** - exclude phase equilibrium terms.}

compressor Indicates whether this unit should be considered a compressor (True (default), pressure increase) or an expander (False, pressure decrease).

thermodynamic_assumption Flag to set the thermodynamic assumption to use for the unit. - ThermodynamicAssumption.isothermal (default) - ThermodynamicAssumption.isentropic - ThermodynamicAssumption.pump - ThermodynamicAssumption.adiabatic

property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PropertyParameterObject** - a PropertyParameterBlock object.}

property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation.}

valve_function The type of valve function, if custom provide an expression rule with the valve_function_rule argument. **default** - ValveFunctionType.linear **Valid values** - { ValveFunctionType.linear, ValveFunctionType.quick_opening, ValveFunctionType.equal_percentage, ValveFunctionType.custom}

valve_function_rule This is a rule that returns a time indexed valve function expression. This is required only if valve_function==ValveFunctionType.custom

phase Expected phase of fluid in valve in {"Liq", "Vap"}

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are BlockData indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (SteamValve) New instance

SteamValveData Class

```
class idaes.power_generation.unit_models.valve_steam.SteamValveData (component)
```

```
    build()
```

Parameters None –

Returns None

```
    initialize (state_args={}, outlvl=0, solver='ipopt', optarg={'max_iter': 30, 'tol': 1e-06})
```

Initialize the turbine stage model. This deactivates the specialized constraints, then does the isentropic turbine initialization, then reactivates the constraints and solves.

Parameters

- **state_args** (*dict*) – Initial state for property initialization
- **outlvl** – sets output level of initialization routine
- **solver** (*str*) – Solver to use for initialization

- **optarg** (*dict*) – Solver arguments dictionary

BoilerHeatExchanger

The BoilerHeatExchanger model can be used to represent boiler heat exchangers in sub-critical and super critical power plant flowsheets (i.e. econmizer, primary superheater, secondary superheater, finishing superheater, reheater, etc.). The model consists of a shell and tube crossflow heat exchanger, in which the shell is used as the gas side and the tube is used as the water or steam side. Rigorous heat transfer calculations (convective heat transfer for shell side, and convective heat transfer for tube side) and shell and tube pressure drop calculations have been included.

The BoilerHeatExchanger model can be imported from `idaes.power_generation.unit_models`, while additional rules and utility functions can be imported from `idaes.power_generation.unit_models.boiler_heat_exchanger`.

Example

The example below demonstrates how to initialize the BoilerHeatExchanger model, and override the default temperature difference calculation.

```
# Import Pyomo libraries
from pyomo.environ import ConcreteModel, SolverFactory, value
# Import IDAES core
from idaes.core import FlowsheetBlock
# Import Unit Model Modules
from idaes.generic_models.properties import iapws95
# import ideal flue gas prop pack
from idaes.power_generation.properties.IdealProp_FlueGas import FlueGasParameterBlock
# Import Power Plant HX Unit Model
from idaes.power_generation.unit_models.boiler_heat_exchanger import _
↳BoilerHeatExchanger, TubeArrangement, \
    DeltaTMethod
import pyomo.environ as pe # Pyomo environment
from idaes.core import FlowsheetBlock, StateBlock
from idaes.unit_models.heat_exchanger import delta_temperature_amtd_callback
from idaes.generic_models.properties import iapws95

# Create a Concrete Model as the top level object
m = ConcreteModel()

# Add a flowsheet object to the model
m.fs = FlowsheetBlock(default={"dynamic": False})

# Add property packages to flowsheet library
m.fs.prop_water = iapws95.Iapws95ParameterBlock()
m.fs.prop_fluegas = FlueGasParameterBlock()

# Create unit models
m.fs.ECON = BoilerHeatExchanger(default={
    "side_1_property_package": m.fs.prop_water,
    "side_2_property_package": m.fs.prop_fluegas,
    "has_pressure_change": True,
    "has_holdup": False,
    "delta_T_method": DeltaTMethod.counterCurrent,
    "tube_arrangement": TubeArrangement.inLine,
    "side_1_water_phase": "Liq",
```

(continues on next page)

(continued from previous page)

```

        "has_radiation": False})

# Set Inputs
# BFW Boiler Feed Water inlet temeperature = 555 F = 563.706 K
# inputs based on NETL Baseline Report v3 (SCPC 650 MW net, no carbon capture case)
h = iapws95.htpx(563.706, 2.5449e7)
m.fs.ECON.side_1_inlet.flow_mol[0].fix(24678.26) # mol/s
m.fs.ECON.side_1_inlet.enth_mol[0].fix(h)
m.fs.ECON.side_1_inlet.pressure[0].fix(2.5449e7) # Pa

# FLUE GAS Inlet from Primary Superheater
FGrate = 28.3876e3 # mol/s equivalent of ~1930.08 klb/hr
# Use FG molar composition to set component flow rates (baseline report)
m.fs.ECON.side_2_inlet.flow_component[0,"H2O"].fix(FGrate*8.69/100)
m.fs.ECON.side_2_inlet.flow_component[0,"CO2"].fix(FGrate*14.49/100)
m.fs.ECON.side_2_inlet.flow_component[0,"N2"].fix(FGrate*(8.69
                                         +14.49+2.47+0.06+0.2)/100)
m.fs.ECON.side_2_inlet.flow_component[0,"O2"].fix(FGrate*2.47/100)
m.fs.ECON.side_2_inlet.flow_component[0,"NO"].fix(FGrate*0.0006)
m.fs.ECON.side_2_inlet.flow_component[0,"SO2"].fix(FGrate*0.002)
m.fs.ECON.side_2_inlet.temperature[0].fix(682.335) # K
m.fs.ECON.side_2_inlet.pressure[0].fix(100145) # Pa
# economizer design variables and parameters
ITM = 0.0254 # inch to meter conversion
# Based on NETL Baseline Report Rev3
m.fs.ECON.tube_di.fix((2-2*0.188)*ITM) # calc inner diameter
# (2 = outer diameter, thickness = 0.188)
m.fs.ECON.tube_thickness.fix(0.188*ITM) # tube thickness
m.fs.ECON.pitch_x.fix(3.5*ITM)
# pitch_y = (54.5) gas path transverse width /columns
m.fs.ECON.pitch_y.fix(5.03*ITM)
m.fs.ECON.tube_length.fix(53.41*12*ITM) # use tube length (53.41 ft)
m.fs.ECON.tube_nrow.fix(36*2.5) # use to match baseline performance
m.fs.ECON.tube_ncol.fix(130) # 130 from NETL report
m.fs.ECON.nrow_inlet.fix(2)
m.fs.ECON.delta_elevation.fix(50)
# parameters
# heat transfer resistance due to tube side fouling (water scales)
m.fs.ECON.tube_rfouling = 0.000176
# heat transfer resistance due to tube shell fouling (ash deposition)
m.fs.ECON.shell_rfouling = 0.00088
if m.fs.ECON.config.has_radiation is True:
    m.fs.ECON.emissivity_wall.fix(0.7) # wall emissivity
# correction factor for overall heat transfer coefficient
m.fs.ECON.fcorrection_htc.fix(1.5)
# correction factor for pressure drop calc tube side
m.fs.ECON.fcorrection_dp_tube.fix(1.0)
# correction factor for pressure drop calc shell side
m.fs.ECON.fcorrection_dp_shell.fix(1.0)

# Initialize the model
m.fs.ECON.initialize()

```

Degrees of Freedom

Aside from the inlet conditions, a heat exchanger model usually has two degrees of freedom, which can be fixed for it to be fully specified. Things that are frequently fixed are two of:

- heat transfer area,
- heat transfer coefficient, or
- temperature approach.

In order to capture off design conditions and heat transfer coefficients at ramp up/down or load following conditions, the `BoilerHeatExchanger` model includes rigorous heat transfer calculations. Therefore, additional degrees of freedom are required to calculate Nusselt, Prandtl, Reynolds numbers, such as:

- `tube_di` (inner diameter)
- tube length
- tube number of rows (`tube_nrow`), columns (`tube_ncol`), and inlet flow (`nrow_inlet`)
- pitch in x and y axis (`pitch_x` and `pitch_y`, respectively)

If pressure drop calculation is enabled, additional degrees of freedom are required:

- elevation with respect to ground level (`delta_elevation`)
- tube fouling resistance (`tube_r_fouling`)
- shell fouling resistance (`shell_r_fouling`)

Model Structure

The `BoilerHeatExchanger` model contains two `ControlVolume0DBlock` blocks. By default the gas side is named `shell` and the water/steam side is named `tube`. These names are configurable. The sign convention is that duty is positive for heat flowing from the hot side to the cold side.

The control volumes are configured the same as the `ControlVolume0DBlock` in the [Heater model](#). The `BoilerHeatExchanger` model contains additional constraints that calculate the amount of heat transferred from the hot side to the cold side.

The `BoilerHeatExchanger` has two inlet ports and two outlet ports. By default these are `shell_inlet`, `tube_inlet`, `shell_outlet`, and `tube_outlet`. If the user supplies different hot and cold side names the inlet and outlets are named accordingly.

Variables

Variable	Symbol	Index Sets	Doc
<code>heat_duty</code>	Q	time	Heat transferred from hot side to the cold side
<code>area</code>	A	None	Heat transfer area
<code>U</code>	U	time	Heat transfer coefficient
<code>delta_temperature</code>	ΔT	time	Temperature difference, defaults to LMTD

Note: `delta_temperature` may be either a variable or expression depending on the callback used. If the specified cold side is hotter than the specified hot side this value will be negative.

Constraints

The default constraints can be overridden by providing *alternative rules* for the heat transfer equation, temperature difference, heat transfer coefficient, shell and tube pressure drop. This section describes the default constraints.

Heat transfer from shell to tube:

$$Q = UA\Delta T$$

Temperature difference is:

$$\Delta T = \frac{\Delta T_1 - \Delta T_2}{\log_e \left(\frac{\Delta T_1}{\Delta T_2} \right)}$$

The overall heat transfer coefficient is calculated as a function of convective heat transfer shell and tube, and wall conduction heat transfer resistance.

Convective heat transfer equations:

$$\frac{1}{U} * f_{correction_{htc}} = \left[\frac{1}{h_{conv_{tube}}} + \frac{1}{h_{conv_{shell}}} + r + tube_{r_{fouling}} + shell_{r_{fouling}} \right]$$

$$h_{conv_{tube}} = \frac{Nu_{tube} k}{tube_{di}}$$

$$Nu_{tube} = 0.023 Re_{tube}^{0.8} Pr_{tube}^{0.4}$$

$$Pr_{tube} = \frac{Cp\mu}{kMw}$$

$$Re_{tube} = \frac{tube_{di} V \rho}{\mu}$$

$$h_{conv_{shell}} = \frac{Nu_{shell} k_{fluegas}}{tube_{do}}$$

$$Nu_{shell} = f_{arrangement} 0.33 Re_{tube}^{0.6} Pr_{tube}^{0.3333}$$

$$Pr_{shell} = \frac{Cp\mu}{kMw}$$

$$Re_{shell} = \frac{tube_{do} V \rho}{\mu}$$

$$tube_{do} = 2 * tube_{thickness} + tube_{di}$$

Wall heat conduction resistance equation:

$$r = 0.5 * tube_{do} * \log \left(\frac{tube_{do}}{tube_{di}} \right) * k$$

where:

- h_{conv_tube} : convective heat transfer resistance tube side (fluid water/steam) (W / m² / K)
- h_{conv_shell} : convective heat transfer resistance shell side (fluid Flue Gas) (W / m² / K)
- Nu : Nusselt number
- Pr : Prandtl number
- Re : Reynolds number
- V : velocity (m/s)

- tube_di : inner diameter of the tube (m)
- tube_do : outer diameter of the tube (m) (expression calculated by the model)
- tube_thickness : tube thickness (m)
- r = wall heat conduction resistance (K m² / W)
- k : thermal conductivity of the tube wall (W / m / K)
- ρ : density (kg/m³)
- μ : viscosity (kg/m/s)
- tube_r_fouling : tube side fouling resistance (K m² / W)
- shell_r_fouling : shell side fouling resistance (K m² / W)
- fcorrection_htc: correction factor for overall heat transfer
- f_arrangement: tube arrangement factor

Note: by default fcorrection_htc is set to 1, however, this variable can be used to match unit performance (i.e. as a parameter estimation problem using real plant data).

Tube arrangement factor is a config argument with two different type of arrangements supported at the moment: 1.- In-line tube arrangement factor (f_arrangement = 0.788), and 2.- Staggered tube arrangement factor (f_arrangement = 1). f_arrangement is a parameter that can be adjusted by the user.

The `BoilerHeatExchanger` includes an argument to compute heat transfer due to radiation of the flue gases. If `has_radiation = True` the model builds additional heat transfer calculations that will be added to the `hconv_shell` resistances. Radiation effects are calculated based on the gas gray fraction and gas-surface radiation (between gas and shell).

$$Gas_{grayfrac} = f(gas_{emissivity})$$

$$f_{rad_{gasgrayfrac}} = f(wall_{emissivity}, gas_{emissivity})$$

$$h_{conv_{shell,ad}} = f(k_{boltzmann}, f_{rad_{gasgrayfrac}}, T_{gasin}, T_{gasout}, T_{fluidin}, T_{fluidout})$$

Note: Gas emissivity is calculated with surrogate models (see more details in `boiler_heat_exchanger.py`). Radiation = True when flue gas temperatures are higher than 700 K (for example, when the model is used for units like Primary superheater, Reheater, or Finishing Superheater; while Radiation = False when the model is used to represent the economizer in a power plant flowsheet).

If pressure change is set to True, ΔP_{uturn} and $\Delta P_{friction}$ are calculated

Tube side:

$$\Delta P_{tube} = \Delta P_{tubefriction} + \Delta P_{tubeuturn} - elevation * g * \frac{\rho_{in} + \rho_{out}}{2}$$

$$\Delta P_{tubefriction} = f(tube_{di}, \rho, V_{tube}, numberoftubes, tube_{length})$$

$$\Delta P_{tubeuturn} = f(\rho, v_{tube}, k_{lossuturn})$$

where:

- $k_{lossuturn}$: pressure loss coefficient of a tube u-turn
- g : is the acceleration of gravity 9.807 (m/s²)

Shell side:

$$\Delta P_{shell} = 1.4 \Delta P_{shellfriction} \rho V_{shell}^2$$

$\Delta P_{shellfriction}$ is calculated based on the tube arrangement type:

$$\text{In-line: } \Delta P_{shellfriction} = \frac{0.044 + \frac{0.08 \left(\frac{P_x}{tube_{do}} \right)}{0.43 + \frac{1.13}{\left(\frac{P_y}{tube_{do}} - 1 \right)}}}{Re^{0.15}}$$

$$\text{Staggered: } \Delta P_{shellfriction} = \frac{0.25 + \frac{0.118}{\left(\frac{P_y}{tube_{do}} - 1 \right)^{1.08}}}{Re^{0.16}}$$

Figure. Tube Arrangement

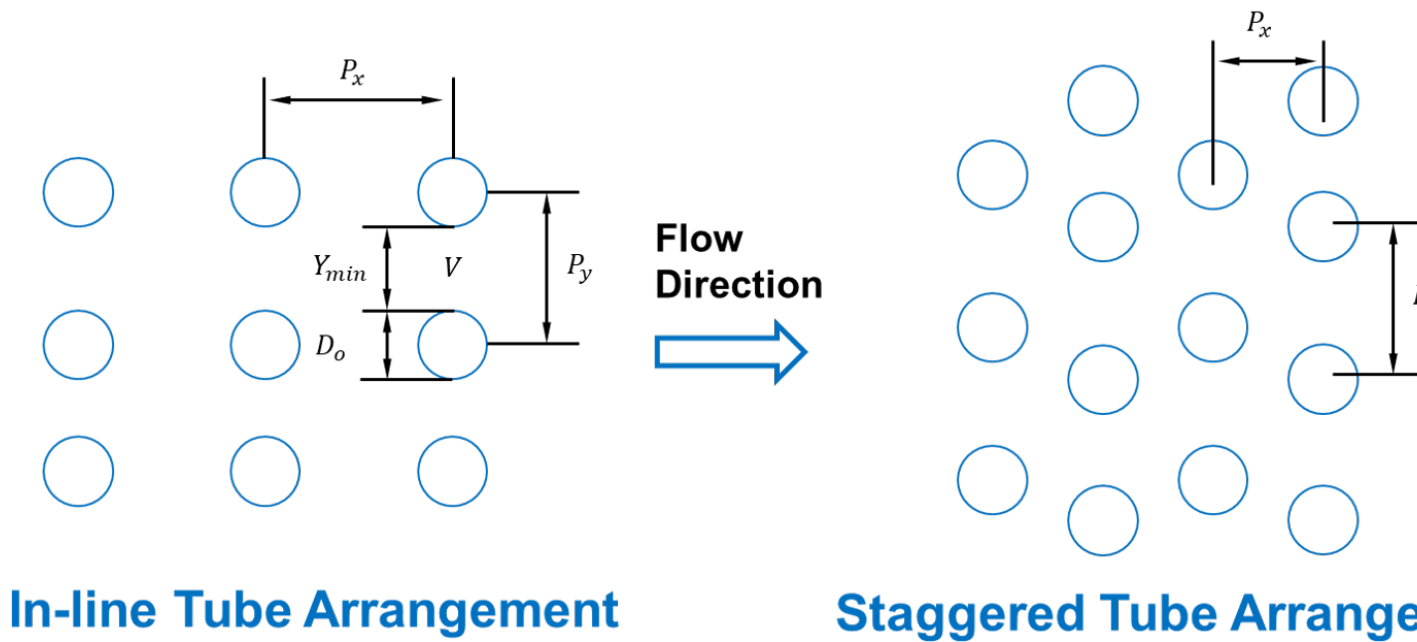


Fig. 3: Tube Arrangement

Class Documentation

Note: The `hot_side_config` and `cold_side_config` can also be supplied using the name of the hot and cold sides (`shell` and `tube` by default) as in [the example](#).

```
class idaes.power_generation.unit_models.boiler_heat_exchanger.BoilerHeatExchanger (*args,
**kwargs)
```

Parameters

- **rule** (*function*) – A rule function or None. Default rule calls `build()`.
- **concrete** (*bool*) – If True, make this a toplevel model. **Default** - False.
- **ctype** (*str*) – Pyomo ctype of the block. **Default** - “Block”

- **default** (*dict*) – Default ProcessBlockData config

Keys

dynamic Indicates whether this model will be dynamic or not, **default** = useDefault. **Valid values:** { **useDefault** - get flag from parent (default = False), **True** - set as a dynamic model, **False** - set as a steady-state model. }

has_holdup Indicates whether holdup terms should be constructed or not. Must be True if dynamic = True, **default** - False. **Valid values:** { **True** - construct holdup terms, **False** - do not construct holdup terms }

side_1_property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PhysicalParameterObject** - a PhysicalParameterBlock object. }

side_1_property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

side_2_property_package Property parameter object used to define property calculations, **default** - useDefault. **Valid values:** { **useDefault** - use default package from parent model or flowsheet, **PhysicalParameterObject** - a PhysicalParameterBlock object. }

side_2_property_package_args A ConfigBlock with arguments to be passed to a property block(s) and used when constructing these, **default** - None. **Valid values:** { see property package for documentation. }

material_balance_type Indicates what type of material balance should be constructed, **default** - MaterialBalanceType.componentPhase. **Valid values:** { **MaterialBalanceType.none** - exclude material balances, **MaterialBalanceType.componentPhase** - use phase component balances, **MaterialBalanceType.componentTotal** - use total component balances, **MaterialBalanceType.elementTotal** - use total element balances, **MaterialBalanceType.total** - use total material balance. }

energy_balance_type Indicates what type of energy balance should be constructed, **default** - EnergyBalanceType.enthalpyTotal. **Valid values:** { **EnergyBalanceType.none** - exclude energy balances, **EnergyBalanceType.enthalpyTotal** - single enthalpy balance for material, **EnergyBalanceType.enthalpyPhase** - enthalpy balances for each phase, **EnergyBalanceType.energyTotal** - single energy balance for material, **EnergyBalanceType.energyPhase** - energy balances for each phase. }

momentum_balance_type Indicates what type of momentum balance should be constructed, **default** - MomentumBalanceType.pressureTotal. **Valid values:** { **MomentumBalanceType.none** - exclude momentum balances, **MomentumBalanceType.pressureTotal** - single pressure balance for material, **MomentumBalanceType.pressurePhase** - pressure balances for each phase, **MomentumBalanceType.momentumTotal** - single momentum balance for material, **MomentumBalanceType.momentumPhase** - momentum balances for each phase. }

has_pressure_change Indicates whether terms for pressure change should be constructed, **default** - False. **Valid values:** { **True** - include pressure change terms, **False** - exclude pressure change terms. }

delta_T_method Flag indicating type of flow arrangement to use for delta **default** - DeltaTMethod.counterCurrent **Valid values:** { **DeltaTMethod.counterCurrent** }

tube_arrangement Tube arrangement could be in-line and staggered

side_1_water_phase Define water phase for property calls

has_radiation Define if side 2 gas radiation is to be considered

- **initialize** (*dict*) – ProcessBlockData config for individual elements. Keys are Block-Data indexes and values are dictionaries described under the “default” argument above.
- **idx_map** (*function*) – Function to take the index of a BlockData element and return the index in the initialize dict from which to read arguments. This can be provided to override the default behavior of matching the BlockData index exactly to the index in initialize.

Returns (BoilerHeatExchanger) New instance

class `idaes.power_generation.unit_models.boiler_heat_exchanger.BoilerHeatExchangerData` (*comp*)
Standard Heat Exchanger Unit Model Class

build ()

Build method for Boiler heat exchanger model

Parameters None –

Returns None

initialize (*state_args_1*={}, *state_args_2*={}, *outlvl*=0, *solver*='ipopt', *optarg*={'max_iter': 100, 'tol': 1e-06})

General Heat Exchanger initialisation routine.

Keyword Arguments

- **state_args_1** – a dict of arguments to be passed to the property package(s) for side 1 of the heat exchanger to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **state_args_2** – a dict of arguments to be passed to the property package(s) for side 2 of the heat exchanger to provide an initial state for initialization (see documentation of the specific property package) (default = {}).
- **outlvl** – sets output level of initialisation routine
 - 0 = no output (default)
 - 1 = return solver state for each step in routine
 - 2 = return solver state for each step in subroutines
 - 3 = include solver output information (tee=True)
- **optarg** – solver options dictionary object (default={'tol': 1e-6})
- **solver** – str indicating which solver to use during initialization (default = 'ipopt')

Returns None

model_check ()

Model checks for unit - calls model checks for both control volume Blocks.

Parameters None –

Returns None

Power Generation Properties

Flue Gas Property Package

A flue gas property package has been developed to provide properties of combustion gases and air. The ideal gas property package includes the main components in flue gas: O₂, N₂, NO, CO₂, H₂O, SO₂

Main parameters:

- molecular weight in kg/kg-mol indexed by component list,
- reference pressure & temperature in Pa and Kelvin,
- critical pressure and temperature in Pa and Kelvin indexed by component list,
- gas constant in J/(mol K),
- constants for specific heat capacity in J/(mol K) indexed by component list and parameter A to H,
- vapor pressure coefficients (Antoine Eq.) P in Bar and T in K indexed by component list and parameters A to C,

Source: NIST webbook (last update: 01/08/2020)

The main methods supported are:

- heat capacity in J/(mol K),
- enthalpy in J/mol,
- entropy in J/(mol K),
- volumetric flowrate m³/s,
- viscosity of mixture in kg/(m s),
- thermal conductivity mixture in J / (m K s),
- molar density m³/mol,
- reduced pressure and temperature (unitless),

Power Generation Flowsheets

Supercritical Coal-Fired Power Plant Flowsheet

This is an example supercritical pulverized coal (SCPC) power plant. This simulation model consist of a ~595 MW gross coal fired

The dimensions and operating conditions used for this simulation do not represent any specific coal-fired power plant.

This model is for demonstration and tutorial purposes only. Before looking at the model, it may be useful to look at the process flow diagram (PFD).

SCPC Power Plant (simplified description)

Inputs:

- Throttle valve opening,
- Feed water pump pressure,
- BFW - boiler feed water (from Feed water heaters),
- Coal from pulverizers

Main Assumptions:

Coal flowrate is a function of the plant load, the coal HHV is fixed and heat duty from fire side to water wall and platen superheater are fixed.

