Tools for Advanced Model Development

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Unit Models

- Commercial process simulation tools have libraries of models for common unit operations. However, libraries offer limited flexibility and lack models for novel processes.
- AMLs offer the ability for users to develop custom models for process systems, but require significant effort to develop , debug and solve.
- IDAES aims to bridge the gap between process simulators and AMLs by offering a flexible, modular framework for constructing models of unit operations.

Property Blocks

- Properties implemented as modular blocks
- Interactions defined at a high level to allow flexible formulation of equations
- Easily switched in and out to allow unit models to be applied to different processes
- Framework automates many interactions

Ports

- Describe points where models can be connected
- Port members are defined by the user via the property package.
- User can pass any state information required
- Can connect to any other Port with the same members

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Example

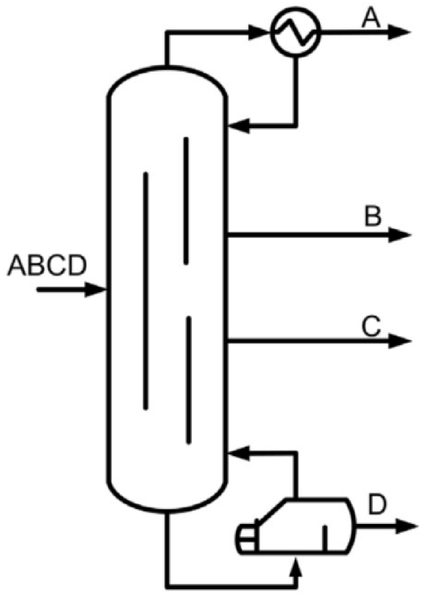
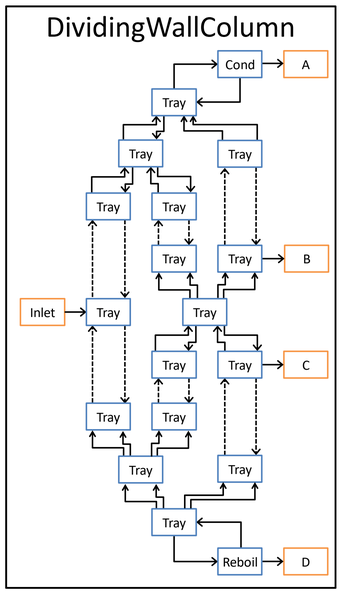
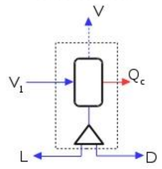


Image from Okoli and Adams, Chem. Eng. and Proc., 2015



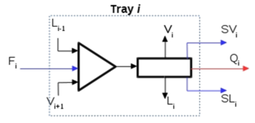
Source: NETL

Condenser Block

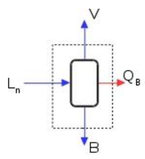


Tray Block

Tray *i*



Reboiler Block



Control Volumes

- Three types of Control Volumes available for different applications
  - 0-D (Inlet-Outlet type)
  - 1-D (Pipes, PFRs)
  - Static (Dead zones)
- Control Volumes can be connected together to form complex units with different levels of detail
- Represent defined volume over which material, energy and momentum balances will be written
- Prebuilt methods for common forms of balance equations, e.g.

$$Acc = In - Out + Gen + Trans$$

IDAES Framework

- Library of models for common unit operations
- All models are fully open and modifiable
- Models are constructed from modular elements for common model features
- Elements provide block-modular structure of process simulators, with the flexibility of AMLs
- Framework provides tools to automate common task, such as writing material, energy and momentum balances to reduce effort required to develop models and reduce errors
- Open source allows for community to contribute new features
- Implementation in Python gives access to wide range of external libraries (e.g. NumPy, SciPy)
- Users are free to use as many or as few of the framework tools as they desire

Initialization

- Each unit model can define a custom initialization routine
- Users can develop custom initialization routines making use of a wide range of tools and solvers
- Routines consider entire unit operation, not just sub-components
- IDAES is developing for solving complex models
  - Decomposition solvers
  - Reliability and convergence tools

Sample output from model reliability and convergence tester

```
  0.0% [----------------] Root Process: Sample-1
 …
 96.0% [***************-] Root Process: Sample-25

==== Scenario Statistics ====
          Parameter        Min        Mean      StdDev        Max
-------------------------------------------------------------------
     Inlet_Flowrate          1      477127      169716      877237
  Inlet_Temperature    202.486     604.057     192.441        1000
-------------------------------------------------------------------

==== Summary ====
Number of Successful Cases (solved=True): 97/100
... Iterations      (min, -1std, mean, +1std, max):     4, 6.136298, 6.835052, 7.533805,     9
... Solver Time (s) (min, -1std, mean, +1std, max): 0.002000, 0.003171, 0.003990, 0.004808, 0.008000

==== Notable Cases ====
Sample-57 : failed solve
            Inlet_Flowrate:     512046 ( 0.06 standard deviations above/below the mean)
         Inlet_Temperature:       1000 ( 2.00 standard deviations above/below the mean)
```