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Progress on IDAES Model Libraries

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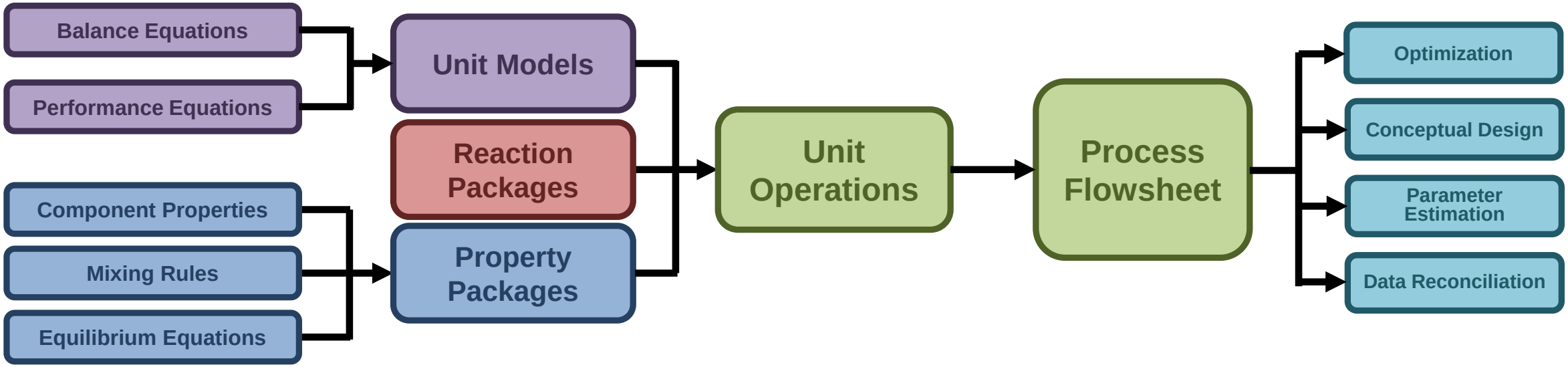
IDAES Model Libraries

Model libraries are a core component of IDAES

- Libraries of models for unit operations and thermophysical properties
- Open, modular structure
- Models are all optimization-ready and extensible
- Models can easily be used directly from libraries

IDAES Modeling Framework

- Combines features of process simulators and equation-oriented packages



- Flexible, modular framework allows for models with different levels of rigor and complexity