Boiler heat exchanger network:

Water Flow: Fresh water -> FWH's -> Economizer -> Water Wall -> Primary SH -> Platen SH -> Finishing Superheater -> HP Turbine -> Reheater -> IP Turbine

Flue Gas Flow:

Fire Ball -> Platen SH -> Finishing SH -> Reheater -> o -> Economizer -> Air Preheater
-> Primary SH -^

Steam Flow: Boiler -> HP Turbine -> Reheater -> IP Turbine -> Condenser HP, IP, and LP steam extractions to Feed Water Heaters

Main Models used:

- Mixers: Attenuator, Flue gas mix
- Heater: Platen SH, Fire/Water side (simplified model), Feed Water Heaters, Hot Tank, Condenser
- **BoilerHeatExchanger: Economizer, Primary SH, Finishing SH, Reheater**
 - **Shell and tube heat exchanger**
 - * tube side: Steam (side 1 holdup)
 - * shell side: flue gas (side 2 holdup)
- Steam Turbines
- Pumps

Property packages used:

- IAPWS: Water/steam side
- IDEAL GAS: Flue Gas side

Figures Process Flow Diagram:

4.10 Data Management Framework

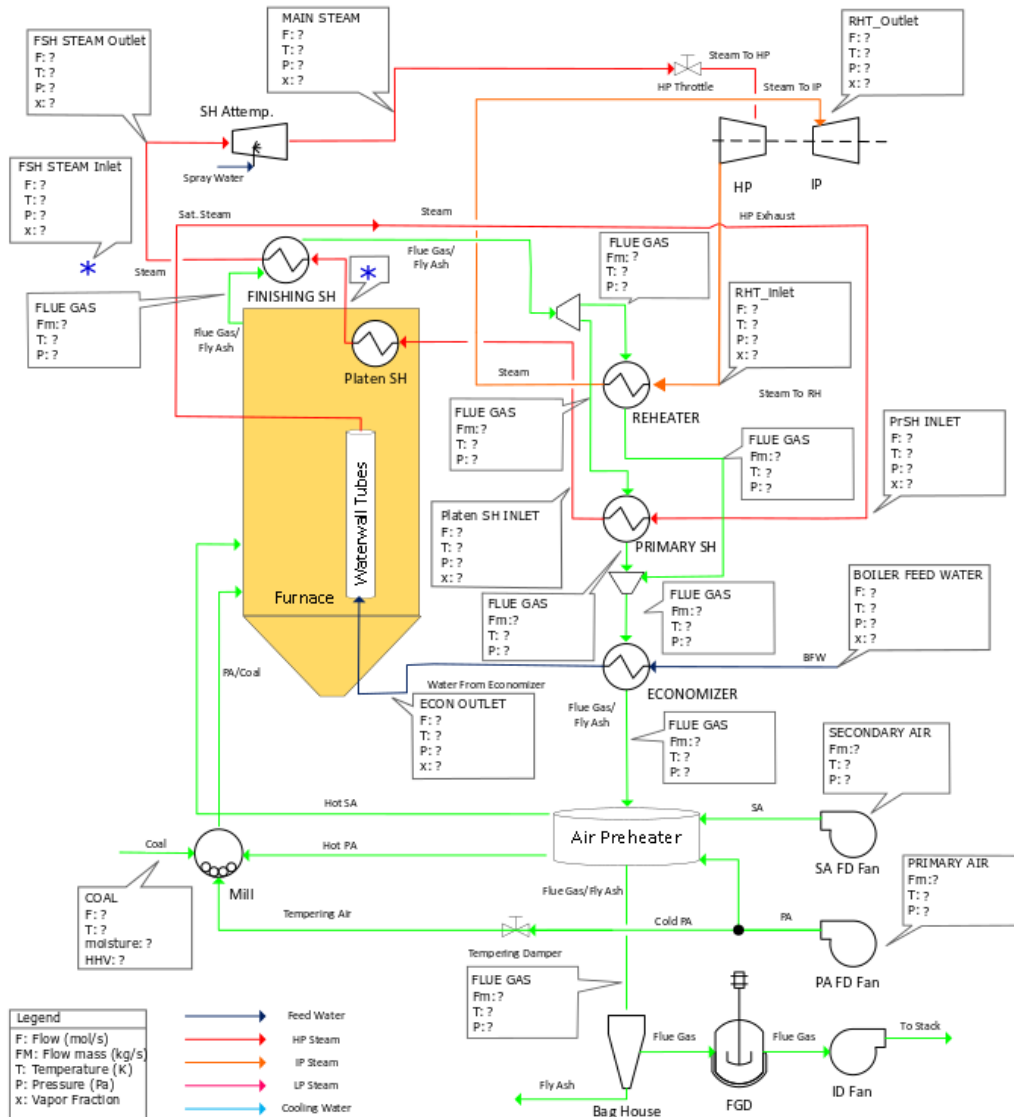
4.10.1 DMF Command-line Interface

This page lists the commands and options for the DMF command-line interface, which is a Python program called *dmf*. There are several usage examples for each sub-command. These examples assume the UNIX *bash* shell.

Contents

- *DMF Command-line Interface*
 - *dmf*
 - *dmf find*
 - *dmf info*
 - *dmf init*
 - *dmf ls*

SUPERCritical BOILER HX NETWORK FLOWSHEET



- *dmf register*
- *dmf related*
- *dmf rm*
- *dmf status*

dmf

Data management framework command wrapper. This base command has some options for verbosity that can be applied to any sub-command.

dmf options

-v

--verbose

Increase verbosity. Show warnings if given once, then info, and then debugging messages.

-q

--quiet

Increase quietness. If given once, only show critical messages. If given twice, show no messages.

dmf usage

Run sub-command with logging at level “error”:

```
$ dmf <sub-command>
```

Run sub-command and log warnings:

```
$ dmf <sub-command>
```

Run sub-command and log informational / warning messages:

```
$ dmf -vv <sub-command>
```

Run sub-command only logging fatal errors:

```
$ dmf -q <sub-command>
```

Run sub-command with no logging at all:

```
$ dmf -qq <sub-command>
```

dmf subcommands

The subcommands are listed alphabetically below. For each, keep in mind that any unique prefix of that command will be accepted. For example, for `dmf init`, the user may also type `dmf ini`. However, `dmf in` will not work because that would also be a valid prefix for `dmf info`.

In addition, there are some aliases for some of the sub-commands:

- `dmf info` => *dmf resource* or *dmf show*
- `dmf ls` => *dmf list*
- `dmf register` => *dmf add*
- `dmf related` => *dmf graph*
- `dmf rm` => *dmf delete*
- `dmf status` => *dmf describe*

usage overview

To give a feel for the context in which you might actually run these commands, below is a simple example that uses each command:

```
# create a new workspace
$ dmf init ws --name workspace --desc "my workspace" --create
Configuration in '/home/dang/src/idaes/dangunter/idaes-dev/docs/ws/config.yaml'

# view status of the workspace
$ dmf status
settings:
  workspace: /home/myuser/ws
workspace:
  location: /home/myuser/ws
  name: workspace
  description: my workspace
  created: 2019-04-20 08:32:59
  modified: 2019-04-20 08:32:59

# add some resources from files
$ echo "one" > oldfile ; echo "two" > newfile
$ dmf register oldfile --version 0.0.1
2792c0ceb0734ed4b302c44884f2d404
$ dmf register newfile --version 0.0.2 --prev 2792c0ceb0734ed4b302c44884f2d404
6ddee9bb2bb3420ab10aaf4c74d186f6

# list the current workspace contents
$ dmf ls
id   type desc      modified
792  data oldfile 2019-04-20 15:33:11
6dde data newfile 2019-04-20 15:33:23

# look at one one resource (newfile)
$ dmf info 6dde
Resource 6ddee9bb2bb3420ab10aaf4c74d186f6
created
  '2019-04-20 15:33:23'
creator
  name: dang
datafiles
  - desc: newfile
    is_copy: true
    path: newfile
    sha1: 7bbef45b3bc70855010e02460717643125c3beca
```

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```

datafiles_dir
  /home/myuser/ws/files/8027bf92628f41a0b146a5167d147e9d
desc
  newfile
doc_id
  2
id_
  6ddee9bb2bb3420ab10aaf4c74d186f6
modified
  '2019-04-20 15:33:23'
relations
  - 2792c0ceb0734ed4b302c44884f2d404 --[version]--> ME
type
  data
version
  0.0.2 @ 2019-04-20 15:33:23

# see relations
$ dmf related 2792
2792 data
    └──version├ 6dde data -

# remove the "old" file
$ dmf rm 2792
id                type desc      modified
2792c0ceb0734ed4b302c44884f2d404 data oldfile 2019-04-20 15:33:11
Remove this resource [y/N]? y
resource removed

$ dmf ls
id  type desc      modified
6dde data newfile 2019-04-20 15:33:23

```

dmf find

Search for resources by a combination of their fields. Several convenient fields are provided. At this time, a comprehensive capability to search on any field is not available.

dmf find options

In addition to the options below, this command also accepts all the *dmf ls options*, although the `--color/` `--no-color` option is ignored for JSON output.

--output value

Output style/format. Possible values:

list (Default) Show results as a listing, as from the *ls* subcommand.

info Show results as individual records, as from the *info* subcommand.

json Show results are JSON objects

--by value

Look for “value” in the value of the *creator.name* field.

--created value

Use “value” as a date or date range and filter on records that have a *created* date in that range. Dates should be in the form:

```
YYYY-MM-DD[*HH[:MM[:SS[.fff[fff]]]]][+HH:MM[:SS[.ffffff]]]
```

To indicate a date range, separate two dates with a “..”.

- 2012-03-19: On March 19, 2012
- 2012-03-19..2012-03-22: From March 19 to March 22, 2012
- 2012-03-19..: After March 19, 2012
- ..2012-03-19: Before March 19, 2012

Note that times may also be part of the date strings.

--file value

Look for “value” in the value of the *desc* field in one of the *datafiles*.

--modified value

Use “value” as a date or date range and filter on records that have a *modified* date in that range. See **--created** for details on the date format.

--name value

Look for “value” as one of the values of the *alias* field.

--type value

Look for “value” as the value of the *type* field.

dmf find usage

By default, find will essentially provide a filtered listing of resources. If used without options, it is basically an alias for *ls*.

```
$ dmf ls
id  type desc      modified
2517 data file1.txt 2019-04-29 17:29:00
344c data file2.txt 2019-04-29 17:29:01
5d98 data A        2019-04-29 17:28:41
602a data B        2019-04-29 17:28:56
8c55 data C        2019-04-29 17:28:58
9cbe data D        2019-04-29 17:28:59
$ dmf find
id  type desc      modified
2517 data file1.txt 2019-04-29 17:29:00
344c data file2.txt 2019-04-29 17:29:01
5d98 data A        2019-04-29 17:28:41
602a data B        2019-04-29 17:28:56
8c55 data C        2019-04-29 17:28:58
9cbe data D        2019-04-29 17:28:59
```

The find-specific options add filters. In the example below, the find filters for files that were modified after the given date and time.

```
$ dmf find --modified 2019-04-29T17:29:00..  
id   type desc      modified  
2517 data file1.txt 2019-04-29 17:29:00  
344c data file2.txt 2019-04-29 17:29:01
```

dmf info

Show detailed information about a resource. This command may also be referred to as `dmf show`.

dmf info options

identifier

Identifier, or unique prefix thereof, of the resource. Any unique prefix of the identifier will work, but if that prefix matches multiple identifiers, you need to add `--multiple` to allow multiple records in the output.

--multiple

Allow multiple records in the output (see *identifier*)

-f, --format value

Output format. Accepts the following values:

term Terminal output (colored, if the terminal supports it), with values that are empty left out and some values simplified for easy reading.

json Raw JSON value for the resource, with newlines and indents for readability.

jsonc Raw JSON value for the resource, “compact” version with no extra whitespace added.

dmf info usage

The default is to show, with some terminal colors, a summary of the resource:

```
$ dmf info 0b62  
  
Resource 0b62d999f0c44b678980d6a5e4f5d37d  
  
created  
  '2019-03-23 17:49:35'  
creator  
  name: dang  
datafiles  
  - desc: foo13  
    is_copy: true  
    path: foo13  
    sha1: feee44ad365b6b1ec75c5621a0ad067371102854  
datafiles_dir  
  /home/dang/src/idaes/dangunter/idaes-dev/ws2/files/  
→ 71d101327d224302aa8875802ed2af52  
desc  
  foo13  
doc_id  
  4
```

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```

id_
  0b62d999f0c44b678980d6a5e4f5d37d
modified
  '2019-03-23 17:49:35'
relations
  - 1e41e6ae882b4622ba9043f4135f2143 --[derived]--> ME
type
  data
version
  0.0.0 @ 2019-03-23 17:49:35

```

The same resource in JSON format:

```

$ dmf info --format json 0b62
{
  "id_": "0b62d999f0c44b678980d6a5e4f5d37d",
  "type": "data",
  "aliases": [],
  "codes": [],
  "collaborators": [],
  "created": 1553363375.817961,
  "modified": 1553363375.817961,
  "creator": {
    "name": "dang"
  },
  "data": {},
  "datafiles": [
    {
      "desc": "foo13",
      "path": "foo13",
      "sha1": "feee44ad365b6b1ec75c5621a0ad067371102854",
      "is_copy": true
    }
  ],
  "datafiles_dir": "/home/dang/src/idaes/dangunter/idaes-dev/ws2/files/
↪ 71d101327d224302aa8875802ed2af52",
  "desc": "foo13",
  "relations": [
    {
      "predicate": "derived",
      "identifier": "1e41e6ae882b4622ba9043f4135f2143",
      "role": "object"
    }
  ],
  "sources": [],
  "tags": [],
  "version_info": {
    "created": 1553363375.817961,
    "version": [
      0,
      0,
      0,
      ""
    ],
    "name": ""
  },
  "doc_id": 4
}

```

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```
}
```

And one more time, in “compact” JSON:

```
$ dmf info --format jsonc 0b62
{"id_": "0b62d999f0c44b678980d6a5e4f5d37d", "type": "data", "aliases": [], "codes":
↪ [], "collaborators": [], "created": 1553363375.817961, "modified": 1553363375.
↪ 817961, "creator": {"name": "dang"}, "data": {}, "datafiles": [{"desc": "foo13",
↪ "path": "foo13", "sha1": "feee44ad365b6blec75c5621a0ad067371102854", "is_copy":
↪ true}], "datafiles_dir": "/home/dang/src/idaes/dangunter/idaes-dev/ws2/files/
↪ 71d101327d224302aa8875802ed2af52", "desc": "foo13", "relations": [{"predicate":
↪ "derived", "identifier": "1e41e6ae882b4622ba9043f4135f2143", "role": "object"}],
↪ "sources": [], "tags": [], "version_info": {"created": 1553363375.817961, "version
↪ ": [0, 0, 0, ""], "name": ""}, "doc_id": 4}
```

dmf init

Initialize the current workspace. Optionally, create a new workspace.

dmf init options

path

Use the provided `path` as the workspace path. This is required.

--create

Create a new workspace at location provided by `path`. Use the `--name` and `--desc` options to set the workspace name and description, respectively. If these are not given, they will be prompted for interactively.

--name

Workspace name, used by `--create`

--desc

Workspace description, used by `--create`

dmf init usage

Note: In the following examples, the current working directory is set to `/home/myuser`.

This command sets a value in the user-global configuration file in `.dmf`, in the user’s home directory, so that all other dmf commands know which workspace to use. With the `--create` option, a new empty workspace can be created.

Create new workspace in sub-directory `ws`, with given name and description:

```
$ dmf init ws --create --name "foo" --desc "foo workspace description"
Configuration in '/home/myuser/ws/config.yaml'
```

Create new workspace in sub-directory `ws`, providing the name and description interactively:

```
$ dmf init ws --create
New workspace name: foo
New workspace description: foo workspace description
Configuration in '/home/myuser/ws/config.yaml'
```

Switch to workspace ws2:

```
$ dmf init ws2
```

If you try to switch to a non-existent workspace, you will get an error message:

```
$ dmf init doesnotexist
Existing workspace not found at path='doesnotexist'
Add --create flag to create a workspace.
$ mkdir some_random_directory
$ dmf init some_random_directory
Workspace configuration not found at path='some_random_directory/'
```

If the workspace exists, you cannot create it:

```
$ dmf init ws --create --name "foo" --desc "foo workspace description"
Configuration in '/home/myuser/ws/config.yaml'
$ dmf init ws --create
Cannot create workspace: path 'ws' already exists
```

And, of course, you can't create workspaces anywhere you don't have permissions to create directories:

```
$ mkdir forbidden
$ chmod 000 forbidden
$ dmf init forbidden/ws --create
Cannot create workspace: path 'forbidden/ws' not accessible
```

dmf ls

This command lists resources in the current workspace.

dmf ls options

--color

Allow (if terminal supports it) colored terminal output. This is the default.

--no-color

Disallow, even if terminal supports it, colored terminal output.

-s, --show

Pick field to show in output table. This option can be repeated to show any known subset of fields. Also the option value can have commas in it to hold multiple fields. Default fields, if this option is not specified at all, are “type”, “desc”, and “modified”. The resource identifier field is always shown first.

codes List name of code(s) in resource. May be shortened with ellipses.

created Date created.

desc Description of resource.

files List names of file(s) in resource. May be shortened with ellipses.

modified Date modified.

type Name of the type of resource.

version Resource version.

You can specify other fields from the schema, as long as they are not arrays of objects, i.e. you can say `--show tags` or `--show version_info.version`, but `--show sources` is too complicated for a tabular listing. To see detailed values in a record use the *dmf info* command.

-S, --sort

Sort by given field; if repeated, combine to make a compound sort key. These fields are a subset of those in *-s*, *--show*, with the addition of `id` for sorting by the identifier: “id”, “type”, “desc”, “created”, “modified”, and/or “version”.

--no-prefix

By default, shown identifier is the shortest unique prefix, but if you don’t want the identifier shortened, this option will force showing it in full.

-r, --reverse

Reverse the order of the sorting given by (or implied by absence of) the *-S*, *--sort* option.

dmf ls usage

Note: In the following examples, the current working directory is set to `/home/myuser` and the workspace is named `ws`.

Without arguments, show the resources in an arbitrary (though consistent) order:

```
$ dmf ls
id  type desc  modified
0b62 data foo13 2019-03-23 17:49:35
1e41 data foo10 2019-03-23 17:47:53
6c9a data foo14 2019-03-23 17:51:59
d3d5 data bar1  2019-03-26 13:07:02
e780 data foo11 2019-03-23 17:48:11
eb60 data foo12 2019-03-23 17:49:08
```

Add a sort key to sort by, e.g. modified date

```
$ dmf ls -S modified
id  type desc  modified
1e41 data foo10 2019-03-23 17:47:53
e780 data foo11 2019-03-23 17:48:11
eb60 data foo12 2019-03-23 17:49:08
0b62 data foo13 2019-03-23 17:49:35
6c9a data foo14 2019-03-23 17:51:59
d3d5 data bar1  2019-03-26 13:07:02
```

Especially for resources of type “data”, showing the first (possibly only) file that is referred to by the resource is useful:


```
$ dmf ls -S modified -s type -s modified -s files
id      type modified      files
1e41 data 2019-03-23 17:47:53 foo10
e780 data 2019-03-23 17:48:11 foo11
eb60 data 2019-03-23 17:49:08 foo12
0b62 data 2019-03-23 17:49:35 foo13
6c9a data 2019-03-23 17:51:59 foo14
d3d5 data 2019-03-26 13:07:02 bar1
```

Note that you don't actually have to show a field to sort by it (compare sort order with results from command above):

```
$ dmf ls -S modified -s type -s files
id      type files
1e41 data foo10
e780 data foo11
eb60 data foo12
0b62 data foo13
6c9a data foo14
d3d5 data bar1
```

Add `--no-prefix` to show the full identifier:

```
$ dmf ls -S modified -s type -s files --no-prefix
id                                     type files
1e41e6ae882b4622ba9043f4135f2143 data foo10
e7809d25b390453487998e1f1ef0e937 data foo11
eb606172dde74aa79eea027e7eb6a1b6 data foo12
0b62d999f0c44b678980d6a5e4f5d37d data foo13
6c9a85629cb24e9796a2d123e9b03601 data foo14
d3d5981106ce4d9d8cccd4e86c2cd184 data bar1
```

dmf register

Register a new resource with the DMF, using a file as an input. An alias for this command is `dmf add`.

dmf register options

`--no-copy`

Do not copy the file, instead remember path to current location. Default is to copy the file under the workspace directory.

`-t, --type`

Explicitly specify the type of resource. If this is not given, then try to infer the resource type from the file. The default will be 'data'. The full list of resource types is in `idaes.dmf.resource.RESOURCE_TYPES`

`--strict`

If inferring the type fails, report an error. With `--no-strict`, or no option, if inferring the type fails, fall back to importing as a generic file.

`--no-unique`

Allow duplicate files. The default is `--unique`, which will stop and print an error if another resource has a file matching this file's name and contents.

--contained resource

Add a 'contained in' relation to the given resource.

--derived resource

Add a 'derived from' relation to the given resource.

--used resource

Add a 'used by' relation to the given resource.

--prev resource

Add a 'version of previous' relation to the given resource.

--is-subject

If given, reverse the sense of any relation(s) added to the resource so that the newly created resource is the subject and the existing resource is the object. Otherwise, the new resource is the object of the relation.

--version

Set the semantic version of the resource. From 1 to 4 part semantic versions are allowed, e.g.

- 1
- 1.0
- 1.0.1
- 1.0.1-alpha

See <http://semver.org> and the function `idaes.dmf.resource.version_list()` for more details.

dmf register usage

Note: In the following examples, the current working directory is set to `/home/myuser` and the workspace is named `ws`.

Register a new file, which is a CSV data file, and use the `--info` option to show the created resource.

```
$ printf "index,time,value\n1,0.1,1.0\n2,0.2,1.3\n" > file.csv
$ dmf reg file.csv --info
Resource 117a42287aec4c5ca333e0ff3ac89639
created
  '2019-04-11 03:58:52'
creator
  name: dang
datafiles
  - desc: file.csv
    is_copy: true
    path: file.csv
    sha1: f1171a6442bd6ce22a718a0e6127866740c9b52c
datafiles_dir
  /home/myuser/ws/files/4db42d92baf3431ab31d4f91ab1a673b
desc
  file.csv
doc_id
  1
```

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```
id_
  117a42287aec4c5ca333e0ff3ac89639
modified
  '2019-04-11 03:58:52'
type
  data
version
  0.0.0 @ 2019-04-11 03:58:52
```

If you try to register (add) the same file twice, it will be an error by default. You need to add the `--no-unique` option to allow it.

```
$ printf "index,time,value\n1,0.1,1.0\n2,0.2,1.3\n" > timeseries.csv
$ dmf add timeseries.csv
2315bea239c147e4bc6d2e1838e4101f
$ dmf add timeseries.csv
This file is already in 1 resource(s): 2315bea239c147e4bc6d2e1838e4101f
$ dmf add --no-unique timeseries.csv
3f95851e4931491b995726f410998491
```

If you register a file ending in “.json”, it will be parsed (unless it is over 1MB) and, if it passes, registered as type JSON. If the parse fails, it will be registered as a generic file *unless* the `--strict` option is given (with this option, failure to parse will be an error):

```
$ echo "totally bogus" > notreally.json
$ dmf reg notreally.json
2019-04-12 06:06:47,003 [WARNING] idaes.dmf.resource: File ending in '.json' is not
↳ valid JSON: treating as generic file
d22727c678a1499ab2c5224e2d83d9df
$ dmf reg --strict notreally.json
Failed to infer resource: File ending in '.json' is not valid JSON
```

You can explicitly specify the type of the resource with the `-t, --type` option. In that case, any failure to validate will be an error. For example, if you say the resource is a Jupyter Notebook file, and it is not, it will fail. But the same file with type “data” will be fine:

```
$ echo "Ceci n'est pas une notebook" > my.ipynb
$ dmf reg -t notebook my.ipynb
Failed to load resource: resource type 'notebook': not valid JSON
$ dmf reg -t data my.ipynb
0197a82abab44ecf980d6e42e299b258
```

You can add links to existing resources with the options `--contained`, `--derived`, `--used`, and `--prev`. For all of these, the new resource being registered is the target of the relation and the option argument is the identifier of an existing resource that is the subject of the relation.

For example, here we add a “shoebox” resource and then some “shoes” that are contained in it:

```
$ touch shoebox.txt shoes.txt closet.txt
$ dmf add shoebox.txt
755374b6503a47a09870dfbdc572e561
$ dmf add shoes.txt --contained 755374b6503a47a09870dfbdc572e561
dba0a5dc7d194040ac646bf18ab5eb50
$ dmf info 7553 # the "shoebox" contains the "shoes"
Resource 755374b6503a47a09870dfbdc572e561
created
```

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```

    '2019-04-11 20:16:50'
  creator
    name: dang
  datafiles
    - desc: shoebox.txt
      is_copy: true
      path: shoebox.txt
      sha1: da39a3ee5e6b4b0d3255bfef95601890afd80709
  datafiles_dir
    /home/dang/src/idaes/dangunter/idaes-dev/docs/ws/files/
→ 7f3ff820676b41689bb32bc325fd2d1b
  desc
    shoebox.txt
  doc_id
    9
  id_
    755374b6503a47a09870dfbdc572e561
  modified
    '2019-04-11 20:16:50'
  relations
    - dba0a5dc7d194040ac646bf18ab5eb50 <--[contains]-- ME
  type
    data
  version
    0.0.0 @ 2019-04-11 20:16:50

$ dmf info dba0 # the "shoes" are in the "shoebox"
                    Resource dba0a5dc7d194040ac646bf18ab5eb50
  created
    '2019-04-11 20:17:28'
  creator
    name: dang
  datafiles
    - desc: shoes.txt
      is_copy: true
      path: shoes.txt
      sha1: da39a3ee5e6b4b0d3255bfef95601890afd80709
  datafiles_dir
    /home/dang/src/idaes/dangunter/idaes-dev/docs/ws/files/
→ a27f98c24d1848eabalb26e5ef87be88
  desc
    shoes.txt
  doc_id
    10
  id_
    dba0a5dc7d194040ac646bf18ab5eb50
  modified
    '2019-04-11 20:17:28'
  relations
    - 755374b6503a47a09870dfbdc572e561 --[contains]--> ME
  type
    data
  version
    0.0.0 @ 2019-04-11 20:17:28

```

To reverse the sense of the relation, add the `--is-subject` flag. For example, we now add a “closet” resource that contains the existing “shoebox”. This means the shoebox now has two different “contains” type of relations.

```

$ dmf add closet.txt --is-subject --contained 755374b6503a47a09870dfbdc572e561
22ace0f8ed914fa3ac3e7582748924e4
$ dmf info 7553
                                Resource 755374b6503a47a09870dfbdc572e561
created
  '2019-04-11 20:16:50'
creator
  name: dang
datafiles
  - desc: shoebox.txt
    is_copy: true
    path: shoebox.txt
    sha1: da39a3ee5e6b4b0d3255bfef95601890afd80709
datafiles_dir
  /home/dang/src/idaes/dangunter/idaes-dev/docs/ws/files/
↪ 7f3ff820676b41689bb32bc325fd2d1b
desc
  shoebox.txt
doc_id
  9
id_
  755374b6503a47a09870dfbdc572e561
modified
  '2019-04-11 20:16:50'
relations
  - dba0a5dc7d194040ac646bf18ab5eb50 <--[contains]-- ME
  - 22ace0f8ed914fa3ac3e7582748924e4 --[contains]--> ME
type
  data
version
  0.0.0 @ 2019-04-11 20:16:50

```

You can give your new resource a version with the `--version` option. You can use this together with the `--prev` option to link between multiple versions of the same underlying data:

```

# note: following command stores the output of "dmf reg", which is the
#       id of the new resource, in the shell variable "oldid"
$ oldid=$( dmf reg oldfile.py --type code --version 0.0.1 )
$ dmf reg newfile.py --type code --version 0.0.2 --prev $oldid
ef2d801ca29a4a0a8c6f79ee71d3fe07
$ dmf ls --show type --show version --show codes --sort version
id  type version codes
44e7 code 0.0.1  oldfile.py
ef2d code 0.0.2  newfile.py
$ dmf related $oldid
44e7 code
    |
    |version| ef2d code -

```

dmf related

This command shows resources related to a given resource.

dmf related options

-d, --direction

Direction of relationships to show / follow. The possible values are:

in Show incoming connection/relationship edges. Since all relations have a bi-directional counterpart, this effectively only shows the immediate neighbors of the root resource. For example, if the root resource is “A”, and “A” *contains* “B” and “B” *contains* “C”, then this option shows the incoming edge from “B” to “A” but not the edge from “C” to “B”.

out (Default) Show the outgoing connection/relationship edges. This will continue until there are no more connections to show, avoiding cycles. For example, if the root resource is “A”, and “A” *contains* “B” and “B” *contains* “C”, then this option shows the outgoing edge from “A” to “B” and also from “B” to “C”.

The default value is `out`.

--color

Allow (if terminal supports it) colored terminal output. This is the default.

--no-color

Disallow, even if terminal supports it, colored terminal output.

--unicode

Allow unicode drawing characters in the output. This is the default.

--no-unicode

Use only ASCII characters in the output.

dmf related usage

In the following examples, we work with 4 resources arranged as a fully connected square (A, B, C, D). This is not currently possible just with the command-line, but the following Python code does the job:

```
from idaes.dmf import DMF, resource
dmf = DMF()
rlist = [resource.Resource(value={"desc": ltr, "aliases": [ltr],
                                "tags": ["graph"]})
          for ltr in "ABCD"]
relation = resource.PR_USES
for r in rlist:
    for r2 in rlist:
        if r is r2:
            continue
        resource.create_relation_args(r, relation, r2)
for r in rlist:
    dmf.add(r)
```

If you save that script as `r4.py`, then the following command-line actions will run it and verify that everything is created.

```
$ python r4.py
$ dmf ls
id  type  desc modified
1e7f other B    2019-04-20 15:43:49
3bc5 other D    2019-04-20 15:43:49
```

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```
ba67 other A    2019-04-20 15:43:49
f7e9 other C    2019-04-20 15:43:49
```

You can then see the connections by looking at any one of the four resource (e.g., A):

```
$ dmf rel ba67
ba67 other A
  |
  |--uses|-- 3bc5 other D
  |
  |--uses|-- f7e9 other C
  |
  |--uses|-- 1e7f other B
  |
  |--uses|-- ba67 other A
  |
  |--uses|-- f7e9 other C
  |
  |--uses|-- 3bc5 other D
  |
  |--uses|-- 1e7f other B
  |
  |--uses|-- ba67 other A
  |
  |--uses|-- 1e7f other B
  |
  |--uses|-- 3bc5 other D
  |
  |--uses|-- f7e9 other C
  |
  |--uses|-- ba67 other A
```

If you change the direction of relations, you will get much the same result, but with the arrows reversed.

dmf rm

Remove one or more resources. This also removes relations (links) to other resources.

dmf rm options

identifier

The identifier, or identifier prefix, of the resource(s) to remove

--list, --no-list

With the `-list` option, which is the default, the resources to remove, or removed, will be listed as if by the `dmf ls` command. With `-no-list`, then do not produce this output.

-y, --yes

If given, do not confirm removal of the resource(s) with a prompt. This is useful for scripts that do not want to bother with input, or people with lots of confidence.

--multiple

If given, allow multiple resources to be selected by an identifier prefix. Otherwise, if the given identifier matches more than one resource, the program will print a message and stop.

dmf rm usage

Note: In the following examples, there are 5 text files named “file1.txt”, “file2.txt”, ..., “file5.txt”, in the workspace. The identifiers for these files may be different in each example.

Remove one resource, by its full identifier:

```
$ dmf ls --no-prefix
id                                type desc          modified
096aa2491e234c4b941f32b537dd3017 data file5.txt     2019-04-16 02:51:30
821fc8f8e54e4c65b481f483be7f5a2d data file4.txt     2019-04-16 02:51:29
c20f3a6e338a40ee8a3a4972544adb74 data file1.txt     2019-04-16 02:51:25
c8f2b5cb80824e649008c414db5287f7 data file3.txt     2019-04-16 02:51:28
cd62e3bcb9a4459c9f2f5405ca442961 data file2.txt     2019-04-16 02:51:26
$ dmf rm c20f3a6e338a40ee8a3a4972544adb74
id                                type desc          modified
c20f3a6e338a40ee8a3a4972544adb74 data file1.txt     2019-04-16 02:51:25
Remove this resource [y/N]? y
resource removed
[dmfcli-167 !?]idaes-dev$ dmf ls --no-prefix
id                                type desc          modified
096aa2491e234c4b941f32b537dd3017 data file5.txt     2019-04-16 02:51:30
821fc8f8e54e4c65b481f483be7f5a2d data file4.txt     2019-04-16 02:51:29
c8f2b5cb80824e649008c414db5287f7 data file3.txt     2019-04-16 02:51:28
cd62e3bcb9a4459c9f2f5405ca442961 data file2.txt     2019-04-16 02:51:26
```

Remove a single resource by its prefix:

```
$ dmf ls
id  type desc          modified
6dd5 data file2.txt     2019-04-16 18:51:10
7953 data file3.txt     2019-04-16 18:51:12
7a06 data file4.txt     2019-04-16 18:51:13
e5d7 data file1.txt     2019-04-16 18:51:08
fe0c data file5.txt     2019-04-16 18:51:15
$ dmf rm 6d
id                                type desc          modified
6dd57ecc50a24efb824a66109dda0956 data file2.txt     2019-04-16 18:51:10
Remove this resource [y/N]? y
resource removed
$ dmf ls
id  type desc          modified
7953 data file3.txt     2019-04-16 18:51:12
7a06 data file4.txt     2019-04-16 18:51:13
e5d7 data file1.txt     2019-04-16 18:51:08
fe0c data file5.txt     2019-04-16 18:51:15
```

Remove multiple resources that share a common prefix. In this case, use the `-y`, `--yes` option to remove without prompting.


```
$ dmf ls
id      type desc      modified
7953 data file3.txt 2019-04-16 18:51:12
7a06 data file4.txt 2019-04-16 18:51:13
e5d7 data file1.txt 2019-04-16 18:51:08
fe0c data file5.txt 2019-04-16 18:51:15
$ dmf rm --multiple --yes 7
id      type desc      modified
7953e67db4a543419b9988c52c820b68 data file3.txt 2019-04-16 18:51:12
7a06435c39b54890a3d01a9eab114314 data file4.txt 2019-04-16 18:51:13
2 resources removed
$ dmf ls
id      type desc      modified
e5d7 data file1.txt 2019-04-16 18:51:08
fe0c data file5.txt 2019-04-16 18:51:15
```

dmf status

This command shows basic information about the current active workspace and, optionally, some additional details. It does not (yet) give any way to modify the workspace configuration. To do that, you need to edit the `config.yaml` file in the workspace root directory. See [Configuration](#).

dmf status options

--color

Allow (if terminal supports it) colored terminal output. This is the default.

--no-color

Disallow, even if terminal supports it, colored terminal output. UNIX output streams to pipes should be detected and have color disabled, but this option can force that behavior if detection is failing.

-s, --show info

Show one of the following types of information:

files Count and total size of files in workspace

htmldocs Configured paths to the HTML documentation (for “%dmf help” magic in the Jupyter Notebook)

logging Configuration for logging

all Show all items above

-a, --all

This option is just an alias for “--show all”.

dmf status usage

Note: In the following examples, the current working directory is set to `/home/myuser` and the workspace is named `ws`.

Also note that the output shown below is plain (black) text. This is due to our limited understanding of how to do colored text in our documentation tool (Sphinx). In a color-capable terminal, the output will be more colorful.

Show basic workspace status:

```
$ dmf status
settings:
  workspace: /home/myuser/ws
workspace:
  location: /home/myuser/ws
  name: myws
  description: my workspace
  created: 2019-04-09 12:46:40
  modified: 2019-04-09 12:46:40
```

Add the file information:

```
$ dmf status --show files
settings:
  workspace: /home/myuser/ws
workspace:
  location: /home/myuser/ws
  name: myws
  description: my workspace
  created: 2019-04-09 12:52:49
  modified: 2019-04-09 12:52:49
files:
  count: 3
  total_size: 1.3 MB
```

You can repeat the `-s`, `--show` option to add more things:

```
$ dmf status --show files --show htmldocs
settings:
  workspace: /home/myuser/ws
workspace:
  location: /home/myuser/ws
  name: myws
  description: my workspace
  created: 2019-04-09 12:54:10
  modified: 2019-04-09 12:54:10
files:
  count: 3
  total_size: 1.3 MB
html_documentation_paths:
  -: /home/myuser/idaes/docs/build
```

However, showing everything is less typing, and not overwhelming:

```
$ dmf status -a
settings:
  workspace: /home/myuser/ws
workspace:
  location: /home/myuser/ws
  name: myws
  description: my workspace
  created: 2019-04-09 12:55:05
  modified: 2019-04-09 12:55:05
```

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```

files:
  count: 3
  total_size: 1.3 MB
html_documentation_paths:
  -: /home/myuser/idaes/docs/build
logging:
  not configured

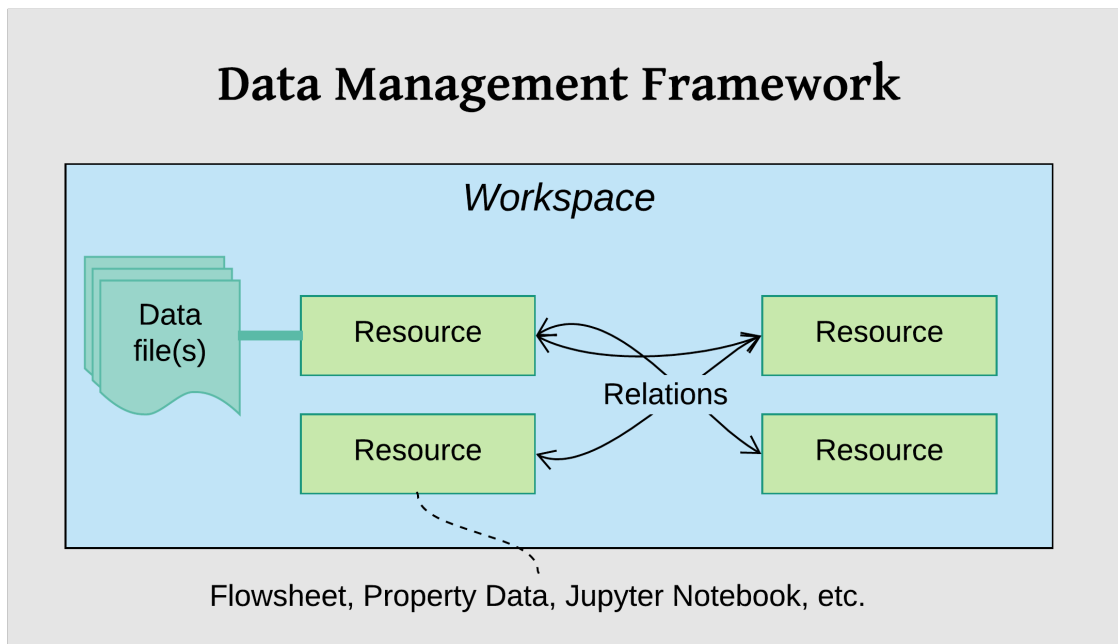
```

4.10.2 Overview

The Data Management Framework (DMF) is used to manage all the data needed by the IDAES framework, including flowsheets, models, and results. It stores metadata and data in persistent storage. It does not require that the user run a server or connect to a remote service. The DMF can be accessed through its Python [API](#) or command-line interfaces. There is work in progress on adding graphical interfaces for Jupyter Notebooks and stand-alone desktop apps.

The DMF is designed to allow multiple separate threads of work. These are organized in *workspaces*. Inside a given workspace, all the information is represented by containers called *resources*. A resource describes some data in the system in a standard way, so it can be searched and manipulated by the rest of the IDAES framework. Resources can be connected to each other with *relations* such as “derived”, “contains”, “uses”, and “version”.

Below is an illustration of these components.



4.10.3 Configuration

The DMF is configured with an optional global configuration file and a required per-workspace configuration file. By default the global file is looked for as `.dmf` in the user’s home directory. Its main function at the moment is to set the default workspace directory with the `workspace` keyword. For example:

```
# global DMF configuration
workspace: ~/data/workspaces/workspace1
```

The per-workspace configuration has more options. See the documentation in the `Workspace` class for details. The configuration file is in YAML (or JSON) format. Here is an example file, with some description in comments:

```
settings:                                # Global settings
  workspace: /home/myuser/ws             # Path to current workspace
workspace:                               # Per-workspace settings
  location: /home/myuser/ws              # Path to this workspace
  name: myws                             # Name of this workspace
  description: my workspace               # Description (if any) of this workspace
  created: 2019-04-09 12:55:05            # Date workspace was created
  modified: 2019-04-09 12:55:05          # Date workspace was modified
  files:                                 # Basic information about data files
    count: 3                             # How many files
    total_size: 1.3 MB                    # Total size of the files
  html_documentation_paths:              # List of paths for HTML documentation
    -: /home/myuser/idaes/docs/build
  logging:                               # Logging configuration
    idaes.dmf:                           # Name of the logger
      level: DEBUG                        # Log level (Python logging constant)
      output: /tmp/debug.log              # File path or "_stdout_" or "_stderr_"
```

This configuration file is used whether you use the DMF from the command-line, Jupyter notebook, or in a Python program. For details see the DMF package documentation.

4.10.4 Jupyter notebook usage

In the Jupyter Notebook, there are some “magics” defined that make initializing the DMF pretty easy. For example:

```
from idaes.dmf import magics
%dmf init path/to/workspace
```

The code above loads the “`%dmf`” line magic in the first line, then uses it to initialize the DMF with the workspace at “`path/to/workspace`”.

From there, other “line magics” will operate in the context of that DMF workspace.

- `%dmf help` - Provide help on IDAES objects and classes. See *dmf-help*.
- `%dmf info` - Provide information about DMF current state for whatever ‘topics’ are provided
- `%dmf list` - List resources in the current workspace
- `%dmf workspaces` - List DMF workspaces; you can do this *before* `%dmf init`

DMF help

The IDAES Python interfaces are documented with [Sphinx](#). This includes automatic translation of the comments and structure of the code into formatted and hyperlinked HTML pages. The `%dmf help` command lets you easily pull up this documentation for an IDAES module, class, or object. Below are a couple of examples:

```
# Initialize the DMF first
from idaes.dmf import magics
%dmf init path/to/workspace create
```

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```

# Get help on a module (imported)
from idaes.core import control_volumeld
%dmf help control_volumeld

# Get help on a module (by name, no import)
%dmf help idaes.core.control_volume0d

# Get help on a class
from idaes.core.control_volumeld import ControlVolume1DBlock
%dmf help ControlVolume1DBlock

# Get help on a class (by name, no import)
%dmf help idaes.core.control_volumeld.ControlVolume1DBlock

# Get help on an object (will show help for the object's class)
# This will end up showing the same help as the previous two examples
obj = control_volumeld.ControlVolume1DBlock()
%dmf help obj

```

The help pages will open in a new window. The location of the built documentation that they use is configured in the per-workspace DMF configuration under the `htmldocs` keyword (a default value is filled in when the DMF is first initialized).

4.10.5 Sharing

The contents of a DMF workspace can be shared quite simply because the data is all contained within a directory in the local file system. So, some ways to share (with one or many people) include:

- Put the workspace directory in a cloud/shared drive like [Dropbox](#) , [Box](#) , [Google Drive](#) , or [OneDrive](#) .
- Put the workspace directory under version control like [Git](#) and share that versioned data using Git commands and a service like [Github](#) , [BitBucket](#) or [Gitlab](#).
- Package up the directory with a standard archiving utility like “zip” or “tar” and share it like any other file (e.g. attach it to an email).

Note: These modes of sharing allow users to see the same data, but are not designed for real-time collaboration (reading and writing) of the same data. That mode of operation requires a proper database server to mediate operations on the same data. This is in the roadmap for the DMF, but not currently implemented.

4.10.6 Reference

See the `idaes.dmf` package documentation that is generated automatically from the source code.

4.11 Surrogate modeling

4.11.1 ALAMOPY : ALAMO Python

ALAMOPY.ALAMO Options

This page lists in more detail the ALAMOPY options and the relation of ALAMO and ALAMOPY.

Contents

- *ALAMOPY.ALAMO Options*
 - *Basic ALAMOPY.ALAMO options*
 - * *Data Arguments*
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 - * *ALAMO Regression Options*
 - * *Validation Capabilities*
 - * *File Options*
 - *ALAMOPY results dictionary*
 - * *Output models*
 - * *Fitness metrics*
 - * *Regression description*
 - * *Performance specs*
 - *Advanced user options in depth*
 - * *Custom Basis Functions*
 - * *Custom Constraints*
 - * *Basis Function Groups and Constraints*

Basic ALAMOPY.ALAMO options

Data Arguments

- **xmin, xmax**: minimum/maximum values of inputs, if not given they are calculated
- **zmin, zmax**: minimum/maximum values of outputs, if not given they are calculated
- **xlabels**: user-specified labels given to the inputs
- **zlabels**: user-specified labels given to the outputs

```
alamo(x_inputs, z_outputs, xlabels=['x1','x2'], zlabels=['z1','z2'])  
alamo(x_inputs, z_outputs, xmin=(-5,0), xmax=(10,15))
```

Available Basis Functions

- **linfens, expfens, logfens, sinfens, cosfens**: 0-1 option to include linear, exponential, logarithmic, sine, and cosine transformations. For example

```
linfcns = 1, expfcns = 1, logfcns = 1, sinfcns = 1, cosfcns = 1
```

This results in basis functions = x_1 , $\exp(x_1)$, $\log(x_1)$, $\sin(x_1)$, $\cos(x_1)$ * **monomialpower**, **multi2power**, **multi3power**: list of monomial, binomial, and trinomial powers. For example

```
monomialpower = (2,3,4), multi2power = (1,2,3), multi3power = (1,2,3)
```

This results in the following basis functions:

- Monomial functions = x^2 , x^3 , x^4
- Binomial functions = x_1*x_2 , $(x_1*x_2)^2$, $(x_1*x_2)^3$
- Trinomial functions = $(x_1*x_2*x_3)$, $(x_1*x_2*x_3)^2$, $(x_1*x_2*x_3)^3$
- **ratio**power: list of ratio powers. For example

```
ratio power = (1,2,3)
```

This results in basis functions = (x_1/x_2) , $(x_1/x_2)^2$, $(x_1/x_2)^3$

```
alamo(x_inputs, z_outputs, linfcns=1, logfcns=1, expfcns=1)
alamo(x_inputs, z_outputs, linfcns=1, multi2power=(2,3))
```

Note: Custom basis functions are discussed in the Advanced User Section.

ALAMO Regression Options

- **showalm**: print ALAMO output to the screen
- **expandoutput**: add a key to the output dictionary for multiple outputs
- **solvemip**, **builder**, **linearerror**: A 01 indicator to solve with an optimizer (GAMSSOLVER), use a greedy heuristic, or use a linear objective instead of squared error.
- **modeler**: Fitness metric to be used for model building (1-8)
 - 1. **BIC**: Bayesian information criterion
 - 2. **Cp**: Mallows's Cp
 - 3. **AICc**: the corrected Akaike's information criterion
 - 4. **HQC**: the Hannan-Quinn information criterion
 - 5. **MSE**: mean square error
 - 6. **SSEp**: sum of square error plus a penalty proportional to the model size (Note: convpen is the weight of the penalty)
 - 7. **RIC**: the risk information criterion
 - 8. **MADp**: the maximum absolute deviation plus a penalty proportional to model size (Note: convpen is the weight of the penalty)
- **regularizer**: Regularization method used to reduce the number of potential basis functions before optimization of the selected fitness metric. Possible values are 0 and 1, corresponding to no regularization and regularization with the lasso, respectively.
- **maxterms**: Maximum number of terms to be fit in the model
- **convpen**: When MODELER is set to 6 or 8 the size of the model is weighted by CONVPEN.

- **almopt**: name of the alamo option file
- **simulator**: a python function to be used as a simulator for ALAMO, a variable that is a python function (not a string)
- **maxiter**: max iteration of runs

Validation Capabilities

- **xval, zval**: validation input/output variables
- **loo**: leave-one-out evaluation
- **lmo**: leave-many-out evaluation
- **cvfun**: cross-validation function (True/False)

File Options

- **almname**: specify a name for the .alm file
- **savescratch**: saves .alm and .lst
- **savetrace**: saves tracefile
- **saveopt**: save .opt options file
- **savegams**: save the .gms gams file

ALAMOPY results dictionary

The results from `alamopy.alamo` are returned as a python dictionary. The data can be accessed by using the dictionary keys listed below. For example

```
regression_results = doalamo(x_input, z_output, **kwargs)
model = regression_results['model']
```

Output models

- **f(model)**: A callable function
- **pymodel**: name of the python model written
- **model**: string of the regressed model

Note: A python script named after the output variables is written to the current directory. The model can be imported and used for further evaluation, for example to evaluate residuals:

```
import z1
residuals = [y-z1.f(inputs[0],inputs[1]) for y,inputs in zip(z,x)]
```


Fitness metrics

- **size**: number of terms chosen in the regression
- **R2**: R2 value of the regression
- **Objective value metrics**: ssr, rmse, madp

Regression description

- **version**: Version of ALAMO
- **xlabels, zlabels**: The labels used for the inputs/outputs
- **xdata, zdata**: array of xdata/zdata
- **ninputs, nbas**: number of inputs/basis functions

Performance specs

There are three types of regression problems that are used: ordinary linear regression (olr), classic linear regression (clr), and a mixed integer program (mip). Performance metrics include the number of each problems and the time spent on each type of problem. Additionally, the time spent on other operations and the total time are included.

- **numolr, olrtime, numclr, clrtime, nummip, miptime**: number of type of regression problems solved and time
- **othertime**: Time spent on other operations
- **totaltime**: Total time spent on the regression

Advanced user options in depth

Similar to ALAMO, there are advanced capabilities for customization and constrained regression facilitated by methods in ALAMOPY including custom basis functions, custom constraints on the response surface, and basis function groups. These methods interact with the regression using the alamo option file.

Custom Basis Functions

Custom basis functions can be added to the built-in functions to expand the functional forms available. In ALAMO, this can be done with the following syntax

```
NCUSTOMBAS #
BEGIN_CUSTOMBAS
x1^2 * x2^2
END_CUSTOMBAS
```

To use this advanced capability in ALAMOPY, the following function is called. Note it is necessary to use the xlabels assigned to the input parameters.

```
addCustomFunctions(fcn_list)
addCustomFunctions(["x1^2 * x2^2", "...", "..."])
```

Custom Constraints

Custom constraints can be placed on response surface or regressed function of the output variable. In ALAMO, this is controlled using custom constraints, CUSTOMCON. The constraints, a function **g(x_inputs, z_outputs)** are applied to a specific output variable, which is the index of the output variable, and are less than or equal to 0 ($g \leq 0$).

```
CRNCUSTOM #
BEGIN_CUSTOMCON
1 z1 - x1 + x2 + 1
END_CUSTOMCON
```

To use this advanced capability in ALAMOPY, the following function is called. Note it is necessary to use the xlabel assigned to the input parameters.

```
addCustomConstraints(custom_constraint_list, **kwargs)
addCustomConstraints(["1 z1 - x1 + x2 +1", "...", "..."])
```

Basis Function Groups and Constraints

In addition to imposing constraints on the response surface it produces, ALAMO has the ability to enforce constraints on groups of selected basis functions. This can be accomplished using NGROUPS and identifying groups of basis functions. For ALAMO, this is achieved by first defining the groups with

```
NGROUPS 3
BEGIN_GROUPS
# Group-id Member-type Member-indices <Powers>
1 LIN 1 2
2 MONO 1 2
3 GRP 1 2
END_GROUPS
```

To add groups to ALAMOPY, you can use the following methods. Each Basis group has an index number that will be used as reference in the group constraints. The groups are defined by three or four parameters. Options for Member-type are LIN, LOG, EXP, SIN, COS, MONO, MULTI2, MULTI3, RATIO, GRP, RBF, and CUST.

```
addBasisGroup(type_of_function, input_indices, powers)
addBasisGroups(groups)

addBasisGroup("MONO", "1", "2")
addBasisGroups([["LIN", "1 2"], ["MONO", "1", "2"], ["GRP", "1 2"]])
```

With the groups defined, constraints can be placed on the groups using the constraint-types NMT (no-more-than), ATL (at-least), REQ (requires), and XCL (exclude). For NMT and ATL the integer-parameter is the number of members in the group that should be selected based on the constraint. For REQ and XCL the integer-parameter is the group-id number of excluded or required basis functions.

```
BEGIN_GROUPCON
# Group-id Output-id Constraint-type Integer-parameter
3 1 NMT 1
END_GROUPCON
```

To add the basis constraints to alamopy, you can use the following methods.

```
addBasisConstraint(group_id, output_id, constraint_type, intParam)
addBasisConstraints(groups_constraint_list)

addBasisConstraint(3,1,"NMT",1)
addBasisConstraints([[3,1,"NMT",1]])
```

The purpose of ALAMOPY (Automatic Learning of Algebraic MOdels PYthon wrapper) is to provide a wrapper for the software ALAMO which generates algebraic surrogate models of black-box systems for which a simulator or experimental setup is available. Consider a system for which the outputs \mathbf{z} are an unknown function \mathbf{f} of the system inputs \mathbf{x} . The software identifies a function \mathbf{f} , i.e., a relationship between the inputs and outputs of the system, that best matches data (pairs of \mathbf{x} and corresponding \mathbf{z} values) that are collected via simulation or experimentation.

Basic Usage

ALAMOPY's main function is **alamopy.alamo**. Data can be read in or simulated using available python packages. The main arguments of the `alamopy.alamo` python function are inputs and outputs, which are 2D arrays of data. For example

```
regression_results =alamopy.alamo(x_inputs, z_outputs, **kwargs)
```

where ****kwargs** is a set of named keyword arguments than can be passed to the `alamo` python function to customize the basis function set, names of output files, and other options available in ALAMO.