- Can mix models of different rigor for individual units and physical properties

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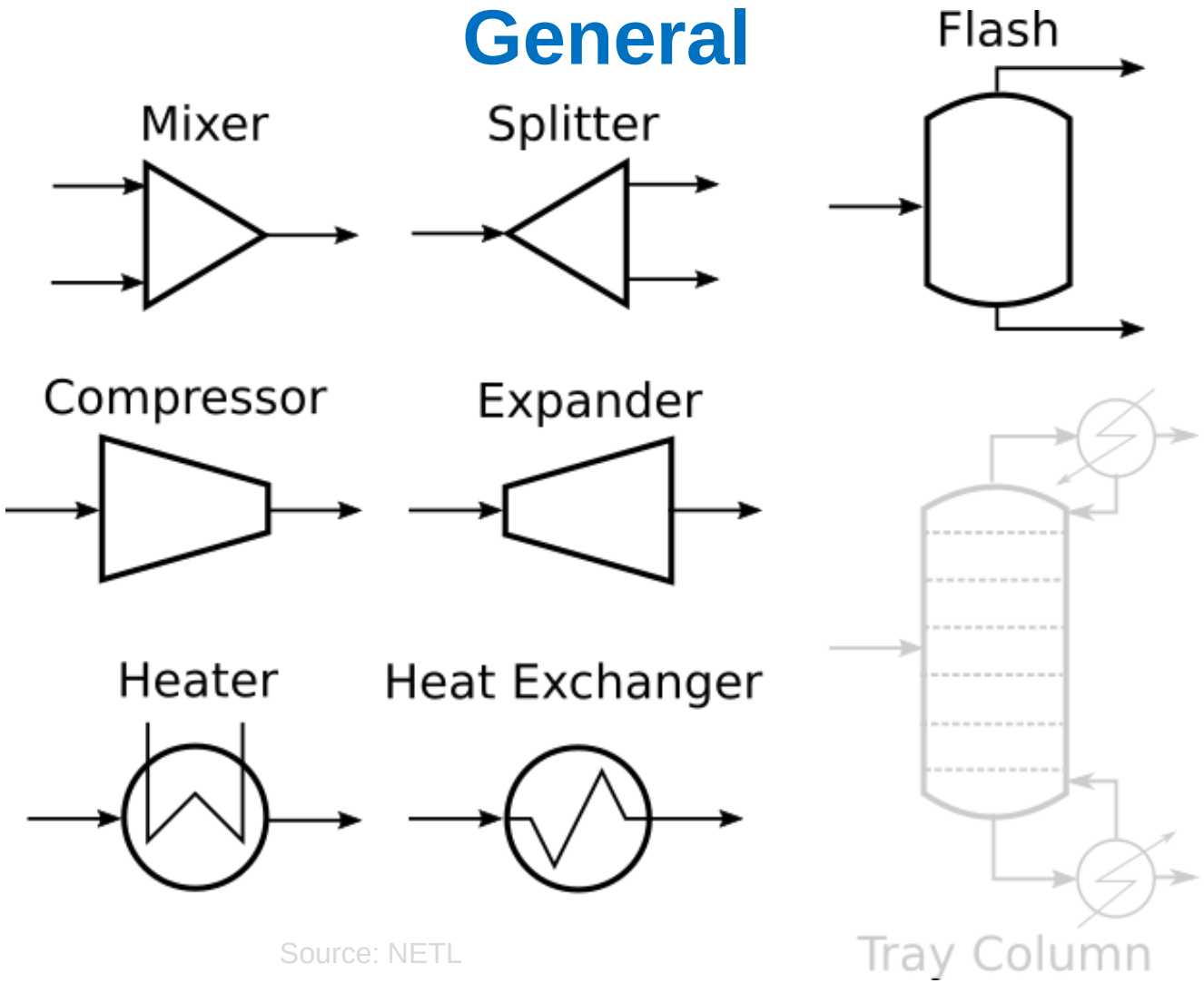
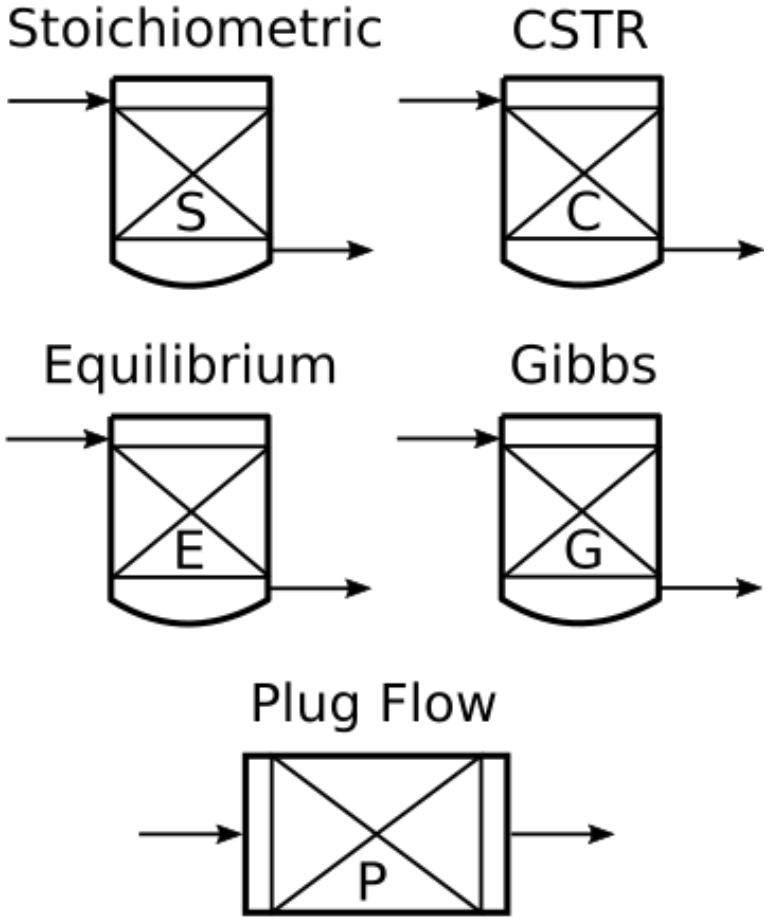
Optimization-Ready Model Library

General



Source: NETL

Reactors



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Libraries are Fully Documented

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).