Warning: The `alamopy.doalamo` function is deprecated. It is being replaced with `alamopy.alamo`

Options for `alamopy.alamo`

Possible arguments to be passed to ALAMO through `do alamo` and additional arguments that govern the behavior of `doalamo`.

- `xlabels` - list of strings to label the input variables
- `zlabels` - list of strings to label the output variables
- `functions` - `logfcns`, `expfcns`, `cosfcns`, `sinfncns`, `linfcns`, `intercept`. These are '0-1' options to activate these functions
- `monomialpower`, `multi2power`, `multi3power`, `ratio`. List of terms to be used in the respective basis functions
- `modeler` - integer 1-7 determines the choice of fitness metric
- `solvemip` - '0-1' option that will force the solving of the `.gms` file

These options are specific to `alamopy` and will not change the behavior of the underlying `.alm` file.

- `expandoutput` - '0-1' option that can be used to collect more information from the ALAMO `.lst` and `.trc` file
- `showalm` - '0-1' option that controlif the ALAMO output is printed to screen
- `almname` - A string that will assign the name of the `.alm` file
- `outkeys` - '0-1' option for dictionary indexing according to the output labels
- `outkeys` - '0-1' option for dictionary indexing according to the output labels
- `outkeys` - '0-1' option for dictionary indexing according to the output labels

- savetrace - '0-1' option that controls the status of the trace file
- savescratch - '0-1' option to save the .alm and .lst files
- almopt - A string option that will append a text file of the same name to the end of each .alm file to facilitate advanced user access in an automated fashion

ALAMOPY Output

There are multiple outputs from the running *alamopy.alamo*. Outputs include:

- f(model): A callable function
- pymodel: name of the python model written
- model: string of the regressed model

Note: A python script named after the output variables is written to the current directory. The model can be imported and used for further evaluation, for example to evaluate residuals:

```
import z1
residuals = [y-z1.f(inputs[0],inputs[1]) for y,inputs in zip(z,x)]
```

Additional Results

After the regression of a model, ALAMOPY provides confidence interval analysis and plotting capabilities using the results output.

Plotting

The plotting capabilities of ALAMOPY are available in the **almplot** function. Almplot will plot the function based on one of the inputs.

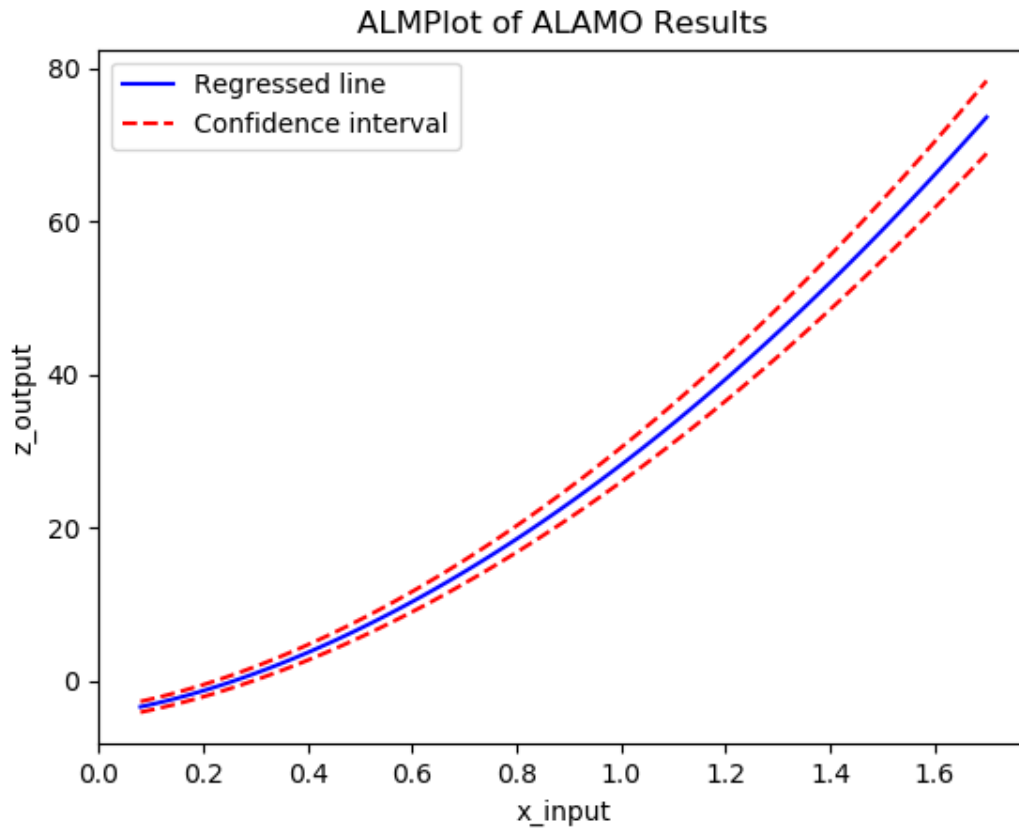
```
result = alamopy.alamo(x_in, z_out, kargs)
alamopy.almplot(result)
```

Confidence intervals

Confidence intervals can similarly be calculated for the weighting of selected basis functions using the **almconfidence** function.

This adds **conf_inv** (confidence intervals) and **covariance** (covariance matrix) to the results dictionary. This also gets incorporated into the plotting function if it is available.

```
result = alamopy.alamo(x_in, z_out, kargs)
result = alamopy.almconfidence(result)
alamopy.almplot(result)
```



Advanced Regression Capabilities

Similar to ALAMO, there are advanced capabilities for customization and constrained regression facilitated by methods in ALAMOPY including custom basis functions, custom constraints on the response surface, and basis function groups. These methods interact with the regression using the `alamo` option file.

Custom Basis Functions

Custom basis functions can be added to the built-in functions to expand the functional forms available. To use this advanced capability in ALAMOPY, the following function is called. Note it is necessary to use the xlabels assigned to the input parameters.

```
addCustomFunctions(fcn_list)
addCustomFunctions(["x1^2 * x2^2", "...", "..."])
```

Custom Constraints

Custom constraints can be placed on response surface or regressed function of the output variable. In ALAMO, this is controlled using custom constraints, `CUSTOMCON`. The constraints, a function $g(\mathbf{x_inputs}, \mathbf{z_outputs})$ are applied to a specific output variable, which is the index of the output variable, and are less than or equal to 0 ($g \leq 0$).

To use this advanced capability in ALAMOPY, the following function is called. Note it is necessary to use the xlabels assigned to the input parameters.

```
addCustomConstraints(custom_constraint_list, **kwargs)
addCustomConstraints(["1 z1 - x1 + x2 +1", "...", "..."])
```

Basis Function Groups and Constraints

In addition to imposing constraints on the response surface it produces, ALAMO has the ability to enforce constraints on groups of selected basis functions. To define groups in ALAMOPY, you can use the following methods. Each Basis group has an index number that will be used as reference in the group constraints. The groups are defined by three or four parameters. Options for Member-type are LIN, LOG, EXP, SIN, COS, MONO, MULTI2, MULTI3, RATIO, GRP, RBF, and CUST.

```
addBasisGroup(type_of_function, input_indices, powers)
addBasisGroups(groups)

addBasisGroup("MONO", "1", "2")
addBasisGroups([["LIN", "1 2"], ["MONO", "1", "2"], ["GRP", "1 2"]])
```

With the groups defined, constraints can be placed on the groups using the constraint-types NMT (no-more-than), ATL (at-least), REQ (requires), and XCL (exclude). For NMT and ATL the integer-parameter is the number of members in the group that should be selected based on the constraint. For REQ and XCL the integer-parameter is the group-id number of excluded or required basis functions.

To add the basis constraints to alamopy, you can use the following methods.

```
addBasisConstraint(group_id, output_id, constraint_type, intParam)
addBasisConstraints(groups_constraint_list)

addBasisConstraint(3, 1, "NMT", 1)
addBasisConstraints([[3, 1, "NMT", 1]])
```

ALAMOPY Examples

Three examples are included with ALMAOPY. These examples demonstrate different use cases, and provide a template for utilizing user-defined mechanisms.

- ackley.py
- branin.py
- camel6.py with a Jupyter notebook

4.11.2 RIPE : Reaction Identification and Parameter Estimation

The RIPE module provides tools for reaction network identification. RIPE uses reactor data consisting of concentration, or conversion, values for multiple species that are obtained dynamically, or at multiple process conditions (temperatures, flow rates, working volumes) to identify probable reaction kinetics. The RIPE module also contains tools to facilitate adaptive experimental design. The experimental design tools in RIPE require the use of the python package RBFopt. More information for RBFopt is available at www.github.com/coin-or/rbfopt

Basic Usage

RIPE can be used to build models for static datasets through the function `ripe.ripemodel`

```
ripe_results = ripe.ripemodel(data, kwargs)
```

- data is provided to RIPE as one, two, or three dimensional python data structures, where the first axis corresponds to observations at different process conditions, the second axis corresponds to observations of different

chemical species, and the third axis corresponds to dynamic observation of a chemical species at a specified process condition.

RIPE adaptive experimental design can be accessed using `ripe.ems`

```
[proposed_x, errors] = ripe.ems(ripe_results, simulator, l_bounds, u_bounds, n_
↪species, kwargs)
```

- `ripe_results` - The results from `ripe.ripemodel`, additional information provided in the results section
- `simulator` - a black-box simulator for the unknown process.
- `l_bounds/u_bounds` - lower and upper bounds for the input variables in the adaptive design
- `nspecies` - the number of chemical species present in the black-box system

Reaction stoichiometries and mechanisms are provided explicitly to `ripemodel` through the keyword arguments `mech` and `stoichiometry`. Detailed explanations of the forms of these arguments are provided in the stoichiometry and mechanism specification section. Additional keyword arguments can be found in the additional options section.

RIPE Output

By default, one file will be generated

- `ripereults.txt` - a file containing the selected reactions and parameter estimates

Reaction Stiochiometry and Mechanism Specification

Considered reaction stiochiometries are provided through keyword arguments.

Stoichiometry

Considered reaction stoichiometries are defiend as a list of list, where reactants and products are defined as negative and positive integers , respectively, according to their stoichiometric coefficeints. A set of considered reaction stoichiometries must be provided. If process data consists of species conversion, a positive coefficient should be specified.

Mechanisms

Considered reaction mechanisms are provided explicitly to RIPE through `q` keyword argument. If no kinetic mechanisms are specified, mass action kinetics are ascribed to every considered stoichiometry. RIPE contains kinetic mechanisms defined internally, and called through `ripe.mechs.<mechanism>`. The available mechanisms include:

- `massact` - mass action kinetics, order informed by reaction stoichiometry

19 empirical rate forms included relate specifically to catalyst conversion in chemical looping combustion reactors include:

- Random nucleation
- Power law models
- Avrami-Erofeev models

These internal kinetics can be specified by calling `ripe.mechs.massact` or `ripe.mechs.clcforms` respectively. User-defined kinetic mechanisms can also be supplied to RIPE as python functions. An example is provided in the file `crac.py`.

Additional Results and Options

In addition to the arguments stoichiometry and mechanism, a number of other optional arguments are available, including:

Arguments relating to process conditions

- x0 - initial concentration at each process condition for every species
- time - time associated with dynamic samples for every process condition
- temp - temperature associated with every process condition
- flow - flow rate at every process condition for every species
- vol - reactor volume at every process condition

Arguments related to RIPE algorithmic function

- tref - reference temperature for reformulated Arrhenius models
- ccon - specified cardinality constraint instead of BIC objective
- sigma - expected variance of noise, estimated if not provided
- onemechper - one mechanism per stoichiometry in selected model, true by default

Additional arguments

- minlp_path - path to baron or other minlp solver, can also be set in shared.py
- alamo_path - path to alamo, can also be set in shared.py
- expand_output - provide estimates for noise variance in model results
- zscale - linear scaling of observed responses between -1 and 1
- ascale - linear scaling of activities between -1 and 1
- hide_output - suppress output to terminal
- keepfiles - keep scratch files for debugging
- showpyomo - show pyomo output to terminal, false by default

RIPE Examples

Three examples are included with RIPE. These examples demonstrate different use cases, and provide a template for utilizing user-defined mechanisms.

- clc.py - a chemical looping combustion example in which catalyst conversion is observed over time
- isoT.py - an example that utilizes both ripe.ripemodel and ripe.ems
- crac.py - an example that utilizes user-defined reaction mechanisms

All of these examples are built for Linux machines. They can be called from the command line by calling python directly, or can be called from inside a python environment using `execfile()`.

4.11.3 HELMET : HELMholtz Energy Thermodynamics

The purpose of HELMET (HELMholtz Energy Thermodynamics) is to provide a framework for regressing multi-parameter equations of state that identify an equation for Helmholtz energy and multiple thermodynamic properties simultaneously. HELMET uses best subset selection to simultaneously model various thermodynamic properties based

on the properties thermodynamic relation to Helmholtz energy. The generated model is a function of reduced density and inverse reduced temperature and uses partial derivatives to calculate the different properties. Constraints are placed on the regression to maintain thermodynamically feasible values and improve extrapolation and behavior of the model based on physical restrictions.

Warning: This is the first public release of HELMET. Future work will include mixtures, regression using Pyomo models, and increased plotting and preprocessing capabilities.

Basic Usage

Warning: To use this software, ALAMOPY and the solver BARON are required.

For the basic use of HELMET, the main regression steps can be imported from `helmet.HELMET`. These functions provide general capabilities of HELMET for new users.

```
import helmet.Helmet as Helmet
```

The methods available in `helmet.Helmet` perform the necessary steps of the regression properties.

1. `initialize(**kargs)`

Initializes key thermodynamic constants, the location of data and sampling, properties to be fit, and optimization settings

- **molecule** - name of the chemical of interest, directs naming of files and where the data should exist
- **fluid_data** - a tuple containing key thermodynamic constants (critical temperature, critical pressure, critical density, molecular weight, triple point, accentric factor)
- **filename** - used for location of data
- **gamsname** - used for naming of files
- **max_time** - max time used for the solver
- **props** - list of thermodynamic properties to be fit

Supported thermodynamic properties are

- Pressure: 'PVT'
- Isochoric heat capacity: 'CV'
- Isobaric heat capacity: 'CP'
- Speed of Sound: 'SND'

- **sample** - sample ratio, ex. sample = 3 then a third of datapoints will be used

2. `prepareAncillaryEquations(plot=True)`

Fits equations to saturated vapor and liquid density and vapor pressure. The keyword argument `plot` defaults to False

3. `viewPropertyData()`

Plots the different thermodynamic properties available and a way to check that the importing of data is successful

4. `setupRegression(numTerms = 12, gams=True)`

Writes the optimization program for modelling the thermodynamic properties. Currently this is through GAMS but in the future it can also be solved using Pyomo.

5. **runRegression()**

Begins the modelling of the multiparameter equation

6. **viewResults(filename)**

Based on the optimization settings, the solution of the regression is parsed and fitness metrics are calculated. The results can be visualized with different plots.

HELMET Output

The output for HELMET is a single equation representing Helmholtz energy. Partial derivatives of this equation will give you the fit thermodynamic properties as well as other properties related to Helmholtz energy.

HELMET Examples

The provided HELMET example uses data modified for this application and made available by the IAPWS organization at <http://www.iapws.org/95data.html> for IAPWS Formulation 1995 for Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use.

4.11.4 PySMO: Python-based Surrogate Modelling Objects

The PySMO toolbox provides tools for generating different types of reduced order models. It provides IDAES users with a set of surrogate modeling tools which supports flowsheeting and direct integration into an equation-oriented modeling framework. It allows users to directly integrate reduced order models with algebraic high-fidelity process models within a single IDAES flowsheet.

PySMO provides two sets of tools necessary for sampling and surrogate model generation.

Sampling

The PySMO package offers five common sampling methods for one-shot design:

Latin Hypercube Sampling (LHS)

LHS is a stratified random sampling method originally developed for efficient uncertainty assessment. LHS partitions the parameter space into bins of equal probability with the goal of attaining a more even distribution of sample points in the parameter space that would be possible with pure random sampling.

The `pysmo.sampling.LatinHypercubeSampling` method carries out Latin Hypercube sampling. This can be done in two modes:

- The samples can be selected from a user-provided dataset, or
- The samples can be generated from a set of provided bounds.

Available Methods

```
class idaes.surrogate.pysmo.sampling.LatinHypercubeSampling(data_input, number_of_samples=None,  
                                                           sampling_type=None)
```

A class that performs Latin Hypercube Sampling. The function returns LHS samples which have been selected randomly after sample space stratification.

It should be noted that no minimax criterion has been used in this implementation, so the LHS samples selected will not have space-filling properties.

To use: call class with inputs, and then run `sample_points` method.

Example:

```
# To select 10 LHS samples from "data"
>>> b = rbf.LatinHypercubeSampling(data, 10, sampling_type="selection")
>>> samples = b.sample_points()
```

```
__init__(data_input, number_of_samples=None, sampling_type=None)
```

Initialization of **LatinHypercubeSampling** class. Two inputs are required.

Parameters

- **data_input** (*NumPy Array*, *Pandas Dataframe* or *list*) – The input data set or range to be sampled.
 - When the aim is to select a set of samples from an existing dataset, the dataset must be a NumPy Array or a Pandas Dataframe and **sampling_type** option must be set to “selection”. The output variable (y) is assumed to be supplied in the last column.
 - When the aim is to generate a set of samples from a data range, the dataset must be a list containing two lists of equal lengths which contain the variable bounds and **sampling_type** option must be set to “creation”. It is assumed that no range contains no output variable information in this case.
- **number_of_samples** (*int*) – The number of samples to be generated. Should be a positive integer less than or equal to the number of entries (rows) in **data_input**.
- **sampling_type** (*str*) – Option which determines whether the algorithm selects samples from an existing dataset (“selection”) or attempts to generate sample from a supplied range (“creation”). Default is “creation”.

Returns `self` function containing the input information

Raises

- `ValueError` – The input data (**data_input**) is the wrong type.
- `Exception` – When **number_of_samples** is invalid (not an integer, too large, zero, or negative)

```
sample_points()
```

`sample_points` generates or selects Latin Hypercube samples from an input dataset or data range. When called, it:

1. generates samples points from stratified regions by calling the `lhs_points_generation`,
2. generates potential sample points by random shuffling, and
3. when a dataset is provided, selects the closest available samples to the theoretical sample points from within the input data.

Returns A numpy array or Pandas dataframe containing **number_of_samples** points selected or generated by LHS.

Return type NumPy Array or Pandas Dataframe

References

- [1] Loeven et al paper titled “A Probabilistic Radial Basis Function Approach for Uncertainty Quantification” <https://pdfs.semanticscholar.org/48a0/d3797e482e37f73e077893594e01e1c667a2.pdf>
- [2] Webpage on low discrepancy sampling methods: <http://planning.cs.uiuc.edu/node210.html>
- [3] Swiler, Laura and Slepoy, Raisa and Giunta, Anthony: “Evaluation of sampling methods in constructing response surface approximations” <https://arc.aiaa.org/doi/abs/10.2514/6.2006-1827>

Full-Factorial Sampling

The `pysmo.sampling.UniformSampling` method carries out Uniform (full-factorial) sampling. This can be done in two modes:

- The samples can be selected from a user-provided dataset, or
- The samples can be generated from a set of provided bounds.

Available Methods

```
class idaes.surrogate.pysmo.sampling.UniformSampling(data_input,  
                                                    list_of_samples_per_variable,  
                                                    sampling_type=None,  
                                                    edges=None)
```

A class that performs Uniform Sampling. Depending on the settings, the algorithm either returns samples from an input dataset which have been selected using Euclidean distance minimization after the uniform samples have been generated, or returns samples from a supplied data range.

Full-factorial samples are based on dividing the space of each variable randomly and then generating all possible variable combinations.

- The number of points to be sampled per variable needs to be specified in a list.

To use: call class with inputs, and then `sample_points` function

Example:

```
# To select 50 samples on a (10 x 5) grid in a 2D space:  
>>> b = rbf.UniformSampling(data, [10, 5], sampling_type="selection")  
>>> samples = b.sample_points()
```

```
__init__(data_input, list_of_samples_per_variable, sampling_type=None, edges=None)
```

Initialization of UniformSampling class. Three inputs are required.

Parameters

- **data_input** (*NumPy Array, Pandas Dataframe or list*) – The input data set or range to be sampled.
 - When the aim is to select a set of samples from an existing dataset, the dataset must be a NumPy Array or a Pandas Dataframe and **sampling_type** option must be set to “selection”. The output variable (Y) is assumed to be supplied in the last column.

- When the aim is to generate a set of samples from a data range, the dataset must be a list containing two lists of equal lengths which contain the variable bounds and **sampling_type** option must be set to “creation”. It is assumed that no range contains no output variable information in this case.

- **list_of_samples_per_variable** (*list*) – The list containing the number of subdivisions for each variable. Each dimension (variable) must be represented by a positive integer variable greater than 1.
- **sampling_type** (*str*) – Option which determines whether the algorithm selects samples from an existing dataset (“selection”) or attempts to generate sample from a supplied range (“creation”). Default is “creation”.

Keyword Arguments **edges** (*bool*) – Boolean variable representing bow the points should be selected. A value of True (default) indicates the points should be equally spaced edge to edge, otherwise they will be in the centres of the bins filling the unit cube

Returns **self** function containing the input information

Raises

- **ValueError** – The **data_input** is the wrong type
- **ValueError** – When **list_of_samples_per_variable** is of the wrong length, is not a list or contains elements other than integers
- **Exception** – When **edges** entry is not Boolean

sample_points()

`sample_points` generates or selects full-factorial designs from an input dataset or data range.

Returns A numpy array or Pandas dataframe containing the sample points generated or selected by full-factorial sampling.

Return type NumPy Array or Pandas Dataframe

References

[1] Loeven et al paper titled “A Probabilistic Radial Basis Function Approach for Uncertainty Quantification” <https://pdfs.semanticscholar.org/48a0/d3797e482e37f73e077893594e01e1c667a2.pdf>

Halton Sampling

Halton sampling is a low-discrepancy sampling method. It is a deterministic sampling method based on the Halton sequence, a sequence constructed by a set of co-prime bases. The Halton sequence is an n-dimensional extension of the Van der Corput sequence; each individual Halton sequence is based on a radix inverse function defined on a prime number.

The `pysmo.sampling.HaltonSampling` method carries out Halton sampling. This can be done in two modes:

- The samples can be selected from a user-provided dataset, or
- The samples can be generated from a set of provided bounds.

The Halton sampling method is only available for low-dimensional problems $n \leq 10$. At higher dimensions, the performance of the sampling method has been shown to degrade.

Available Methods

```
class idaes.surrogate.pysmo.sampling.HaltonSampling(data_input, num-  
                                                    ber_of_samples=None, sam-  
                                                    pling_type=None)
```

A class that performs Halton Sampling.

Halton samples are based on the reversing/flipping the base conversion of numbers using primes.

To generate n samples in a p -dimensional space, the first p prime numbers are used to generate the samples.

Note: Use of this method is limited to use in low-dimensionality problems (less than 10 variables). At higher dimensions, the performance of the sampling method has been shown to degrade.

To use: call class with inputs, and then `sample_points` function.

Example:

```
# For the first 10 Halton samples in a 2-D space:  
>>> b = rbf.HaltonSampling(data, 10, sampling_type="selection")  
>>> samples = b.sample_points()
```

`__init__` (*data_input*, *number_of_samples=None*, *sampling_type=None*)

Initialization of **HaltonSampling** class. Two inputs are required.

Parameters

- **data_input** (*NumPy Array*, *Pandas Dataframe* or *list*) – The input data set or range to be sampled.
 - When the aim is to select a set of samples from an existing dataset, the dataset must be a NumPy Array or a Pandas Dataframe and **sampling_type** option must be set to “selection”. The output variable (Y) is assumed to be supplied in the last column.
 - When the aim is to generate a set of samples from a data range, the dataset must be a list containing two lists of equal lengths which contain the variable bounds and **sampling_type** option must be set to “creation”. It is assumed that no range contains no output variable information in this case.
- **number_of_samples** (*int*) – The number of samples to be generated. Should be a positive integer less than or equal to the number of entries (rows) in **data_input**.
- **sampling_type** (*str*) – Option which determines whether the algorithm selects samples from an existing dataset (“selection”) or attempts to generate sample from a supplied range (“creation”). Default is “creation”.

Returns `self` function containing the input information.

Raises

- `ValueError` – The **data_input** is the wrong type.
- `Exception` – When the **number_of_samples** is invalid (not an integer, too large, zero or negative.)

sample_points ()

The `sample_points` method generates the Halton samples. The steps followed here are:

1. Determine the number of features in the input data.

2. Generate the list of primes to be considered by calling `prime_number_generator` from the sampling superclass.
3. Create the first **number_of_samples** elements of the Halton sequence for each prime.
4. Create the Halton samples by combining the corresponding elements of the Halton sequences for each prime.
5. When in “selection” mode, determine the closest corresponding point in the input dataset using Euclidean distance minimization. This is done by calling the `nearest_neighbours` method in the sampling superclass.

Returns A numpy array or Pandas dataframe containing **number_of_samples** Halton sample points.

Return type NumPy Array or Pandas Dataframe

References

- [1] Loeven et al paper titled “A Probabilistic Radial Basis Function Approach for Uncertainty Quantification” <https://pdfs.semanticscholar.org/48a0/d3797e482e37f73e077893594e01e1c667a2.pdf>
- [2] Webpage on low discrepancy sampling methods: <http://planning.cs.uiuc.edu/node210.html>

Hammersley Sampling

Hammersley sampling is a low-discrepancy sampling method based on the Hammersley sequence. The Hammersley sequence is the same as the Halton sequence except in the first dimension where points are located equidistant from each other.

The `pysmo.sampling.HammersleySampling` method carries out Hammersley sampling. This can be done in two modes:

- The samples can be selected from a user-provided dataset, or
- The samples can be generated from a set of provided bounds.

The Hammersley sampling method is only available for low-dimensional problems $n \leq 10$. At higher dimensions, the performance of the sampling method has been shown to degrade.

Available Methods

```
class idaes.surrogate.pysmo.sampling.HammersleySampling(data_input,          num-
                                                         ber_of_samples=None,
                                                         sampling_type=None)
```

A class that performs Hammersley Sampling.

Hammersley samples are generated in a similar way to Halton samples - based on the reversing/flipping the base conversion of numbers using primes.

To generate n samples in a p -dimensional space, the first $(p - 1)$ prime numbers are used to generate the samples. The first dimension is obtained by uniformly dividing the region into **no_samples points**.

Note: Use of this method is limited to use in low-dimensionality problems (less than 10 variables). At higher dimensionalities, the performance of the sampling method has been shown to degrade.

To use: call class with inputs, and then `sample_points` function.

Example:

```
# For the first 10 Hammersley samples in a 2-D space:
>>> b = rbf.HammersleySampling(data, 10, sampling_type="selection")
>>> samples = b.sample_points()
```

`__init__` (*data_input*, *number_of_samples=None*, *sampling_type=None*)

Initialization of **HammersleySampling** class. Two inputs are required.

Parameters

- **data_input** (*NumPy Array*, *Pandas Dataframe* or *list*) – The input data set or range to be sampled.
 - When the aim is to select a set of samples from an existing dataset, the dataset must be a NumPy Array or a Pandas Dataframe and **sampling_type** option must be set to “selection”. The output variable (Y) is assumed to be supplied in the last column.
 - When the aim is to generate a set of samples from a data range, the dataset must be a list containing two lists of equal lengths which contain the variable bounds and **sampling_type** option must be set to “creation”. It is assumed that no range contains no output variable information in this case.
- **number_of_samples** (*int*) – The number of samples to be generated. Should be a positive integer less than or equal to the number of entries (rows) in **data_input**.
- **sampling_type** (*str*) – Option which determines whether the algorithm selects samples from an existing dataset (“selection”) or attempts to generate sample from a supplied range (“creation”). Default is “creation”.
- **Returns** – **self** function containing the input information.
- **Raises** – **ValueError**: When **data_input** is the wrong type.

Exception: When the **number_of_samples** is invalid (not an integer, too large, zero, negative)

sample_points ()

The **sampling_type** method generates the Hammersley sample points. The steps followed here are:

1. Determine the number of features n_f in the input data.
2. Generate the list of $(n_f - 1)$ primes to be considered by calling `prime_number_generator`.
3. Divide the space $[0, **number_of_samples*-1]$ into **number_of_samples** places to obtain the first dimension for the Hammersley sequence.
4. For the other $(n_f - 1)$ dimensions, create first **number_of_samples** elements of the Hammersley sequence for each of the $(n_f - 1)$ primes.
5. Create the Hammersley samples by combining the corresponding elements of the Hammersley sequences created in steps 3 and 4
6. When in “selection” mode, determine the closest corresponding point in the input dataset using Euclidean distance minimization. This is done by calling the `nearest_neighbours` method in the sampling superclass.

Returns A numpy array or Pandas dataframe containing **number_of_samples** Hammersley sample points.

Return type NumPy Array or Pandas Dataframe

References

- [1] Loeven et al paper titled “A Probabilistic Radial Basis Function Approach for Uncertainty Quantification” <https://pdfs.semanticscholar.org/48a0/d3797e482e37f73e077893594e01e1c667a2.pdf>
- [2] Webpage on low discrepancy sampling methods: <http://planning.cs.uiuc.edu/node210.html>
- [3] Holger Dammertz’s webpage titled “Hammersley Points on the Hemisphere” which discusses Hammersley point set generation in two dimensional spaces, http://holger.dammertz.org/stuff/notes_HammersleyOnHemisphere.html

Centroidal voronoi tessellation (CVT) sampling

In CVT, the generating point of each Voronoi cell coincides with its center of mass; CVT sampling locates the design samples at the centroids of each Voronoi cell in the input space. CVT sampling is a geometric, space-filling sampling method which is similar to k-means clustering in its simplest form.

The `pysmo.sampling.CVTSampling` method carries out CVT sampling. This can be done in two modes:

- The samples can be selected from a user-provided dataset, or
- The samples can be generated from a set of provided bounds.

The CVT sampling algorithm implemented here is based on McQueen’s method which involves a series of random sampling and averaging steps, see <http://kmh-lanl.hansonhub.com/uncertainty/meetings/gunz03vgr.pdf>.

Available Methods

```
class idaes.surrogate.pysmo.sampling.CVTSampling (data_input, num-  
                                                ber_of_samples=None, toler-  
                                                ance=None, sampling_type=None)
```

A class that constructs Centroidal Voronoi Tessellation (CVT) samples.

CVT sampling is based on the generation of samples in which the generators of the Voronoi tessellations and the mass centroids coincide.

To use: call class with inputs, and then `sample_points` function.

Example:

```
# For the first 10 CVT samples in a 2-D space:
>>> b = rbf.CVTSampling(data_bounds, 10, tolerance = 1e-5, sampling_type="creation
↪")
>>> samples = b.sample_points()
```

```
__init__ (data_input, number_of_samples=None, tolerance=None, sampling_type=None)
```

Initialization of CVTSampling class. Two inputs are required, while an optional option to control the solution accuracy may be specified.

Parameters

- **data_input** (*NumPy Array, Pandas Dataframe or list*) – The input data set or range to be sampled.
 - When the aim is to select a set of samples from an existing dataset, the dataset must be a NumPy Array or a Pandas Dataframe and **sampling_type** option must be set to “selection”. The output variable (Y) is assumed to be supplied in the last column.

- When the aim is to generate a set of samples from a data range, the dataset must be a list containing two lists of equal lengths which contain the variable bounds and **sampling_type** option must be set to “creation”. It is assumed that no range contains no output variable information in this case.

- **number_of_samples** (*int*) – The number of samples to be generated. Should be a positive integer less than or equal to the number of entries (rows) in **data_input**.
- **sampling_type** (*str*) – Option which determines whether the algorithm selects samples from an existing dataset (“selection”) or attempts to generate sample from a supplied range (“creation”). Default is “creation”.

Keyword Arguments **tolerance** (*float*) – Maximum allowable Euclidean distance between centres from consecutive iterations of the algorithm. Termination condition for algorithm.

- The smaller the value of tolerance, the better the solution but the longer the algorithm requires to converge. Default value is 10^{-7} .

Returns **self** function containing the input information.

Raises

- **ValueError** – When **data_input** is the wrong type.
- **Exception** – When the **number_of_samples** is invalid (not an integer, too large, zero, negative)
- **Exception** – When the tolerance specified is too loose (tolerance > 0.1) or invalid
- **warnings.warn** – when the tolerance specified by the user is too tight (tolerance < 10^{-9})

sample_points()

The **sample_points** method determines the best/optimal centre points (centroids) for a data set based on the minimization of the total distance between points and centres.

Procedure based on McQueen’s algorithm: iteratively minimize distance, and re-position centroids. Centre re-calculation done as the mean of each data cluster around each centre.

Returns A numpy array or Pandas dataframe containing the final **number_of_samples** centroids obtained by the CVT algorithm.

Return type NumPy Array or Pandas Dataframe

References

- [1] Loeven et al paper titled “A Probabilistic Radial Basis Function Approach for Uncertainty Quantification” <https://pdfs.semanticscholar.org/48a0/d3797e482e37f73e077893594e01e1c667a2.pdf>
- [2] Centroidal Voronoi Tessellations: Applications and Algorithms by Qiang Du, Vance Faber, and Max Gunzburger <https://doi.org/10.1137/S0036144599352836>
- [3] D. G. Loyola, M. Pedernana, S. G. García, “Smart sampling and incremental function learning for very large high dimensional data” <https://www.sciencedirect.com/science/article/pii/S0893608015001768?via%3Dihub>

More Information about PySMO’s Sampling Methods

The sampling methods are able to generate samples based from variable bounds or select samples from a user-provided dataset. To use any of the method, the class is first initialized with the required parameters, and then the

`sample_points` method is called.

Examples

The following code snippet shows basic usage of the package for generating samples from a set of bounds:

```
# Required imports
>>> from idaes.surrogates.pyomo import sampling as sp

# Declaration of lower and upper bounds of 3D space to be sampled
>>> bounds = [[0, 0, 0], [1.2, 0.1, 1]]

# Initialize the Halton sampling method and generate 10 samples
>>> space_init = sp.HaltonSampling(bounds_list, sampling_type='creation', number_of_
↳ samples=10)
>>> samples = space_init.sample_points()
```

The following code snippet shows basic usage of the package for selecting sample points from an existing dataset:

```
# Required imports
>>> from idaes.surrogates.pyomo import sampling as sp
>>> import pandas as pd

# Load dataset from a csv file
>>> xy_data = pd.read_csv('data.csv', header=None, index_col=0)

# Initialize the CVT sampling method and generate 25 samples
>>> space_init = sp.CVTSampling(xy_data, sampling_type='selection', number_of_
↳ samples=25)
>>> samples = space_init.sample_points()
```

Note: The results of the sampling process will be a Numpy array or Pandas dataframe, depending on the format of the input data.

Characteristics of sampling methods available in PySMO

Table 6: Characteristics of the different sampling methods

	Deterministic	Stochastic	Low-discrepancy	Space-filling	Geometric
LHS		✓			✓
Full-factorial	✓				✓
Halton	✓		✓		
Hammersley	✓		✓		
CVT	✓			✓	✓

Further information about the sampling tools and their input options may be found by accessing the individual sampling methods. Examples and details of the characteristics of the sampling methods may be found at [More Information about PySMO's Sampling Methods](#).

Surrogate Generation

PySMO offers tools for generating three types of surrogates:

Generating Polynomial Models with PySMO

The `pysmo.polynomial_regression` method learns polynomial models from data. Presented with a small number of samples generated from experiments or computer simulations, the approach determines the most accurate polynomial approximation by comparing the accuracy and performance of polynomials of different orders and basis function forms.

`pysmo.polynomial_regression` considers three types of basis functions

- univariate polynomials,
- second-degree bivariate polynomials, and
- user-specified basis functions.

Thus, for a problem with m sample points and n input variables, the resulting polynomial is of the form

$$y_k = \sum_{i=1}^n \beta_i x_{ik}^\alpha + \sum_{i,j>i}^n \beta_{ij} x_{ik} x_{jk} + \beta_\Phi \Phi(x_{ik}) \quad i, j = 1, \dots, n; i \neq j; k = 1, \dots, m; \alpha \leq 10 \quad (4.1)$$

Basic Usage

To generate a polynomial model with PySMO, the `pysmo.polynomial_regression` class is first initialized, and then the method `poly_training` is called on the initialized object:

```
# Required imports
>>> from idaes.surrogates.pysmo import polynomial_regression
>>> import pandas as pd

# Load dataset from a csv file
>>> xy_data = pd.read_csv('data.csv', header=None, index_col=0)

# Initialize the PolynomialRegression class, extract the list of features and train_
↳ the model
>>> pr_init = polynomial_regression.PolynomialRegression(xy_data, xy_data, maximum_
↳ polynomial_order=3, *kwargs)
>>> features = pr_init.get_feature_vector()
>>> polyfit = pr_init.poly_training()
```

- **xy_data** is a two-dimensional python data structure containing the input and output training data. The output values **MUST** be in the last column.
- **maximum_polynomial_order** refers to the maximum polynomial order to be considered when training the surrogate.

Optional Arguments

- **multinomials** - boolean option which determines whether bivariate terms are considered in polynomial generation.

- **training_split** - option which determines fraction of training data to be used for training (the rest will be for testing). Default is 0.8.
- **number_of_crossvalidations** - Number of cross-validations during training. Default number is 3.

pysmo.polynomial_regression Output

The result of the `pysmo.polynomial_regression` method (polyfit in above example) is a python object containing information about the optimal polynomial order, the polynomial coefficients and different error and quality-of-fit metrics such as the mean-squared-error (MSE) and the R^2 coefficient-of-fit. A Pyomo expression can be generated from the object simply passing a list of variables into the function `generate_expression`:

```
# Create a python list from the headers of the dataset supplied for training
>>> list_vars = []
>>> for i in features.keys():
>>>     list_vars.append(features[i])
# Pass list to generate_expression function to obtain a Pyomo expression as output
>>> print(polyfit.generate_expression(list_vars))
```

Prediction with *pysmo.polynomial_regression* models

Once a polynomial model has been trained, predictions for values at previously unsampled points :math:x_{unsampled} can be evaluated by calling the `poly_predict_output()` method on the resulting model object and the unsampled points:

```
# Create a python list from the headers of the dataset supplied for training
>>> y_unsampled = pr_init.poly_predict_output(rbf_fit, x_unsampled)
```

Flowsheet Integration

The result of the polynomial training process can be passed directly into a process flowsheet as an objective or a constraint. The following code snippet demonstrates how an output polynomial model may be integrated directly into a Pyomo flowsheet as an objective:

```
# Required imports
>>> import pyomo.environ as pyo
>>> from idaes.surrogates.pysmo import polynomial_regression
>>> import pandas as pd

# Create a Pyomo model
>>> m = pyo.ConcreteModel()
>>> i = pyo.Set(initialize=[1, 2])

# Create a Pyomo variable with indexed by the 2D-set i with initial values {0, 0}
>>> init_x = {1: 0, 2: 0}
>>> def x_init(m, i):
>>>     return (init_x[i])
>>> m.x = pyo.Var(i, initialize=x_init)

# Train a simple polynomial model on data available in csv format, resulting in the
↳ Python object polyfit
>>> xy_data = pd.read_csv('data.csv', header=None, index_col=0)
```

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```

>>> pr_init = polynomial_regression.PolynomialRegression(xy_data, xy_data, maximum_
↳ polynomial_order=3)
>>> features = pr_init.get_feature_vector()
>>> polyfit = pr_init.poly_training()

# Use the resulting polynomial as an objective, passing in the Pyomo variable x
>>> m.obj = pyo.Objective(expr=polyfit.generate_expression([m.x[1], m.x[2]]))

# Solve the model
>>> instance = m
>>> opt = pyo.SolverFactory("ipopt")
>>> result = opt.solve(instance, tee=True)

```

Further details about *pysmo.polynomial_regression* may be found by consulting the examples or reading the paper [...]

Available Methods

class `idaes.surrogate.pysmo.polynomial_regression.FeatureScaling`

A class for scaling and unscaling input and output data. The class contains two main methods: `data_scaling` and `data_unscaling`

static `data_scaling(data)`

`data_scaling` performs column-wise minimax scaling on the input dataset.

Parameters `data` – The input data set to be scaled. Must be a numpy array or dataframe.

Returns

tuple containing:

- **scaled_data** : A 2-D Numpy Array containing the scaled data. All array values will be between [0, 1].
- **data_minimum** : A 2-D row vector containing the column-wise minimums of the input data.
- **data_maximum** : A 2-D row vector containing the column-wise maximums of the input data.

Return type (tuple)

Raises `TypeError` – Raised when the input data is not a numpy array or dataframe

static `data_unscaling(x_scaled, x_min, x_max)`

`data_unscaling` performs column-wise un-scaling on the a minmax-scaled input dataset.

Parameters

- **x_scaled** (*NumPy Array*) – Data to be un-scaled. Data values should be between 0 and 1.
- **x_min** (*NumPy vector*) – $n \times 1$ vector containing the actual minimum value for each column. Must contain same number of elements as the number of columns in `x_scaled`.
- **x_max** (*NumPy vector*) – $n \times 1$ vector vector containing the actual minimum value for each column. Must contain same number of elements as the number of columns in `x_scaled`.

Returns A 2-D numpy array containing the scaled data, $x_{min} + x_{scaled} * (x_{max} - x_{min})$

Return type NumPy Array

Raises `IndexError` – Raised when the dimensions of the arrays are inconsistent.

```
class idaes.surrogate.pysmo.polynomial_regression.PolynomialRegression(original_data_input,
                                                                    re-
                                                                    gres-
                                                                    sion_data_input,
                                                                    max-
                                                                    i-
                                                                    imum_polynomial_order,
                                                                    num-
                                                                    ber_of_crossvalidations=None,
                                                                    no_adaptive_samples=None,
                                                                    train-
                                                                    ing_split=None,
                                                                    max_fraction_training_samples=None,
                                                                    max_iter=None,
                                                                    so-
                                                                    lu-
                                                                    tion_method=None,
                                                                    multi-
                                                                    no-
                                                                    mi-
                                                                    als=None)
```

The PolynomialRegression class performs polynomial regression on a training data set.

The class must first be initialized by calling PolynomialRegression. Regression is then carried out by calling `poly_training`.

For a given dataset with n features x_1, x_2, \dots, x_n , Polyregression is able to consider three types of basis functions:

- Monomial terms ($x_i^p, p \leq 10$) for all individual features. The maximum degree to be considered can be set by the user (**maximum_polynomial_order**)
- All first order interaction terms x_1x_2, x_1x_3 etc. This can be turned on or off by the user (set **multinomials**)
- User defined input features, e.g. $\sin(x_1)$. These must be Pyomo functions and should be provided as a list by the user calling `set_additional_terms` method before the polynomial training is done.

Example:

```
# Initialize the class and set additional terms
>>> d = PolynomialRegression(full_data, training_data, maximum_polynomial_order=2,
    ↪ max_iter=20, multinomials=1, solution_method='pyomo')
>>> p = d.get_feature_vector()
>>> d.set_additional_terms([...extra terms...])

# Train polynomial model and predict output for an test data x_test
>>> results = d.poly_training()
>>> predictions = d.poly_predict_output(results, x_test)
```

Parameters

- regression_data_input** (NumPy Array of Pandas Dataframe) – The dataset for regression training. It is expected to contain the features (X) and output (Y) data, with the output values (Y) in the last column.

- **original_data_input** (*NumPy Array of Pandas Dataframe*) – If **regression_data_input** was drawn from a larger dataset by some sampling approach, the larger dataset may be provided here. When additional data is not available, the same data supplied for training_data can be supplied - this tells the algorithm not to carry out adaptive sampling.
- **maximum_polynomial_order** (*int*) – The maximum polynomial order to be considered.

Further details about the optional inputs may be found under the `__init__` method.

`__init__` (*original_data_input, regression_data_input, maximum_polynomial_order, number_of_crossvalidations=None, no_adaptive_samples=None, training_split=None, max_fraction_training_samples=None, max_iter=None, solution_method=None, multinomials=None*)

Initialization of PolynomialRegression class.

Parameters

- **regression_data_input** (*NumPy Array of Pandas Dataframe*) – The dataset for regression training. It is expected to contain features and output data, with the output values (Y) in the last column.
- **original_data_input** (*NumPy Array of Pandas Dataframe*) – If **regression_data_input** was drawn from a larger dataset by some sampling approach, the larger dataset may be provided here.
- **maximum_polynomial_order** (*int*) – The maximum polynomial order to be considered.

Keyword Arguments

- **number_of_crossvalidations** (*int*) – The number of polynomial fittings and cross-validations to be carried out for each polynomial function/expression. Must be a positive, non-zero integer. Default=3.
- **training_split** (*float*) – The training/test split to be used for regression_data_input. Must be between 0 and 1. Default = 0.75
- **solution_method** (*str*) – The method to be used for solving the least squares optimization problem for polynomial regression. Three options are available:
 - (a) "MLE" : The mle (maximum likelihood estimate) method solves the least squares problem using linear algebra. Details of the method may be found in Forrester et al.
 - (b) "BFGS" : This approach solves the least squares problem using scipy's BFGS algorithm.
 - (c) "pyomo": This option solves the optimization problem in pyomo with IPOPT as solver. This is the default option.
- **multinomials** (*bool*) – This option determines whether or not multinomial terms are considered during polynomial fitting. Takes 0 for No and 1 for Yes. Default = 1.

Returns `self` object containing all the input information.

Raises

- `ValueError` – - The input datasets (**original_data_input** or **regression_data_input**) are of the wrong type (not Numpy arrays or Pandas Dataframes)
- `Exception` – * **maximum_polynomial_order** is not a positive, non-zero integer or **maximum_polynomial_order** is higher than the number of training samples available
- `Exception` – * **solution_method** is not 'mle', 'pyomo' or 'bfgs'

- `Exception` -- **multinomials** is not binary (0 or 1)
- `Exception` -- **training_split** is not between 0 and 1
- `Exception` -- **number_of_crossvalidations** is not a positive, non-zero integer
- `Exception` -- **max_fraction_training_samples** is not between 0 and 1
- `Exception` -- **no_adaptive_samples** is not a positive, non-zero integer
- `Exception` -- **max_iter** is not a positive, non-zero integer
- `warnings.warn` -- When the number of cross-validations is too high, i.e. `number_of_crossvalidations > 10`

`get_feature_vector()`

The `get_feature_vector` method generates the list of regression features from the column headers of the input dataset.

Returns An indexed parameter list of the variables supplied in the original data

Return type Pyomo IndexedParam

Example:

```
# Create a small dataframe with three columns ('one', 'two', 'three') and two
↳ rows (A, B)
>>> xy_data = pd.DataFrame.from_items([('A', [1, 2, 3]), ('B', [4, 5, 6])],
↳ orient='index', columns=['one', 'two', 'three'])

# Initialize the **PolynomialRegression** class and print the column headers
↳ for the variables
>>> f = PolynomialRegression(xy_data, xy_data, maximum_polynomial_order=1,
↳ multinomials=True, training_split=0.8)
>>> p = f.get_feature_vector()
>>> for i in p.keys():
>>>     print(i)
one
two
```

`poly_predict_output(results_vector, x_data)`

The `poly_predict_output` method generates output predictions for input data `x_data` based a previously generated polynomial fitting.

Parameters

- **results_vector** – Python object containing results of polynomial fit generated by calling the `poly_training` function.
- **x_data** – Numpy array of designs for which the output is to be evaluated/predicted.

Returns Output variable predictions based on the polynomial fit.

Return type Numpy Array

`poly_training()`

The `poly_training` method trains a polynomial model to an input dataset. It calls the core method which is called in the `PolynomialRegression` class (`polynomial_regression_fitting`). It accepts no user input, inheriting the information passed in class initialization.

Returns

Python Object (results) containing the results of the polynomial regression process including:

- the polynomial order (**self.polynomial_order**)
- polynomial coefficients (**self.optimal_weights_array**), and
- MAE and MSE errors as well as the R^2 (**results.errors**).

Return type `tuple`

set_additional_terms (*term_list*)

`set_additional_terms` accepts additional user-defined features for consideration during regression.

Parameters **term_list** (*list*) – List of additional terms to be considered as regression features. Each term in the list must be a Pyomo-supported intrinsic function.

Example:

```
# To add the sine and cosine of a variable with header 'X1' in the dataset as
↳additional regression features:
>>> xy_data = pd.DataFrame.from_items([('A', [1, 2, 3]), ('B', [4, 5, 6])],
↳orient='index', columns=['X1', 'X2', 'Y'])
>>> A = PolynomialRegression(xy_data, xy_data, maximum_polynomial_order=5)
>>> p = A.get_feature_vector()
>>> A.set_additional_terms([ pyo.sin(p['X1']) , pyo.cos(p['X1']) ])
```

class `idaes.surrogate.pysmo.polynomial_regression.ResultReport` (*optimal_weight_vector*,
polynomial_order,
multinomials,
mae_error,
mse_error,
R2, *adjusted_R2*, *number_of_iterations*,
results_vector,
additional_features_array,
final_regression_data,
df_coefficients,
extra_terms_coeffs,
extra_terms_feature_vector,
extra_terms_expressions)

generate_expression (*variable_list*)

The `generate_expression` method returns the Pyomo expression for the polynomial model trained.

The expression is constructed based on a supplied list of variables **variable_list** and the output of `poly_training`.

Parameters **variable_list** (*list*) – List of input variables to be used in generating expression. This can be the a list generated from the results of `get_feature_vector`. The user can also choose to supply a new list of the appropriate length.

Returns Pyomo expression of the polynomial model based on the variables provided in **variable_list**.

Return type Pyomo Expression

References:

[1] Forrester et al.'s book "Engineering Design via Surrogate Modelling: A Practical Guide", <https://onlinelibrary.wiley.com/doi/pdf/10.1002/9780470770801>

Generating Radial Basis Function (RBF) models with PySMO

The `pysmo.radial_basis_function` package has the capability to generate different types of RBF surrogates from data based on the basis function selected. RBFs models are usually of the form where

$$y_k = \sum_{j=1}^{\Omega} w_j \psi(\|x_k - z_j\|) \quad k = 1, \dots, m \quad (4.2)$$

where z_j are basis function centers (in this case, the training data points), w_j are the radial weights associated with each center z_j , and ψ is a basis function transformation of the Euclidean distances.

PySMO offers a range of basis function transformations ψ , as shown in the table below.

Table 7: List of available RBF basis transformations, $d = \|x_k - z_j\|$

Transformation type	PySMO option name	$\psi(d)$
Linear	'linear'	d
Cubic	'cubic'	d^3
Thin-plate spline	'spline'	$d^2 \ln(d)$
Gaussian	'gaussian'	$e^{(-d^2 \sigma^2)}$
Multiquadric	'mq'	$\sqrt{1 + (\sigma d)^2}$
Inverse mMultiquadric	'imq'	$1/\sqrt{1 + (\sigma d)^2}$

Selection of parametric basis functions increase the flexibility of the radial basis function but adds an extra parameter (σ) to be estimated.

Basic Usage

To generate an RBF model with PySMO, the `pysmo.radial_basis_function` class is first initialized, and then the function `rbf_training` is called on the initialized object:

```
# Required imports
>>> from idaes.surrogates.pysmo import radial_basis_function
>>> import pandas as pd

# Load dataset from a csv file
>>> xy_data = pd.read_csv('data.csv', header=None, index_col=0)

# Initialize the RadialBasisFunctions class, extract the list of features and train
↳ the model
>>> rbf_init = radial_basis_function.RadialBasisFunctions(xy_data, *kwargs)
>>> features = rbf_init.get_feature_vector()
>>> rbf_fit = rbf_init.rbf_training()
```

- *xy_data* is a two-dimensional python data structure containing the input and output training data. The output values **MUST** be in the last column.

Optional Arguments

- *basis_function* - option to specify the type of basis function to be used in the RBF model. Default is 'gaussian'.
- *regularization* - boolean which determines whether regularization of the RBF model is considered. Default is True.
 - When regularization is turned on, the resulting model is a regressing RBF model.
 - When regularization is turned off, the resulting model is an interpolating RBF model.

pysmo.radial_basis_function Output

The result of *pysmo.radial_basis_function* (*rbf_fit* in above example) is a python object containing information about the optimal radial basis function weights w_j and different error and quality-of-fit metrics such as the mean-squared-error (MSE) and the R^2 coefficient-of-fit. A Pyomo expression can be generated from the object simply passing a list of variables into the function *rbf_generate_expression*:

```
# Create a python list from the headers of the dataset supplied for training
>>> list_vars = []
>>> for i in features.keys():
>>>     list_vars.append(features[i])

# Pass list to generate_expression function to obtain a Pyomo expression as output
>>> print(rbf_fit.rbf_generate_expression(list_vars))
```

Similar to the *pysmo.polynomial_regression* module, the output of the *rbf_generate_expression* function can be passed into an IDAES or Pyomo module as a constraint, objective or expression.

Prediction with *pysmo.radial_basis_function* models

Once an RBF model has been trained, predictions for values at previously unsampled points $x_{\text{unsampled}}$ can be evaluated by calling the *rbf_predict_output()* function on the resulting Python object and the unsampled points:

```
# Create a python list from the headers of the dataset supplied for training
>>> y_unsampled = rbf_init.rbf_predict_output(rbf_fit, x_unsampled)
```

Further details about *pysmo.radial_basis_function* module may be found by consulting the examples or reading the paper [...]

Available Methods

class `idaes.surrogate.pysmo.radial_basis_function.FeatureScaling`

A class for scaling and unscaling input and output data. The class contains two main methods: `data_scaling_minmax` and `data_unscaling_minmax`

static `data_scaling_minmax(data)`

`data_scaling_minmax` performs column-wise min-max scaling on the input dataset.

Parameters `data` – The input data set to be scaled. Must be a numpy array or dataframe.

Returns

tuple containing:

- **scaled_data** : A 2-D Numpy Array containing the scaled data. All array values will be between [0, 1].
- **data_minimum** : A 2-D row vector containing the column-wise minimums of the input data.
- **data_maximum** : A 2-D row vector containing the column-wise maximums of the input data.

Return type (tuple)

Raises `TypeError` – Raised when the input data is not a numpy array or dataframe

static data_unscaling_minmax (*x_scaled*, *x_min*, *x_max*)

`data_unscaling_minmax` performs column-wise un-scaling on the a minmax-scaled input dataset.

Parameters

- **x_scaled** (*NumPy Array*) – Data to be un-scaled. Data values should be between 0 and 1.
- **x_min** (*NumPy vector*) – $n \times 1$ vector containing the actual minimum value for each column. Must contain same number of elements as the number of columns in *x_scaled*.
- **x_max** (*NumPy vector*) – $n \times 1$ vector vector containing the actual minimum value for each column. Must contain same number of elements as the number of columns in *x_scaled*.

Returns A 2-D numpy array containing the scaled data, $x_{min} + x_{scaled} * (x_{max} - x_{min})$

Return type NumPy Array

Raises `IndexError` – Raised when the dimensions of the arrays are inconsistent.