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Variables

CSTR units add the following additional Variables beyond those created by the ControlVolume Block.

Variable	Name	Notes
V_t	volume	If `has_holdup` = `True` this is a reference to `control_volume.volume`, otherwise a Var attached to the Unit Model
Q_t	heat	Only if `has_heat_transfer` = `True`, reference to `control_volume.heat`

CSTR Class

class **idaes.unit_models.cstr.CSTR**(**args, **kwargs*)

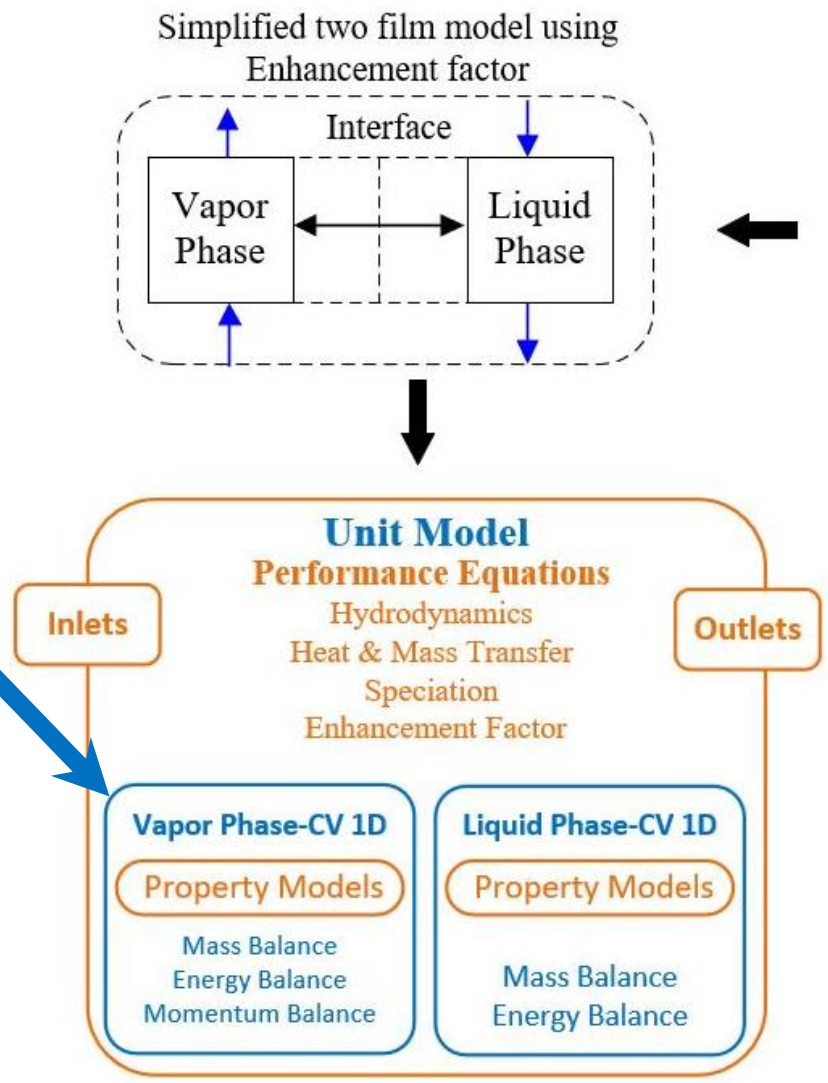
Parameters:

- **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*) –

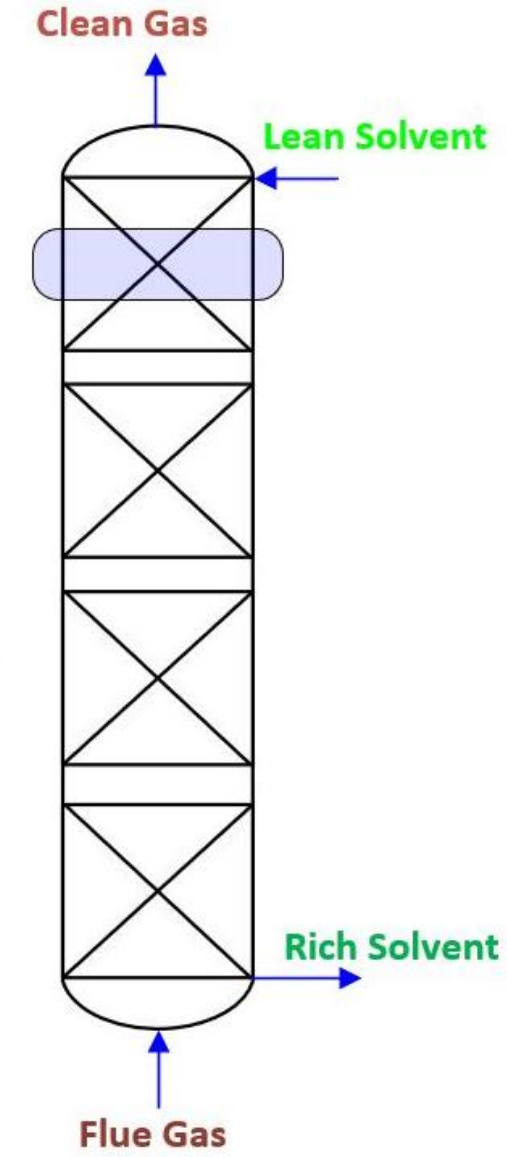
Modular Framework for Complex Processes

Control Volumes

- Automatically links to property packages
- Tools for automating:
  - Material balances
  - Energy balances
  - Momentum balances
- 0- and 1-D forms
- Steady-state and dynamic
- Methods to assist with initialization



Continuous Differential Contactor Model



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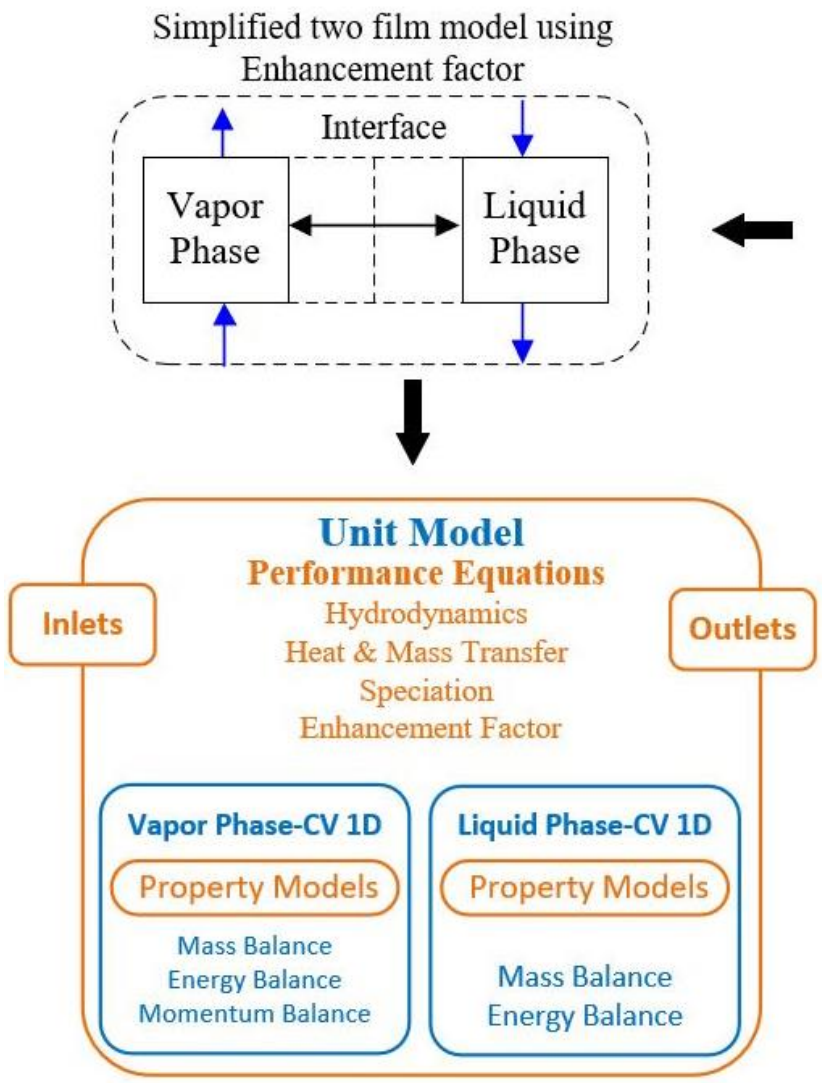
Modular Framework for Complex Processes