```
class idaes.surrogate.pysmo.radial_basis_function.RadialBasisFunctions (XY_data,
                                                                    ba-
                                                                    sis_function=None,
                                                                    so-
                                                                    lu-
                                                                    tion_method=None,
                                                                    reg-
                                                                    u-
                                                                    lar-
                                                                    iza-
                                                                    tion=None)
```

The `RadialBasisFunctions` class generates a radial basis function fitting for a training data set.

The class must first be initialized by calling **RadialBasisFunctions**. Regression is then carried out by calling the method `rbf_training`.

For a given dataset with n features x_1, \dots, x_n , `RadialBasisFunctions` is able to consider six types of basis transformations:

- Linear ('linear')
- Cubic ('cubic')
- Gaussian ('gaussian')
- Multiquadric ('mq')
- Inverse multiquadric ('imq')
- Thin-plate spline ('spline')

`rbf_training` selects the best hyperparameters (regularization parameter λ and shape parameter σ , where necessary) by evaluating the leave-one-out cross-validation error for each (λ, σ) pair.

It should be noted that all the training points are treated as centres for the RBF, resulting in a square system.

Example:

```
# Initialize the class
>>> d = RadialBasisFunctions(training_data, basis_function='gaussian', solution_
↪method='pyomo', regularization=True))
>>> p = d.get_feature_vector()

# Train RBF model and predict output for an test data x_test
>>> results = d.rbf_training()
>>> predictions = d.rbf_predict_output(results, x_test)
```

Parameters `XY_data` (*Numpy Array or Pandas Dataframe*) – The dataset for RBF training. **`XY_data`** is expected to contain the features (X) and output (Y) data, with the output values (Y) in the last column.

Further details about the optional inputs may be found under the `__init__` method.

`__init__` (*XY_data, basis_function=None, solution_method=None, regularization=None*)
Initialization of **`RadialBasisFunctions`** class.

Parameters `XY_data` (*Numpy Array or Pandas Dataframe*) – The dataset for RBF training. **`XY_data`** is expected to contain feature and output information, with the output values (y) in the last column.

Keyword Arguments

- **`basis_function`** (*str*) – The basis function transformation to be applied to the training data. Two classes of basis transformations are available for selection:
 - Fixed basis transformations, which require no shape parameter σ :
 - (a) 'cubic' : Cubic basis transformation
 - (b) 'linear' : Linear basis transformation
 - (c) 'spline' : Thin-plate spline basis transformation
 - Parametric basis transformations which require a shape parameter:
 - (a) 'gaussian' : Gaussian basis transformation (Default)
 - (b) 'mq' : Multiquadric basis transformation
 - (c) 'imq' : Inverse multiquadric basis transformation
- **`solution_method`** (*str*) – The method to be used for solving the RBF least squares optimization problem. Three options are available:
 - (a) 'algebraic' : The explicit algebraic method solves the least squares problem using linear algebra.
 - (b) 'BFGS' : This approach solves the least squares problem using SciPy's BFGS algorithm.
 - (c) 'pyomo' : This option solves the optimization problem in Pyomo with IPOPT as solver. This is the default.
- **`regularization`** (*bool*) – This option determines whether or not the regularization parameter λ is considered during RBF fitting. Default setting is True.

Returns `self` object with the input information

Raises

- `ValueError` – The input dataset is of the wrong type (not a NumPy array or Pandas Dataframe)
- `Exception` – * `basis_function` entry is not valid.
- `Exception` – * `solution_method` is not ‘algebraic’, ‘pyomo’ or ‘bfgs’.
- `Exception` – λ is not boolean.

Example:

```
# Specify the gaussian basis transformation
>>> d = RadialBasisFunctions(XY_data, basis_function='gaussian')
```

get_feature_vector()

The `get_feature_vector` method generates the list of regression features from the column headers of the input dataset.

Returns An indexed parameter list of the variables supplied in the original data

Return type Pyomo IndexedParam

Example:

```
# Create a small dataframe with three columns ('one', 'two', 'three') and two
↳ rows (A, B)
>>> xy_data = pd.DataFrame.from_items([('A', [1, 2, 3]), ('B', [4, 5, 6])],
↳ orient='index', columns=['one', 'two', 'three'])

# Initialize the **RadialBasisFunctions** class with a linear kernel and
↳ print the column headers for the variables
>>> f = RadialBasisFunctions(xy_data, basis_function='linear')
>>> p = f.get_feature_vector()
>>> for i in p.keys():
>>>     print(i)
one
two
```

static r2_calculation(y_true, y_predicted)

`r2_calculation` returns the R^2 as a measure-of-fit between the true and predicted values of the output variable.

Parameters

- `y_true` (NumPy Array) – Vector of actual values of the output variable
- `y_predicted` (NumPy Array) – Vector of predictions for the output variable based on the surrogate

Returns R^2 measure-of-fit between actual and predicted data

Return type float

rbf_predict_output(results_vector, x_data)

The `rbf_predict_output` method generates output predictions for input data `x_data` based a previously generated RBF fitting.

Parameters

- **results_vector** (*tuple*) – Results of RBF training generated by calling the `rbf_training` function.
- **x_data** (*NumPy Array*) – Designs for which the output is to be evaluated/predicted.

Returns Output variable predictions based on the rbf fit.

Return type Numpy Array

rbf_training()

Main function for RBF training.

To train the RBF:

- (1) The best values of the hyperparameters (σ , λ) are selected via LOOCV.
- (2) The necessary basis transformation at the optimal hyperparameters is generated.
- (3) The condition number for the transformed matrix is calculated.
- (4) The optimal radial weights are evaluated using the selected optimization method.
- (5) The training predictions, prediction errors and r-square coefficient of fit are evaluated by calling the methods `error_calculation` and `r2_calculation`
- (6) A results object is generated by calling the `ResultsReport` class.

The LOOCV error for each (σ , λ) pair is evaluated by calling the function `loo_error_estimation_with_rippa_method`.

The pre-defined shape parameter set considers 24 irregularly spaced values ranging between 0.001 - 1000, while the regularization parameter set considers 21 values ranging between 0.00001 - 1.

Returns

Python object (results) containing the all information about the best RBF fitting obtained, including:

- the optimal radial weights (**results.radial_weights**),
- when relevant, the optimal shape parameter found σ (**results.sigma**),
- when relevant, the optimal regularization parameter found λ (**results.regularization**),
- the RBF predictions for the training data (**results.output_predictions**), and
- the R^2 value on the training data (**results.R2**)

Return type *tuple*

```
class idaes.surrogate.pyomo.radial_basis_function.ResultReport (radial_weights,
                                                                best_r_value,
                                                                best_lambda_param,
                                                                centres,
                                                                y_training_predictions,
                                                                rmse_error,
                                                                x_condition_number,
                                                                reg_setting,
                                                                r_square,  ba-
                                                                sis_function,
                                                                data_min,
                                                                data_max)
```

rbf_generate_expression (*variable_list*)

The `rbf_generate_expression` method returns the Pyomo expression for the RBF model trained.

The expression is constructed based on the supplied list of variables **variable_list** and the results of the previous RBF training process.

Parameters **variable_list** (*list*) – List of input variables to be used in generating expression. This can be the a list generated from the output of `get_feature_vector`. The user can also choose to supply a new list of the appropriate length.

Returns Pyomo expression of the RBF model based on the variables provided in **variable_list**

Return type Pyomo Expression

References:

- [1] Forrester et al.'s book "Engineering Design via Surrogate Modelling: A Practical Guide", <https://onlinelibrary.wiley.com/doi/pdf/10.1002/9780470770801>
- [2] Hongbing Fang & Mark F. Horstemeyer (2006): Global response approximation with radial basis functions, <https://www.tandfonline.com/doi/full/10.1080/03052150500422294>
- [3] Rippa, S. (1999): An algorithm for selecting a good value for the parameter c in radial basis function interpolation, <https://doi.org/10.1023/A:1018975909870>
- [4] Mongillo M.A. (2011) Choosing Basis Functions and Shape Parameters for Radial Basis Function Methods, <https://doi.org/10.1137/11S010840>

Generating Kriging Models with PySMO

The *pysmo.kriging* trains Ordinary Kriging models. Interpolating kriging models assume that the outputs $\hat{y} \in \mathbb{R}^{m \times 1}$ are correlated and may be treated as a normally distributed stochastic process. For a set of input measurements $X = \{x_1, x_2, \dots, x_m\}; x_i \in \mathbb{R}^n$, the output \hat{y} is modeled as the sum of a mean (μ) and a Gaussian process error,

$$\hat{y}_k = \mu + \epsilon(x_k) \quad k = 1, \dots, m \quad (4.3)$$

Kriging models assume that the errors in the outputs ϵ are correlated proportionally to the distance between corresponding points,

$$\text{cor}[\epsilon(x_j), \epsilon(x_k)] = \exp\left(-\sum_{i=1}^n \theta_i |x_{ij} - x_{ik}|^{\tau_i}\right) \quad j, k = 1, \dots, m; \tau_i \in [1, 2]; \theta_i \geq 0 \quad (4.4)$$

The hyperparameters of the Kriging model $(\mu, \sigma^2, \theta_1, \dots, \theta_n, \tau_1, \dots, \tau_n)$ are selected such that the concentrated log likelihood function is maximized.

Basic Usage

To generate a Kriging model with PySMO, the *pysmo.kriging* class is first initialized, and then the function *kriging_training* is called on the initialized object:

```
# Required imports
>>> from idaes.surrogates.pysmo import kriging
>>> import pandas as pd

# Load dataset from a csv file
>>> xy_data = pd.read_csv('data.csv', header=None, index_col=0)

# Initialize the KrigingModel class, extract the list of features and train the model
>>> krg_init = kriging.KrigingModel(xy_data, *kwargs)
>>> features = krg_init.get_feature_vector()
>>> krg_fit = krg_init.kriging_training()
```

- *xy_data* is a two-dimensional python data structure containing the input and output training data. The output values **MUST** be in the last column.

Optional Arguments

- *numerical_gradients*: Whether or not numerical gradients should be used in training. This choice determines the algorithm used to solve the problem.
 - True: The problem is solved with BFGS using central differencing with $\Delta = 10^{-6}$ to evaluate numerical gradients.
 - False: The problem is solved with Basinhopping, a stochastic optimization algorithm.
- *regularization* - Boolean option which determines whether or not regularization is considered during Kriging training. Default is True.
 - When regularization is turned on, the resulting model is a regressing kriging model.
 - When regularization is turned off, the resulting model is an interpolating kriging model.

pysmo.kriging Output

The result of *pysmo.kriging* (*krg_fit* in above example) is a python object containing information about the optimal Kriging hyperparameters $(\mu, \sigma^2, \theta_1, \dots, \theta_n)$ and different error and quality-of-fit metrics such as the mean-squared-error (MSE) and the R^2 coefficient-of-fit. A Pyomo expression can be generated from the object simply passing a list of variables into the function *kriging_generate_expression*:

```
# Create a python list from the headers of the dataset supplied for training
>>> list_vars = []
>>> for i in features.keys():
>>>     list_vars.append(features[i])

# Pass list to generate_expression function to obtain a Pyomo expression as output
>>> print(krg_fit.kriging_generate_expression(list_vars))
```

Similar to the *pysmo.polynomial_regression* module, the output of the *kriging_generate_expression* function can be passed into an IDAES or Pyomo module as a constraint, objective or expression.

Prediction with *pysmo.kriging* models

Once a Kriging model has been trained, predictions for values at previously unsampled points *x_unsampled* can be evaluated by calling the *kriging_predict_output()* function on the resulting Python object and the unsampled points:

```
# Create a python list from the headers of the dataset supplied for training
>>> y_unsampled = kriging_init.kriging_predict_output(krg_fit, x_unsampled)
```

Further details about *pysmo.kriging* module may be found by consulting the examples or reading the paper [...]

Available Methods

class `idaes.surrogate.pysmo.kriging.KrigingModel` (*XY_data*, *numerical_gradients=True*,
regularization=True)

The `KrigingModel` class trains a Kriging model for a training data set.

The class must first be initialized by calling **KrigingModel**. Model training is then carried out by calling the `kriging_training` method.

KrigingModel is able to generate either an interpolating or a regressing Kriging model depending on the settings used during initialization..

Example:

```
# Initialize the class
>>> d = KrigingModel(training_data, numerical_gradients=True,
    ↪regularization=True)
>>> p = d.get_feature_vector()

# Train Kriging model and predict output for an test data x_test
>>> results = d.kriging_training()
>>> predictions = d.kriging_predict_output(results, x_test)
```

Parameters **XY_data** (*NumPy Array or Pandas Dataframe*) – The dataset for Kriging training. **XY_data** is expected to contain both the features (X) and output (Y) information, with the output values (Y) in the last column.

Further details about the optional inputs may be found under the `__init__` method.

__init__ (*XY_data*, *numerical_gradients=True*, *regularization=True*)
Initialization of **KrigingModel** class.

Parameters **XY_data** (*NumPy Array or Pandas Dataframe*) – The dataset for Kriging training. **XY_data** is expected to contain feature and output data, with the output values (y) in the last column.

Keyword Arguments

- **numerical_gradients** (*bool*) – Whether or not numerical gradients should be used in training. This choice determines the algorithm used to solve the problem.
 - `numerical_gradients = True`: The problem is solved with BFGS using central differencing with a step size of 10^{-6} to evaluate numerical gradients.
 - `numerical_gradients = False`: The problem is solved with Basinhopping, a stochastic optimization algorithm.
- **regularization** (*bool*) – This option determines whether or not regularization is considered during Kriging training. Default is `True`.
 - When regularization is turned off, the model generates an interpolating kriging model.

Returns self object with the input information and settings.

Raises

- `ValueError` – - The input dataset is of the wrong type (not a NumPy array or Pandas Dataframe)

- `Exception` -- numerical_gradients is not boolean
- `Exception` -- regularization is not boolean

Example:

```
# Initialize Kriging class with no numerical gradients - solution algorithm_  
↪ will be Basinhopping  
>>> d = KrigingModel(XY_data, numerical_gradients=False)
```

get_feature_vector()

The `get_feature_vector` method generates the list of regression features from the column headers of the input dataset.

Returns An indexed parameter list of the variables supplied in the original data

Return type Pyomo IndexedParam

kriging_predict_output(kriging_params, x_pred)

The `kriging_predict_output` method generates output predictions for input data `x_pred` based a previously trained Kriging model.

Parameters

- **kriging_params** (*tuple*) – Results of Kriging training generated by calling the `kriging_training` method.
- **x_pred** (*NumPy Array*) – Array of designs for which the output is to be evaluated/predicted.

Returns Output variable predictions based on the Kriging model.

Return type NumPy Array

kriging_training()

Main function for Kriging training.

To train the Kriging model:

- (1) The Kriging exponent τ_i is fixed at 2.
- (2) The optimal Kriging hyperparameters $(\mu, \sigma^2, \theta_1, \dots, \theta_n)$ are evaluated by calling the `optimal_parameter_evaluation` method using either BFGS or Basinhopping.
- (3) The training predictions, prediction errors and r-square coefficient of fit are evaluated by calling the functions `error_calculation` and `self.r2_calculation`
- (4) A results object is generated by calling the `ResultsReport` class.

Returns

Python object (results) containing the all information about the best Kriging model obtained, including:

- the Kriging model hyperparameters (**results.optimal_weights**),
- when relevant, the optimal regularization parameter found λ (**results.regularization_parameter**),
- the Kriging mean (**results.optimal_mean**),
- the Kriging variance (**results.optimal_variance**),
- the Kriging model regularized co-variance matrix (**results.optimal_covariance_matrix**),

- the inverse of the co-variance matrix (**results.covariance_matrix_inverse**),
- the RBF predictions for the training data (**results.output_predictions**),
- the RMSE of the training output predictions (**results.training_rmse**), and
- the R^2 value on the training data (**results.R2**)

Return type `tuple`

static `r2_calculation` (*y_true*, *y_predicted*)

`r2_calculation` returns the R^2 as a measure-of-fit between the true and predicted values of the output variable.

Parameters

- **y_true** (*NumPy Array*) – Vector of actual values of the output variable
- **y_predicted** (*NumPy Array*) – Vector of predictions for the output variable based on the surrogate

Returns R^2 measure-of-fit between actual and predicted data

Return type `float`

```
class idaes.surrogate.pysmo.kriging.ResultReport (theta, reg_param, mean, variance,
                                                cov_mat, cov_inv, ymu, y_training,
                                                r2_training, rmse_error, p, x_data,
                                                x_data_scaled,      x_data_min,
                                                x_data_max)
```

kriging_generate_expression (*variable_list*)

The `kriging_generate_expression` method returns the Pyomo expression for the Kriging model trained.

The expression is constructed based on the supplied list of variables **variable_list** and the results of the previous Kriging training process.

Parameters **variable_list** (*list*) – List of input variables to be used in generating expression. This can be the a list generated from the output of `get_feature_vector`. The user can also choose to supply a new list of the appropriate length.

Returns Pyomo expression of the Kriging model based on the variables provided in **variable_list**

Return type Pyomo Expression

References:

- [1] Forrester et al.'s book "Engineering Design via Surrogate Modelling: A Practical Guide", <https://onlinelibrary.wiley.com/doi/pdf/10.1002/9780470770801>
- [2] D. R. Jones, A taxonomy of global optimization methods based on response surfaces, Journal of Global Optimization, <https://link.springer.com/article/10.1023%2FA%3A1012771025575>



ALAMOpPy, RIPE, and HELMET are data driven machine learning (ddm-learning) tools. They are regression tools for the development of property models for kinetics and thermodynamics of a system. The provided tools include both ALAMOpPy and RIPE that can access ALAMO and other solvers through the Python API.



Python-based Surrogate Modeling Objects (PySMO) is a framework for general-purpose surrogate modeling techniques, integrated with the Pyomo mathematical optimization framework (on which IDAES is also based).

4.12 Applications

This section contains applications that can be used in conjunction with the IDAES framework and libraries, but which are not closely tied to the implementation.

4.12.1 Contents

MatOpt : Materials Optimization

The MatOpt module provides tools for nanomaterials design using Mathematical Optimization. MatOpt can be used to design crystalline nanostructured materials, including but not limited to particles, wires, surfaces, and periodic bulk structures.

The main goals of this package are as follows:

- To automate many of the steps that are necessary for utilizing mathematical optimization to design materials, speeding up the development of new mathematical models and accelerating new materials discovery.
- To simplify the representation of nanostructured materials and their structure-function relationships as Pyomo objects, streamlining the creation of materials optimization problems in the Pyomo modeling language.
- To provide a simple interface so that users need not handle the details of casting efficient mathematical optimization models, invoking mathematical optimization solvers, or utilizing specialized Pyomo syntax to do this.

Thank you for your interest in MatOpt. We would love to hear your feedback! Please report any thoughts, questions or bugs to: gounaris@cmu.edu

If you are using MatOpt, please consider citing:

- Hanselman, C.L., Yin, X., Miller, D.C. and Gounaris, C.E., 2020. MatOpt: A Python package for nanomaterials design using discrete optimization. *In preparation*.

Basic Usage

There are two main sub-modules contained in the package serving two distinct purposes:

- The `matopt.materials` module contains objects and methods for efficiently representing and manipulating a nanomaterial and its design space.
- The `matopt.opt` module contains objects and methods for speeding up the casting of a Mixed-integer Linear Programming (MILP) model with simplified modeling syntax and automatic model formulation.

Dependencies

User access to the MILP solver CPLEX through Pyomo is assumed. For users who do not have access to CPLEX, the use of [NEOS-CPLEX](#) is suggested as an alternative.

Define design canvas

Several pieces of information about the material and design space need to be specified in order to formulate a materials optimization problem. To fulfill this need, the `matopt.materials` module defines generic and simple objects for describing the type of material to be designed and its design space, also referred to as a “canvas”.

Some key objects are listed as follows:

class `apps.matopt.materials.lattices.lattice.Lattice`

A class used to represent crystal lattice locations.

The class encodes methods for determining which Cartesian coordinates to consider as sites on an infinite crystal lattice. A `Lattice` can be constructed from a point on the lattice (i.e., a shift from the origin), an alignment (i.e., rotation from a nominal orientation), and appropriate scaling factors. With these attributes, we generally support the translation, rotation, and rescaling of lattices. Additionally, `Lattice` objects include a method for determining which sites should be considered neighbors.

class `apps.matopt.materials.canvas.Canvas` (*Points=None, NeighborhoodIndexes=None, DefaultNN=0*)

A class for combining geometric points and neighbors.

This class contains a list of Cartesian points coupled with a graph of nodes for sites and arcs for bonds. A `Canvas` object establishes a mapping from the abstract, mathematical modeling of materials as graphs to the geometry of the material lattice. The list of points and neighbor connections necessary to create a `Canvas` object can be obtained from the combination of `Lattice`, `Shape`, and `Tiling` objects.

class `apps.matopt.materials.design.Design` (*Canvas_=None, Contents=None*)

A class used to represent material designs.

This class combines a `Canvas` objects and a list of contents. It assigns an element (possibly `None`) to each point in the `Canvas`. This generally works for any type of content, but it is intended to work with `Atom` objects and can be used to generate CFG, PDB, POSCAR, and XYZ files.

Build model via descriptors

The material type and design space specified provide indices, sets, and parameters for the optimization model. Using simple syntax, inspired by materials-related terminology, MatOpt users define a `MatOptModel` object, which will be translated into a Pyomo `ConcreteModel` object automatically.

MatOpt uses `MaterialDescriptor` objects to represent variables, constraints, and objectives. A `MatOptModel` object holds lists of `MaterialDescriptor` objects. By default, several universal site descriptors are pre-defined in the model.

Descriptor	Explanation
Y_{ik}	Presence of a building block of type k at site i
Y_i	Presence of any type of building block at site i
X_{ijkl}	Presence of a building block of type k at site i and a building block of type l at site j
X_{ij}	Presence of any building block at site i and any building block at site j
C_{ikl}	Count of neighbors of type l next to a building block of type k at site i
C_i	Count of any type of neighbors next to a building block at site i

User-specified descriptors are defined by `DescriptorRule` objects in conjunction with `Expr` expression objects. Available expressions include:

Expression	Explanation
<code>LinearExpr</code>	Multiplication and addition of coefficients to distinct descriptors
<code>SiteCombination</code>	Summation of site contributions from two sites
<code>SumNeighborSites</code>	Summation of site contributions from all neighboring sites
<code>SumNeighborBonds</code>	Summation of bond contributions to all neighboring sites
<code>SumSites</code>	Summation across sites
<code>SumBonds</code>	Summation across bonds
<code>SumSiteTypes</code>	Summation across site types
<code>SumBondTypes</code>	Summation across bond types
<code>SumSitesAndTypes</code>	Summation across sites and site types
<code>SumBondsAndTypes</code>	Summation across bonds and bond types
<code>SumConfs</code>	Summation across conformation types
<code>SumSitesAndConfs</code>	Summation across sites and conformation types

Several types of `DescriptorRules` are available.

Rule	Explanation
<code>LessThan</code>	Descriptor less than or equal to an expression
<code>EqualTo</code>	Descriptor equal to an expression
<code>GreaterThan</code>	Descriptor greater than or equal to an expression
<code>FixedTo</code>	Descriptor fixed to a scalar value
<code>PiecewiseLinear</code>	Descriptor equal to the evaluation of a piecewise linear function
<code>Implies</code>	Indicator descriptor that imposes other constraints if equal to 1
<code>NegImplies</code>	Indicator descriptor that imposes other constraints if equal to 0
<code>ImpliesSiteCombination</code>	Indicator bond-indexed descriptor that imposes constraints on the two sites
<code>ImpliesNeighbors</code>	Indicator site-indexed descriptor that imposes constraints on neighboring sites

From the combination of the above pre-defined descriptors, expressions, and rules, a user can specify a wide variety of other descriptors, as necessary.

```
class apps.matopt.opt.mat_modeling.MaterialDescriptor (name,          canv=None,
                                                         atoms=None, confDs=None,
                                                         bounds=(None, None), in-
                                                         teger=False,  binary=False,
                                                         rules=[], **kwargs)
```

A class to represent material geometric and energetic descriptors.

This class holds the information to define mathematical optimization variables for the properties of materials. Additionally, each descriptor has a ‘rules’ list to which the user can append rules defining the descriptor and constraining the design space.

name
A unique (otherwise Pyomo will complain) name
Type string

canv
The canvas that the descriptor will be indexed over
Type Canvas

atoms
The building blocks to index the descriptor over.
Type list<BBlock>

confDs
The designs for conformations to index over.
Type list<Design>

integer
Flag to indicate if the descriptor takes integer values.
Type bool

binary
Flag to indicate if the descriptor takes boolean values.
Type bool

rules
List of rules to define and constrain the material descriptor design space.
Type list<DescriptorRules>

bounds
If tuple, the lower and upper bounds on the descriptor values across all indices. If dict, the bounds can be individually set for each index.
Type tuple/dict/func

See `IndexedElem` for more information on indexing. See `DescriptorRule` for information on defining descriptors.

Solve optimization model

Once the model is fully specified, the user can optimize it in light of a chosen descriptor to serve as the objective to be maximized or minimized, as appropriate. Several functions are provided for users to choose from.

class `apps.matopt.opt.mat_modeling.MatOptModel` (*canv*, *atoms=None*, *confDs=None*)
A class for the specification of a materials optimization problem.

Once all the material information is specified, we use this class to specify the material design problem of interest. This class is intended to be interpretable without mathematical optimization background while the conversion to Pyomo optimization models happens automatically.

canv
The canvas of the material design space
Type Canvas

atoms
The list of building blocks to consider. Note: This list does not need to include a void-atom type. We use 'None' to represent the absence of any building block at a given site.
Type list<BBlock>

confDs

The list of conformations to consider.

Type list<Design>

maximize (*func*, ***kwargs*)

Method to maximize a target functionality of the material model.

Parameters

- **func** (MaterialDescriptor/Expr) – Material functionality to optimize.
- ****kwargs** – Arguments to MatOptModel.optimize

Returns (Design/list<Design>) Optimal designs.

Raises pyutilib.ApplicationError if MatOpt can not find usable solver (CPLEX or NEOS-CPLEX)

See MatOptModel.optimize method for details.

minimize (*func*, ***kwargs*)

Method to minimize a target functionality of the material model.

Parameters

- **func** (MaterialDescriptor/Expr) – Material functionality to optimize.
- ****kwargs** – Arguments to MatOptModel.optimize

Returns (Design/list<Design>) Optimal designs.

Raises pyutilib.ApplicationError if MatOpt can not find usable solver (CPLEX or NEOS-CPLEX)

See MatOptModel.optimize method for details.

optimize (*func*, *sense*, *nSolns=1*, *tee=True*, *disp=1*, *keepfiles=False*, *tilim=3600*, *trelim=None*, *solver='cplex'*)

Method to create and optimize the materials design problem.

This method automatically creates a new optimization model every time it is called. Then, it solves the model via Pyomo with the CPLEX solver.

If multiple solutions (called a ‘solution pool’) are desired, then the nSolns argument can be provided and the populate method will be called instead.

Parameters

- **func** (MaterialDescriptor/Expr) – Material functionality to optimize.
- **sense** (*int*) – flag to indicate the choice to minimize or maximize the functionality of interest. Choices: minimize/maximize (Pyomo constants 1,-1 respectively)
- **nSolns** (*int*) – Optional, number of Design objects to return. Default: 1 (See MatOptModel.populate for more information)
- **tee** (*bool*) – Optional, flag to turn on solver output. Default: True
- **disp** (*int*) – Optional, flag to control level of MatOpt output. Choices: 0: No MatOpt output (other than solver tee) 1: MatOpt output for outer level method 2: MatOpt output for solution pool & individual solns. Default: 1
- **keepfiles** (*bool*) – Optional, flag to save temporary pyomo files. Default: True
- **tilim** (*float*) – Optional, solver time limit (in seconds). Default: 3600

- **trelim** (*float*) – Optional, solver tree memory limit (in MB). Default: None (i.e., Pyomo/CPLEX default)
- **solver** (*str*) – Solver choice. Currently only cplex or neos-cplex are supported Default: cplex

Returns (Design/list<Design>) Optimal design or designs, depending on the number of solutions requested by argument nSolns.

Raises pyutilib.ApplicationError if MatOpt can not find usable solver (CPLEX or NEOS-CPLEX)

populate (*func, sense, nSolns, tee=True, disp=1, keepfiles=False, tilim=3600, trelim=None, solver='cplex'*)

Method to a pool of solutions that optimize the material model.

This method automatically creates a new optimization model every time it is called. Then, it solves the model via Pyomo with the CPLEX solver.

The populate method iteratively solves the model, interprets the solution as a Design object, creates a constraint to disallow that design, and resolves to find the next best design. We build a pool of Designs that are guaranteed to be the nSolns-best solutions in the material design space.

Parameters

- **func** (MaterialDescriptor/Expr) – Material functionality to optimize.
- **sense** (*int*) – flag to indicate the choice to minimize or maximize the functionality of interest. Choices: minimize/maximize (Pyomo constants 1,-1 respectively)
- **nSolns** (*int*) – Optional, number of Design objects to return. Default: 1 (See MatOptModel.populate for more information)
- **tee** (*bool*) – Optional, flag to turn on solver output. Default: True
- **disp** (*int*) – Optional, flag to control level of MatOpt output. Choices: 0: No MatOpt output (other than solver tee) 1: MatOpt output for outer level method 2: MatOpt output for solution pool & individual solns. Default: 1
- **keepfiles** (*bool*) – Optional, flag to save temporary pyomo files. Default: True
- **tilim** (*float*) – Optional, solver time limit (in seconds). Default: 3600
- **trelim** (*float*) – Optional, solver tree memory limit (in MB). Default: None (i.e., Pyomo/CPLEX default)
- **solver** (*str*) – Solver choice. Currently only cplex or neos-cplex are supported Default: cplex

Returns (list<Design>) A list of optimal Designs in order of decreasing optimality.

Raises pyutilib.ApplicationError if MatOpt can not find usable solver (CPLEX or NEOS-CPLEX)

MatOpt Output

The results of the optimization process will be loaded into Design objects automatically. Users can then save material design(s) into files for further analysis and visualization using suitable functions provided. MatOpt provides interfaces to several standard crystal structure file formats, including CFG, PDB, POSCAR, and XYZ.

MatOpt Examples

Five [case studies](#) are provided to illustrate the detailed usage of MatOpt. In each case, a Jupyter notebook with explanations as well as an equivalent Python script is provided.

References

- Hanselman, C.L. and Gounaris, C.E., 2016. [A mathematical optimization framework for the design of nanopatterned surfaces](#). *AIChE Journal*, 62(9), pp.3250-3263.
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- Hanselman, C.L., Zhong, W., Tran, K., Ulissi, Z.W. and Gounaris, C.E., 2019. [Optimization-based design of active and stable nanostructured surfaces](#). *The Journal of Physical Chemistry C*, 123(48), pp.29209-29218.
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- Yin, X., Isenberg, N.M., Hanselman, C.L., Mpourmpakis, G. and Gounaris, C.E., 2020. [A mathematical optimization-based design framework for identifying stable bimetallic nanoclusters](#). *In preparation*.
- Hanselman, C.L., Yin, X., Miller, D.C. and Gounaris, C.E., 2020. MatOpt: A Python package for nanomaterials design using discrete optimization. *In preparation*.

4.13 IDAES Versioning

The IDAES Python package is versioned according to the general guidelines of [semantic versioning](#), following the recommendations of [PEP 440](#) with respect to extended versioning descriptors (alpha, beta, release candidate, etc.).

4.13.1 Basic usage

You can see the version of the package at any time interactively by printing out the `__version__` variable in the top-level package:

```
import idaes
print(idaes.__version__)
# prints a version like "1.2.3"
```

4.13.2 Advanced usage

This section describes the module's variables and classes.

Overview

The API in this module is mostly for internal use, e.g. from 'setup.py' to get the version of the package. But `Version` has been written to be usable as a general versioning interface.

Example of using the class directly:

```
>>> from idaes.ver import Version
>>> my_version = Version(1, 2, 3)
>>> print(my_version)
1.2.3
>>> tuple(my_version)
(1, 2, 3)
>>> my_version = Version(1, 2, 3, 'alpha')
>>> print(my_version)
1.2.3.a
>>> tuple(my_version)
(1, 2, 3, 'alpha')
>>> my_version = Version(1, 2, 3, 'candidate', 1)
>>> print(my_version)
1.2.3.rc1
>>> tuple(my_version)
(1, 2, 3, 'candidate', 1)
```

If you want to add a version to a class, e.g. a model, then simply inherit from `HasVersion` and initialize it with the same arguments you would give the `Version` constructor:

```
>>> from idaes.ver import HasVersion
>>> class MyClass(HasVersion):
...     def __init__(self):
...         super(MyClass, self).__init__(1, 2, 3, 'alpha')
...
>>> obj = MyClass()
>>> print(obj.version)
1.2.3.a
```

```
idaes.ver.package_version = <idaes.ver.Version object>
Package's version as an object
```

```
idaes.ver.__version__ = '1.5.1.rc0'
Package's version as a simple string
```

Version class

The versioning semantics are encapsulated in a class called *Version*.

class `idaes.ver.Version` (*major*, *minor*, *micro*, *releaselevel*=*'final'*, *serial*=*None*, *label*=*None*)
This class attempts to be compliant with a subset of [PEP 440](#).

Note: If you actually happen to read the PEP, you will notice that pre- and post- releases, as well as “release epochs”, are not supported.

__init__ (*major*, *minor*, *micro*, *releaselevel*=*'final'*, *serial*=*None*, *label*=*None*)
Create new version object.

Provided arguments are stored in public class attributes by the same name.

Parameters

- **major** (*int*) – Major version
- **minor** (*int*) – Minor version
- **micro** (*int*) – Micro (aka patchlevel) version
- **releaselevel** (*str*) – Optional PEP 440 specifier

- **serial** (*int*) – Optional number associated with releaselevel
- **label** (*str*) – Optional local version label

__iter__()
Return version information as a sequence.

__str__()
Return version information as a string.

HasVersion class

For adding versions to other classes in a simple and standard way, you can use the *HasVersion* mixin class.

class `idaes.ver.HasVersion` (*args)
Interface for a versioned class.

__init__ (*args)
Constructor creates a *version* attribute that is an instance of *Version* initialized with the provided args.

Parameters ***args** – Arguments to be passed to Version constructor.

4.14 Developer Documentation

This section of the documentation is intended for developers, and **much of it is targeted at the IDAES internal team**. Hopefully many of the principles and ideas are also applicable to external contributors.

4.14.1 Developer Contents

Developer introductory material

This section gives a high-level introduction for collaborative software development on the IDAES project. It serves as background for understanding the collaborative development procedures.

Please refer to the [IDAES contributor guide](#) for specifics on writing, testing, and documenting code for the IDAES project.

There are many more useful things to learn about git and Github. For more information, please refer to the excellent [Atlassian Github tutorials](#) and the online [Git documentation](#) and [Github help](#).

Terminology

Git A “version control system”, for keeping track of changes in a set of files

Github A hosting service for Git repositories that adds many other features that are useful for collaborative software development.

branch A name for a series of commits. See [Branches](#).

fork Copy of a repository in Github. See [Forks](#).

pull request (PR) A request to compare and merge code in a Github repository. See [Pull Requests](#).

Git commands

The Git tool has many different commands, but there are several really important ones that tend to get used as verbs in software development conversations, and therefore are good to know:

add Put a file onto the list of “things I want to commit” (see “commit”), called “staging” the file.

commit Save the changes in “staged” files into Git (since the last time you did this), along with a user-provided description of what the changes mean (called the “commit message”).

push Move local committed changes to the Github-hosted “remote” repository by “pushing” them across the network.

pull Update your local files with changes from the Github-hosted “remote” repository by “pulling” them across the network.

Note that the *push* and *pull* commands require Github (or some other service that can host a remote copy of the repository).

Branches

There is a good description of what git branches are and [how they work here](#). Understanding this takes a little study, but this pays off by making git’s behavior much less mysterious. The short, practical version is that a branch is a name for a series of commits that you want to group together, and keep separable from other series of commits. From git’s perspective, the branch is just a name for the first commit in that series.

It is recommended that you create new branches on which to develop your work, and reserve the “master” branch for merging in work that has been completed and approved on Github. One way to do this is to create branches that correspond directly to issues on Github, and include the issue number in the branch name.

Forks

A *fork* is a copy of a repository, in the Github shared space (a copy of a repository from Github down to your local disk is called a “clone”). In this context, that means a copy of the “idaes-dev” repository from the IDAES organization (<https://github.com/IDAES/idaes-dev>) to your own user space, e.g., <https://github.com/myname/idaes-dev>). The mechanics of creating and using forks on Github [are given here](#).

Pull Requests

A fundamental procedure in the development lifecycle is what is called a “pull request”. Understanding what these are, and do, is important for participating fully in the software development process. First, understand that pull requests are for collaborative development (Github) and not part of the core revision control functionality that is offered by Git. The official Github description of pull requests is [here](#). However, it gets technical rather quickly, so a higher-level explanation may be helpful:

Pull requests are a mechanism that Github provides to look at what the code on some branch from your fork of the repository would be like if it were merged with the master branch in the main (e.g., `idaes/idaes-dev`) repository. You can think of it as a staging area where the code is merged and all the tests are run, without changing the target repository. Everyone on the team can see a pull request, comment on it, and review it.

Github repository overview

This section describes the layout of the [Github repositories](#). Later sections will give guidelines for contributing code to these repositories.

Repositories

Repository name	Public?	Description
idaes-pse	Yes	Main public repository, including core framework and integrated tools
idaes-dev	No	Main private repository, where code is contributed before being “mirrored” to the public <i>ideas-pse</i> repository
workspace	No	Repository for code that does not belong to any particular CRADA or NDA, but also is never intended to be released open-source

The URL for an IDAES repository, e.g. “some-repo”, will be `https://github.com/IDAES/some-repo`.

Public vs. Private

All these repositories except for “idaes-pse” will only be visible on Github, on the web, for people who have been added to the IDAES developer team in the IDAES “organization” (See [About Github organizations](#)). If you are a member of the IDAES team and not in the IDAES Github organization, please contact one of the core developers. The *ideas-pse* repository will be visible to anyone, even people without a Github account.

Collaborative software development

This page gives guidance for all developers on the project.

Note: Many details here are targeted at members of the IDAES project team. However, we strongly believe in the importance of transparency in the project’s software practices and approaches. Also, understanding how we develop the software internally should be generally useful to understand the review process to expect for external contributors.

Although the main focus of this project is developing open source software (OSS), it is also true that some of the software may be developed internally or in coordination with industry under a [CRADA](#) or [NDA](#).

It is the developer’s responsibility, for a given development effort, to keep in mind what role you must assume and thus which set of procedures must be followed.

CRADA/NDA If you are developing software covered by a CRADA, NDA, or other legal agreement that does not explicitly allow the data and/or code to be released as open-source under the IDAES license, then you must follow procedures under [Developing Software with Proprietary Content](#).

Internal If you are developing non-CRADA/NDA software, which is not intended to be part of the core framework or (ever) released as open-source then follow procedures under [Developing Software for Internal Use](#).

Core/open-source If you are developing software with no proprietary data or code, which is intended to be released as open-source with the core framework, then follow procedures under [Developing software for Open-source Release](#).

Developing Software with Proprietary Content

Proprietary content is not currently being kept on Github, or any other collaborative version control platform. When this changes, this section will be updated.

Developing Software for Internal Use

Software for internal use should be developed in the `workspace` repository of the IDAES github organization. The requirements for reviews and testing of this code are not as strict as for the `idaes-dev` repository, but otherwise the procedures are the same as outlined for *open-source development*.

Developing software for Open-source Release

We can break the software development process into five distinct phases, illustrated in Figure 1 and summarized below:

1. <i>Setup</i> : Prepare your local system for collaborative development
2. <i>Initiate</i> : Notify collaborators of intent to make some changes
3. <i>Develop</i> : Make local changes
4. <i>Collaborate</i> : Push the changes to Github, get feedback and merge

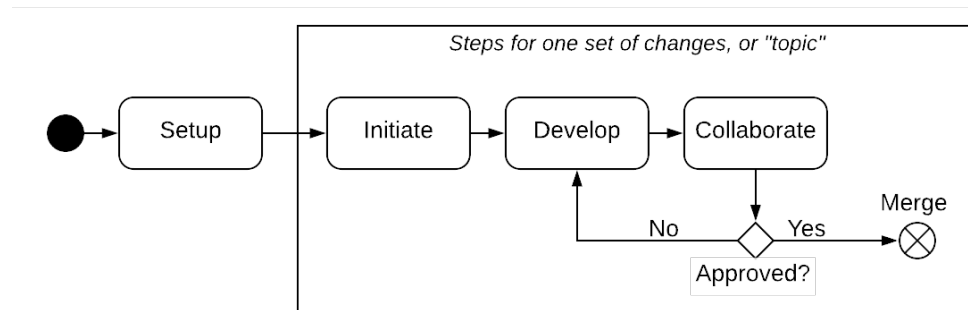


Fig. 4: Figure 1. Overview of software development workflow

The rest of this page describes the what and how of each of these phases.

1. Setup

Before you can start developing software collaboratively, you need to make sure you are set up in Github and set up your local development environment.

Github setup

To work within the project, you need to create a login on [Github](#). You also need to make sure that this login has been added to the IDAES organization by contacting one of the core developers.

If these steps are successful, you should be able to login to Github, visit the [IDAES Github organization](#), and see “Private” repositories such as `idaes-dev` and `workspace`.

Fork the repo

You use a “fork” of a repository (or “repo” for short) to create a space where you can save changes without directly affecting the main repository. Then, as we will see, you *request* that these changes be incorporated (after review).

This section assumes that the repository in question is `idaes-dev`, but the idea is the same for any other repo.

You should first visit the repo on Github by pointing your browser to <https://github.com/IDAES/idaes-dev/>. Then you should fork the repo into a repo of the same name under your name.

Clone your fork

A “clone” is a copy of a Github repository on your local machine. This is what you need to do in order to actually edit and change the files. To make a clone of the fork you created in the previous step, change to a directory where you want to put the source code and run the command:

```
git clone git@github.com:MYNAME/idaes-dev.git
cd idaes-dev
```

Of course, replace MYNAME with your login name. This will download all the files in the latest version of the repository onto your local disk.

Note: After the `git clone`, subsequent `git` commands should be performed from the “idaes-dev” directory.

Add upstream remote

In order to guarantee that your fork can be synchronized with the “main” `idaes-dev` repo in the Github IDAES organization, you need to add a pointer to that repository as a *remote*. This repository is called *upstream* (changes made there by the whole team flow down to your fork), so we will use that name for it in our command:

```
git remote add upstream git@github.com:IDAES/idaes-dev.git
```

Create the Python environment

Once you have the repo cloned, you can change into that directory (by default, it will be called “idaes-dev” like the repo) and install the Python packages.

But before you do that, you need to get the Python package manager fully up and running. We use a Python packaging system called [Conda](#). Below are instructions for installing a minimal version of Conda, called [Miniconda](#). The full version installs a large number of scientific analysis and visualization libraries that are not required by the IDAES framework.

```
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
bash Miniconda3-latest-Linux-x86_64.sh
```

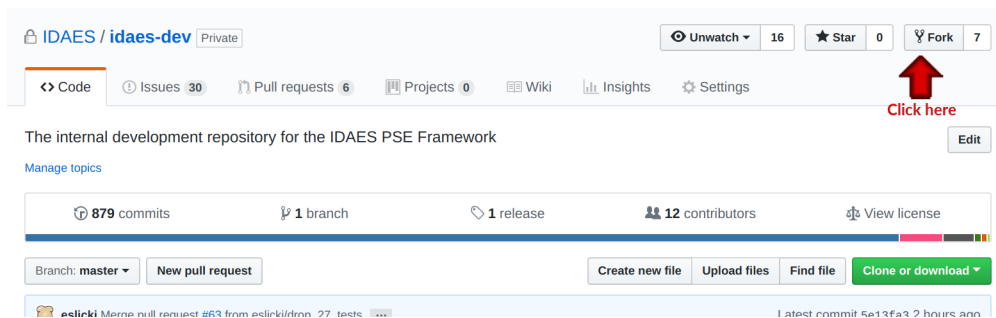


Fig. 5: Figure 2. Screenshot showing where to click to fork the Github repo

Create and activate a conda environment (along with its own copy of `pip`) for the new IDAES installation (**you will need to** `conda activate idaes` **when you open a fresh terminal window and wish to use IDAES**):

```
conda create -n idaes pip
conda activate idaes
```

Now that conda and pip are installed, and you are in the “idaes” conda environment, you can run the standard steps for installing a Python package in development mode:

```
pip install -r requirements.txt
python setup.py develop
```

You can test that everything is installed properly by running the tests with `Pytest`:

```
pytest
```

2. Initiate

We will call a set of changes that belong together, e.g. because they depend on each other to work, a “topic”. This section describes how to start work on a new topic. The workflow for initiating a topic is shown in Figure 3 below.

Create an issue on Github

To create an issue on Github, simply navigate to the repository page and click on the “Issues” tab. Then click on the “Issues” button and fill in a title and brief description of the issue. You do not need to list details about sub-steps required for the issue, as this sort of information is better put in the (related) pull request that you will create later. Assign the issue to the appropriate people, which is often yourself.

There is one more important step to take, that will allow the rest of the project to easily notice your issue: add the issue to the “Priorities” project. The screenshot below shows where you need to click to do this.

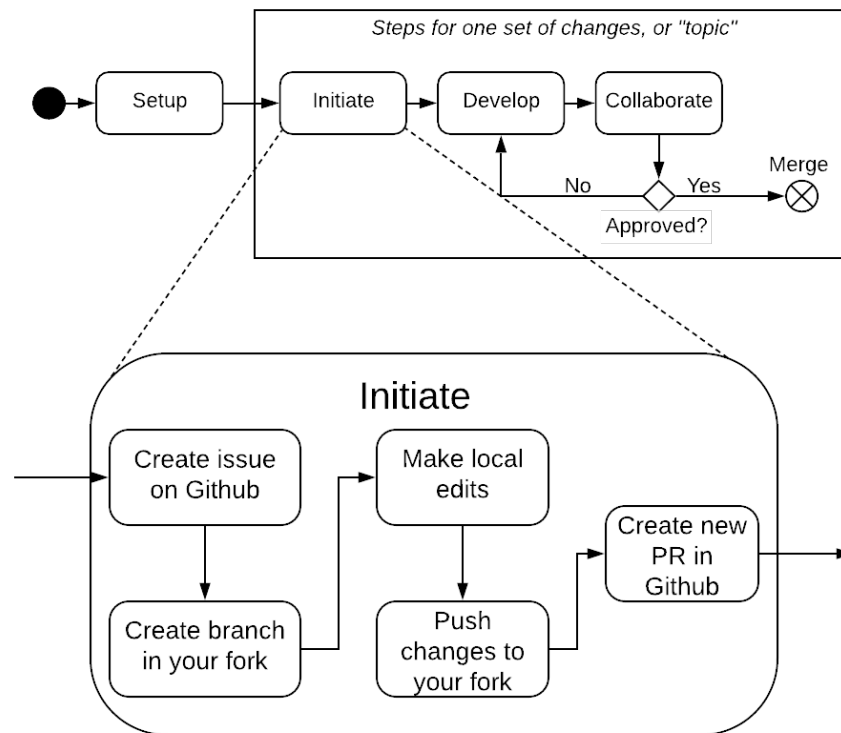


Fig. 6: Figure 3. Initiate topic workflow

Create a branch on your fork

It is certainly possible to do your work on your fork in the

“master” branch. The problem that can arise here is if

you need to do two unrelated things at the same time, for example working on a new feature and fixing a bug in the current code. This can be quite tricky to manage as a single set of changes, but very easy to handle by putting each new set of changes in its own branch, which we call a *topic* branch. When all the changes in the branch are done and merged, you can delete it both locally and in your fork so you don’t end up with a bunch of old branches cluttering up your git history.

The command for doing this is simple:

```
git_
  ↳ checkout -b_
  ↳ <BRANCH-NAME>
```

The branch name should be one word, with dashes or under-scores as needed. One convention for the name that can be helpful is to include the issue number at the end, e.g. git co -b

mytopic-issue42. This is especially useful later when you are cleaning up old branches, and you can quickly see which branches are related to issues that are completed.

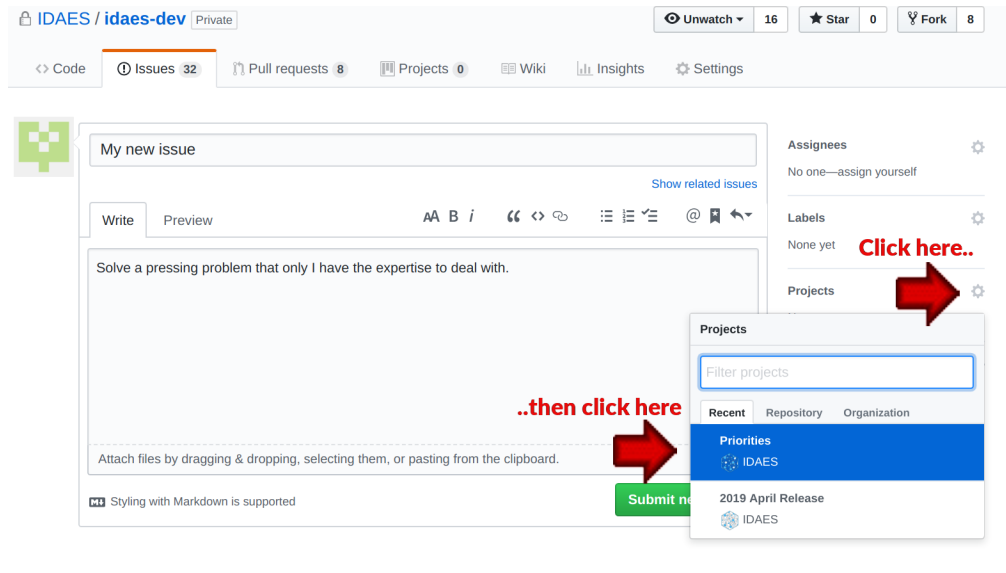


Fig. 7: Figure 4. Screenshot for creating an issue on Github

Make local edits and push changes

A new branch, while it feels like a change, is not really a change in the eyes of Git or Github, and by itself will not allow you to start a new pull request (which is the goal of this whole phase). The easiest thing to do is a special “empty” commit:

```
git commit --allow-empty -m 'Empty commit so I can open a PR'
```

Since this is your first “push” to this branch, you are going to need to set an upstream branch on the remote that should receive the changes. If this sounds complicated, it’s OK because git actually gives you cut-and-paste instructions. Just run the `git push` command with no other arguments:

```
$ git push
fatal: The current branch mybranch-issue3000 has no upstream branch.
To push the current branch and set the remote as upstream, use
```

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```
git push --set-upstream origin mybranch-issue3000
```

Cut and paste the suggested command, and you're ready to go. Subsequent calls to "push" will not require any additional arguments to work.