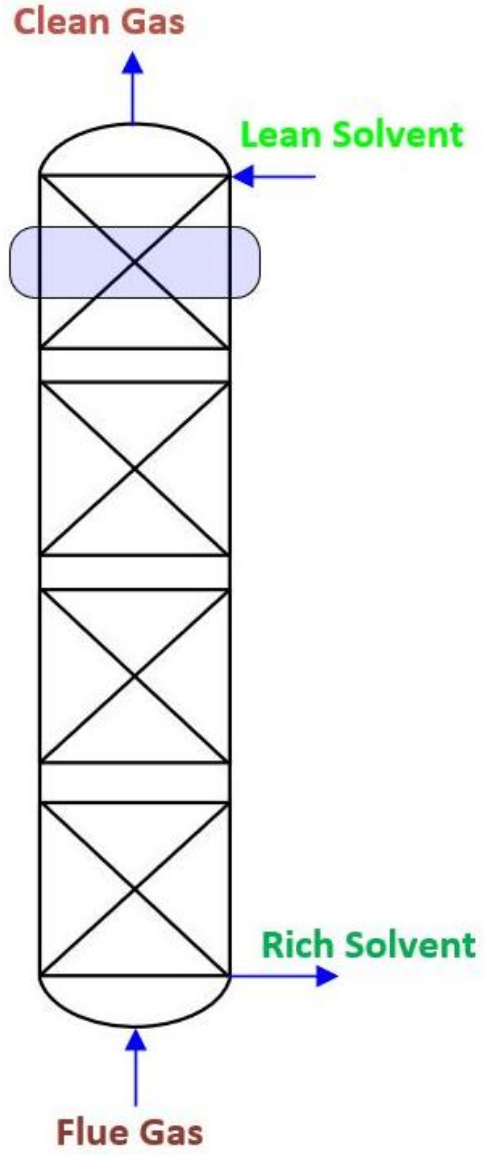
Control Volumes

Ports

- Points to link between units
- Coupled with control volumes
- Automatically determines variables to link



Continuous Differential Contactor Model



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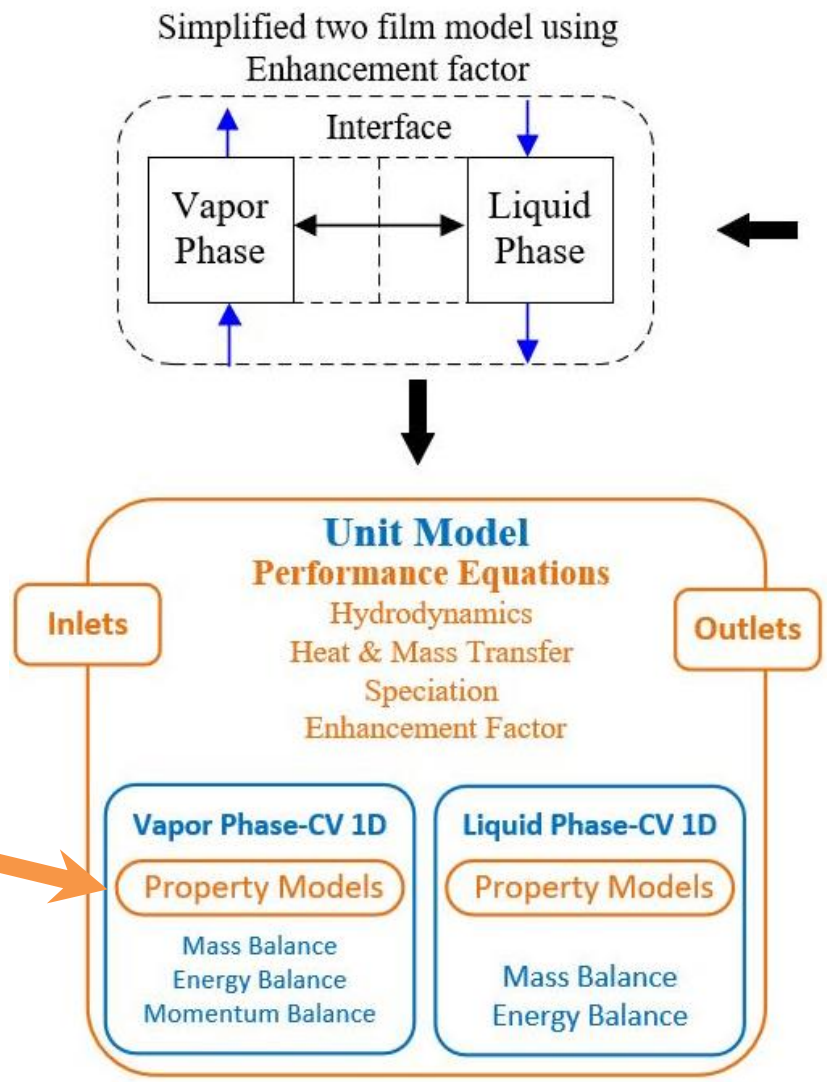
Modular Framework for Complex Processes