Start a new Pull Request on Github

Finally, you are ready to initiate the pull request. Right after you perform the push command above, head to the repository URL in Github (<https://github.com/IDAES/idaes-dev>) and you should see a highlighted bar below the tabs, as in Figure 5 below, asking if you want to start a pull-request.

Click on this and fill in the requested information. Remember to link to the issue you created earlier.

Depending on the Github plan, there may be a pull-down menu for creating the pull request that lets you create a "draft" pull request. If that is not present, you can signal this the old-fashioned way by adding "[WIP]" (for Work-in-Progress) at the beginning of the pull request title.

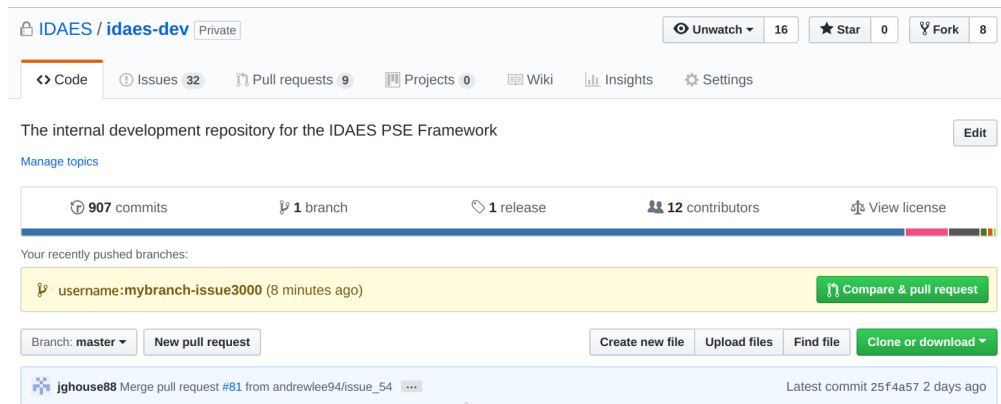


Fig. 8: Figure 5. Screenshot for starting a Pull Request on Github

Either way, create the pull request. Do *not* assign reviewers until you are done making your changes (which is probably not now). This way the assigning of reviewers becomes an unambiguous signal that the PR is actually ready for review.

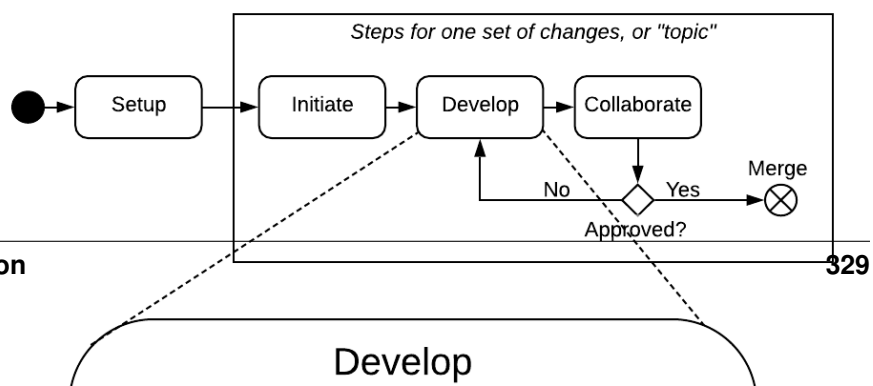
Note: Avoid having pull requests that take months to complete. It is better to divide up the work, even artificially, into a piece that can be reviewed and merged into the main repository within a week or two.

3. Develop

The development process is a loop of adding code, testing and debugging, and committing and pushing to Github. You may go through many (many!) iterations of this loop before the code is ready for review. This workflow is illustrated in Figure 6.

Running tests

After significant edits, you should make sure you have tests for the new/changed



functionality. This involves writing *Unit tests* as well as running the test suite and examining the results of the *Code coverage*.

This project uses *Pytest* to help with running the unit tests. From the top-level directory of the working tree, type:

```
pytest
```

Alternatively users of an IDE like PyCharm can run the tests from within the IDE.

Commit changes

The commands: `git add`, `git status`, and `git commit` are all used in combination to save a snapshot of a Git project's current state.¹.

The *commit* command is the equivalent of “saving” your changes. But unlike editing a document, the set of changes may cover multiple files, including newly created files.

To allow the user flexibility in specifying exactly which changes to save with each commit, the *add* command is used first to indicate files to “stage” for the next commit command. The *status* command is used to show the current status of the working tree.

A typical workflow goes like this:

```
$ ls
file1 file2
$ echo 'a' > file1 # edit existing file
$ echo '1' > file3 # create new file
$ git status --short # shows changed/unstaged and unknown file
M file1
?? file3
$ git add file1 file3 # stage file1, file3 for commit
$ git status --short # M=modified, A=added
M file1
A file3
$ git commit -m "made some changes"
[master 067c16e] made some changes
2 files changed, 2 insertions(+)
create mode 100644 file3
```

¹ Git has an additional saving mechanism called ‘the stash’. The stash is an ephemeral storage area for changes that are not ready to be committed. The stash operates on the working directory and has extensive usage options.* See the documentation for [git stash](#) for more information.

Of course, in most IDEs you could use built-in commands for committing and adding files. The basic flow would be the same.

Synchronize with upstream changes

Hopefully you are not the only one on the team doing work, and therefore you should expect that the main repository may have new and changed content while you are in the process of working. To synchronize with the latest content from the “upstream” (IDAES organization) repository, you should periodically run one of the two following commands:

```
git pull
# OR -- explicit
git fetch --all
git merge upstream/master
```

You’ll notice that this merge command is using the name of the “upstream” remote that you *created earlier*.

Push changes to Github

Once changes are *tested* and committed, they need to be synchronized up to Github. This is done with the git push command, which typically takes no options (assuming you have set up your fork, etc., as described so far):

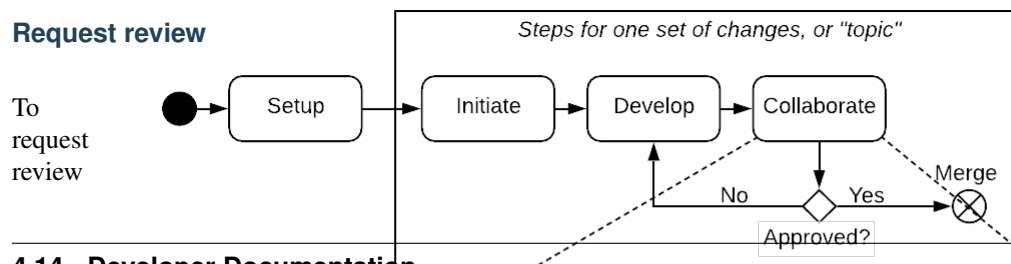
```
git push
```

The output of this command on the console should be an informative, if slightly cryptic, statement of how many changes were pushed and, at the bottom, the name of your remote fork and the local/remote branches (which should be the same). For example:

```
Counting objects: 5, done.
Delta compression using up to 8 threads.
Compressing objects: 100% (5/5), done.
Writing objects: 100% (5/5), 528 bytes | 528.00 KiB/s, done.
Total 5 (delta 4), reused 0 (delta 0)
remote: Resolving deltas: 100% (4/4), completed with 4 local objects.
To github.com:dangunter/idaes-dev.git
    d535552..fe61fcc  devdocs-issue65 -> devdocs-issue65
```

4. Collaborate

The collaboration phase of our journey, shown in Figure 7, is mostly about communicating what you did to the other developers. Through the Github “review” mechanism, people will be able to suggest changes and improvements. You can make changes to the code (other people can also make changes, see *Shared forks*), and then push those changes up into the same Pull Request. When you get enough approving reviews, the code is merged into the master repository. At this point, you can delete the “topic branch” used for the pull request, and go back to *initiate* your next set of changes.



of a
pull
request,
navigate to
the pull
request
in the
main
(e.g.,
“idaes-
dev”)
repository
and
select
some
names
in the
“Review-
ers”
pull-
down
on the

right-hand side. You need to have two approving reviews. The reviewers should get an email, but you can also “@” people in a comment in the pull request to give them a little extra nudge.

See the full [code review](#) procedure for more details.

Make changes

You need to keep track of the comments and reviews, and make changes accordingly. Think of a pull request as a discussion. Normally, the person who made the pull request will make any requested edits. Occasionally, it may make sense for one or more other developers to jump in and make edits too, so how to do this is covered in the sub-section below.

Changes made while the code is being reviewed use the normal [Develop](#) workflow.

Shared forks

Other developers can also make changes in your fork. All they need to do is `git clone` your fork (not the main repository), switch to the correct topic branch, and then `git push` work directly to that branch. Note since this does not use the whole pull-request mechanism, all developers working on the same branch this way need to make sure the `git pull` to synchronize with updates from the other developers.

For example, if Jack wants to make some edits on Rose’s fork, on a topic branch called “changes-issue51” he could do the following:

```
$ git clone https://github.com/rose/idaes-dev # clone Rose's fork
$ git checkout changes-issue51 # checkout the topic branch
$ echo "Hello" >> README.txt # make some important changes
$ pytest # always run tests!!
```

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```
$ git add README.txt ; git commit -m "important changes"
$ git push # push changes to the fork
```

Hopefully it also is obvious that developers working this way have less safeguards for overwriting each other's work, and thus should make an effort to communicate clearly and in a timely manner.

Merge

Once all the tests pass and you have enough approving reviews, it's time to merge the code! This is the easy part: go to the bottom of the Pull Request and hit the big green "merge" button.

Before you close the laptop and go down to the pub, you should tidy up. First, delete your local branch (you can also delete that branch on Github):

```
git checkout master # switch back to master branch
git branch -d mychanges-issue3000
```

Next, you should make sure your master reflects the current state of the main master branch, i.e. go back and *synchronize with the upstream remote*, i.e. run `git pull`.

Now you can go and enjoy a tasty beverage. Cheers!



Testing

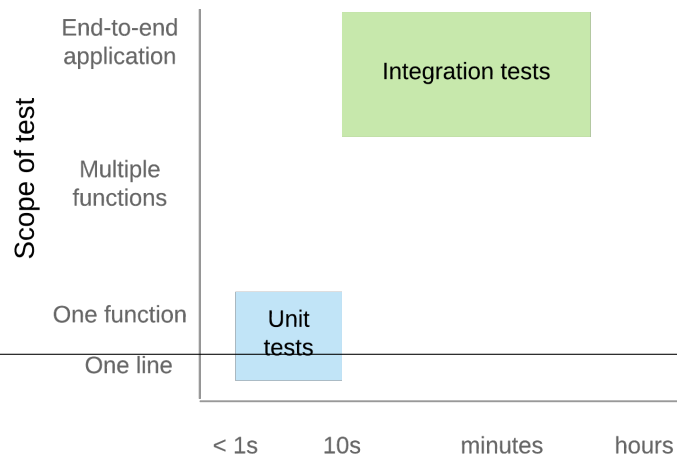
Testing is essential to the process of creating software. "If it isn't tested, it doesn't work" is a good rule of thumb.

For some specific advice for adding new tests in the IDAES code, see *IDAES contributor guide*.

There are different kinds of tests: functional, acceptance, performance, usability. We will primarily concern ourselves with *functional* testing here, i.e. whether the thing being tested produces correct outputs for expected inputs, and gracefully handles everything else. Within functional testing, we can classify the testing according to the axes of *time*, i.e. how long the test takes to run, and *scope*, i.e. the amount of the total functionality being tested. Along these two axes we will pick out just two points, as depicted in Figure 1. The main tests you will write are "unit tests", which run very quickly and test a focused amount of functionality. But sometimes you need something more involved (e.g. running solvers, using data on disk), and here we will label that kind of test "integration tests".

Unit tests

Testing individual pieces of functionality, including the ability to report the correct kind of errors from bad inputs. Unit tests must always run quickly. If it takes more than 10 seconds, it is not a unit test, and it is expected that most



unit tests take well under 1 second. The reason for this is that the entire unit test suite is run on every change in a Pull Request, and should also be run relatively frequently on local developer machines. If this suite of hundreds of tests takes more than a couple of minutes to run, it will introduce a significant bottleneck in the development workflow.

For Python code, we use the `pytest` testing framework. This is compatible with the built-in Python `unittest` framework, but has many nice features that make it easier and more powerful.

The best way to learn how to use `pytest` is to look at existing unit tests, e.g. the file `idaes/core/tests/test_process_block.py`. Test files are found in a directory named `“test/”` in every Python package (directory with an `“__init__.py”`). The tests are named `“test_{something}.py”`; this naming convention is important so `pytest` can automatically find all the tests.

When writing your own tests, make sure to remember to keep each test focused on a single piece of functionality. If a unit test fails, it should be obvious which code is causing the problem.

Mocking

Mocking is a common, but important, technique for avoiding dependencies that make your tests slow, fragile, and harder to understand. The basic idea is to replace dependencies with fake, or “mock”, versions of them that will provide just enough realism for the test. Python provides a library, `unittest.mock`, to help with this process by providing objects that can report how they were used, and easily pretend to have certain functionality (returning, for example, fixed values). To make this all more concrete, consider a simple problem where you want to test a function that makes a system call (in this case, `os.remove`):

```
# file: mymodule.py
import os
def rm(filename):
    os.remove(filename)
```

Normally, to test this you would create a temporary file, and then see if it got removed. However, with mocking you can take a different approach entirely:

```
# file: test_mymodule.py
from mymodule import rm
from unittest import mock

@mock.patch('mymodule.os')
def test_rm(mock_os):
    rm("any path")
    # test that rm called os.remove with the right parameters
    mock_os.remove.assert_called_with("any path")
```

Here, we have “patched” the `os` module that got imported into `“mymodule”` (note: had to do `mymodule.os` instead of simply `os`, or the one `mymodule` uses would not get patched) so that when `rm` calls `os.remove`, it is really calling a fake method in `mock_os` that does nothing but record how it was called. The patched module is passed in to the

test as an argument so you can examine it. So, now, you are not doing any OS operations at all! You can imagine how this is very useful with large files or external services.

Integration tests

Integration tests exercise an end-to-end slice of the overall functionality. At this time, the integration tests are all housed in Jupyter Notebooks, which serve double-duty as examples and tutorials for end users. We execute these notebooks and verify that they run correctly to completion at least once before each new release of the software.

Code coverage

The “coverage” of the code refers to what percentage of the code (“lines covered” divided by total lines) is executed by the automated tests. This is important because passing automated tests is only meaningful if the automated tests cover the majority of the code’s behavior. This is not a perfect measure, of course, since simply executing a line of code under one condition does not mean it would execute correctly under all conditions. The code coverage is evaluated locally and then integrated with Github through a tool called [Coveralls](#).

Code Review

“It’s a simple 3-step process. Step one: Fix! Step two: It! Step three: Fix it!” – Oscar Rogers (Kenan Thompson), Saturday Night Live, 2/2009

Code review is the last line of defense between a mistake that the IDAES team will see and a mistake the whole world will see. In the case of that mistake being a leak of proprietary information, the entire project is jeopardized, so we need to take this process seriously.

Summary

Warning: This section is an incomplete set of notes

Every piece of code must be reviewed by at least two people.

In every case, one of those people will be a designated “gatekeeper” and the one or more others will be “technical reviewers”.

The technical reviewers are expected to consider various aspects of the proposed changes (details below), and engage the author in a discussion on any aspects that are deemed lacking or missing.

The gatekeeper is expected to make sure all criteria have been met, and actually merge the PR.

Assigning Roles

The gatekeeper is a designated person, who will always be added to review a Pull Request (PR)

Gatekeeper is a role that will be one (?) person for some period like a week or two weeks

The role should rotate around the team, it’s expected to be a fair amount of work and should be aligned with availability and paper deadlines, etc.

The originator of the PR will add as reviewers the gatekeeper and 1+ technical reviewers.

Originator responsibilities

The originator of the PR should include in the PR itself information about where to find:

Changes to code/data

Tests of the changes

Documentation of the changes

The originator should be responsive to the reviewers

Technical reviewer responsibilities

The technical reviewer(s) should look at the proposed changes for

Technical correctness (runs properly, good style, internal code documentation, etc.)

Tests

Documentation

No proprietary / sensitive information

Until they approve, the conversation in the PR is between the technical reviewers and the originator (the gatekeeper is not required to participate, assuming they have many PRs to worry about)

Gatekeeper responsibilities

The gatekeeper does not need to engage until there is at least one approving technical review.

Once there is, they should verify that:

Changes do not contain proprietary data

Tests are adequate and do not fail

Documentation is adequate

Once everything is verified, the gatekeeper merges the PR

Automated Checks

The first level of code review is a set of automated checks that *must* pass before the code is ready for people to review it. These checks will run on the initiation of a [pull request](#) and on every new commit to that pull request that is pushed to Github (thus the name “continuous integration”).

The “continuous integration” of the code is hosted by an online service – we use [CircleCI](#) – that can automatically rerun the tests after every change (in this case, every new Pull Request or update to the code in an existing Pull Request) and report the results back to Github for display in the web pages. This status information can then be used as an automatic gatekeeper on whether the code can be merged into the master branch – if tests fail, then no merge is allowed. Following this procedure, it is not possible for the master branch to ever be failing its own tests.

Docker container

This page documents information needed by developers for working with the IDAES docker container.

As is expected by Docker, the main file for creating the Docker image is the “Dockerfile” in the top-level directory.

docker-idaes script

You can build new Docker images using the `create` option to the `docker-idaes` script. For example:

```
./docker-idaes create
```

You need to have the IDAES installation activated. The script will automatically find the current version and attempt to build a Docker image with the same version. If it detects an existing image, it will skip the image build. Next, the script will try to use `docker save` to save the image as a compressed archive. This will also be skipped if an existing image file, with the same version as the “idaes” Python package, is detected.

Pushing an image to S3

The Docker images are stored on Amazon S3. Before you can upload a new image, you need to be part of the “IDAES-admin” group that is part of Amazon’s IAM (Identity Access Management) system. Please contact one of the core developers to learn how to join this IAM group.

Once you have the IAM keys, you need to create a file `~/.aws/credentials` that has the access key id and key from the IAM account. It will look like this:

```
[default]
aws_access_key_id = IDGOESHERE
aws_secret_access_key = accesskeygoeshere
```

The values for the ID and Access key are available from the AWS “IAM” service console.

Next you need to use the AWS command-line tools to copy the local image up to Amazon S3. For example, if the image was version “1.0.1”, you would use the following command:

```
aws s3 cp idaes-pse-docker-1.0.1.tgz \
s3://idaes/idaes-pse/idaes-pse-docker-1.0.1.tgz
```

If the new image should be the latest, you also need to do an S3 -> S3 copy to create a new latest image:

```
aws s3 cp s3://idaes/idaes-pse/idaes-pse-docker-1.0.1.tgz \
s3://idaes/idaes-pse/idaes-pse-docker-latest.tgz
```

IDAES contributor guide

About

This page tries to give all the essential information needed to contribute software to the IDAES project. It is designed to be useful to both internal and external collaborators.

Code and other file locations

Source code The main Python package is under the *idaes/* directory. Sub-directories, aka subpackages, should be documented elsewhere. If you add a new directory in this tree, be sure to add a `__init__.py` in that directory so Python knows it is a subpackage with Python modules. Code that is not part of the core package is under *apps/*. This code can have any layout that the creator wants.

Documentation The documentation for the core package is under *docs*.

Examples Examples are under the *examples/* directory. Tutorials from workshops are under the *examples/workshops/* subdirectory.

Developer environment

Development of IDAES will require an extra set of required package not needed by regular users. To install those extra developer tools use the command `pip install -r requirements-dev.txt` rather than `pip install -r requirements.txt`

Code style

The code style is not entirely consistent. But some general guidelines are:

- follow the [PEP8](#) style (or variants such as [Black](#))
- use [Google-style](#) docstrings on classes, methods, and functions
- format your docstrings as [reStructuredText](#) so they can be nicely rendered as HTML by Sphinx
- add logging to your code by creating and using a global log object named for the module, which can be created like: `_log = logging.getLogger(__name__)`
- take credit by adding a global author variable: `__author__ = 'yourname'`

Tests

For general information about writing tests in Python, see [Testing](#).

There are three types of tests:

Python source code The Python tests are integrated into the Python source code directories. Every package (directory with `.py` modules and an `__init__.py` file) should also have a `tests/` sub-package, in which are test files. These, by convention are named `test_<something>.py`.

Doctests With some special [reStructuredText](#) “directives” (see “Writing tests”), the documentation can contain tests. This is particularly useful for making sure examples in the documentation still run without errors.

Jupyter notebook tests (coming soon)

Writing tests

We use [pytest](#) to run our tests. The main advantage of this framework over the built-in `unittest` that comes with Python is that almost no boilerplate code is required. You write a function named `test_<something>()` and, inside it, use the (pytest-modified) `assert` keyword to check that things are correct.

Writing the Python unit tests in the `tests/` directory is, hopefully, quite straightforward. Here is an example (out of context) that tests a couple of things related to configuration in the core unit model library:

```
def test_config_block():
    m = ConcreteModel()

    m.u = Unit()

    assert len(m.u.config) == 2
    assert m.u.config.dynamic == useDefault
```

See the existing tests for many more examples.

For tests in the documentation, you need to wrap the test itself in a directive called `testcode`. Here is an example:

```

.. testcode::

    from pyomo.environ import *
    from pyomo.common.config import ConfigValue
    from idaes.core import ProcessBlockData, declare_process_block_class

    @declare_process_block_class("MyBlock")
    class MyBlockData(ProcessBlockData):
        CONFIG = ProcessBlockData.CONFIG()
        CONFIG.declare("xinit", ConfigValue(default=1001, domain=float))
        CONFIG.declare("yinit", ConfigValue(default=1002, domain=float))
        def build(self):
            super(MyBlockData, self).build()
            self.x = Var(initialize=self.config.xinit)
            self.y = Var(initialize=self.config.yinit)

```

First, note that `reStructuredText` directive and indented Python code. The indentation of the Python code is important. You have to write an entire program here, so all the imports are necessary (unless you use the `testsetup` and `testcleanup` directives, but honestly this isn't worth it unless you are doing a lot of tests in one file). Then you write your Python code as usual.

Running tests

Running all tests is done by, at the top directory, running the command: `pytest`.

The documentation test code will actually be run by a special hook in the `pytest` configuration that treats the `Makefile` like a special kind of test. As a result, *when you run `pytest` in any way that includes the “docs/” directory (including the all tests mode), then all the documentation tests will run, and errors/etc. will be reported through `pytest`*. A useful corollary is that, to run documentation tests, do: `pytest docs/Makefile`

You can run specific tests using the `pytest` syntax, see its documentation or `pytest -h` for details.

Documentation

The documentation is built from its sources with a tool called Sphinx. The sources for the documentation are:

- hand-written text files, under `docs/`, with the extension “`.rst`” for `reStructuredText`.
- the Python source code
- selected Jupyter Notebooks

Building documentation

Note: To build the documentation locally, you will need to have the Sphinx tools installed. This will be done for you by running `pip install requirements-dev.txt` (“developer” setup) as opposed to the regular `pip install requirements.txt` (“user” setup).

To build the documentation locally, use our custom `build.py` script.

```
cd docs python build.py
```

The above commands will do a completely clean build to create HTML output.

If the command succeeds, the final line will look like:

```
=== SUCCESS
```

If it fails, it will instead print something like:

```
*** ERROR in 'html'
***
*** message about the command that failed
*** and any additional info
***
```

If you want to see the commands actually being run, add `-v` to the command line.

By default the build command removes all existing built files before running the Sphinx commands. To turn this off, and rebuild only “new” things, add `-dirty` to the command line.

Previewing documentation

The generated documentation can be previewed locally by opening the generated HTML files in a web browser. The files are under the `docs/build/` directory, so you can open the file `docs/build/index.html` to get started.

4.15 Glossary

API Acronym for “Application Programming Interface”, this is the set of functions used by an external program to invoke the functionality of a library or application. For IDAES, it usually refers to Python functions and classes/methods in a Python module. By analogy, the APIs are to the IDAES library what a steering wheel, gearshift and pedals are to a car.

CRADA Cooperative Research and Development Agreement. A legal agreement between two or more parties that involves a statement of work and terms for sharing non-public data.

NDA Non-Disclosure Agreement. A legal agreement between two or more parties that involves terms for sharing non-public data.

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