Control Volumes

Ports

Property Models

- Instances of property models



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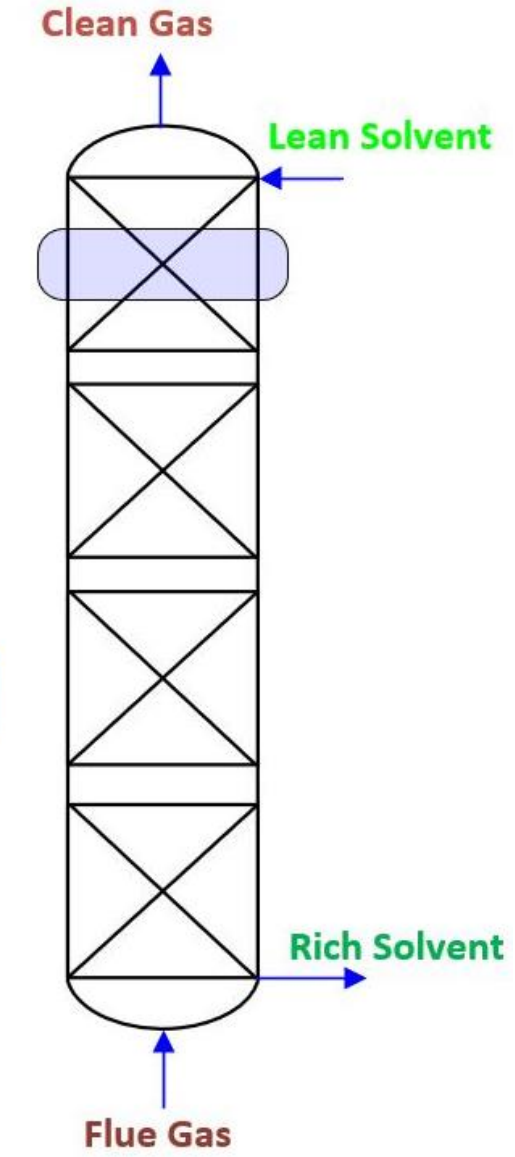

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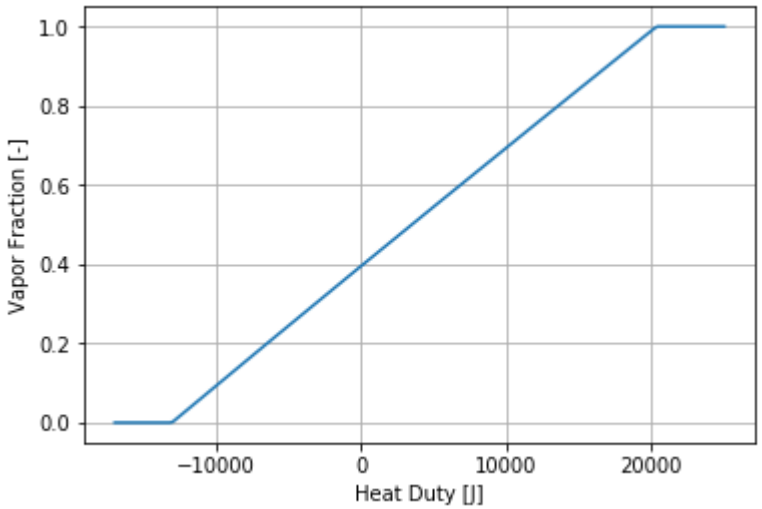
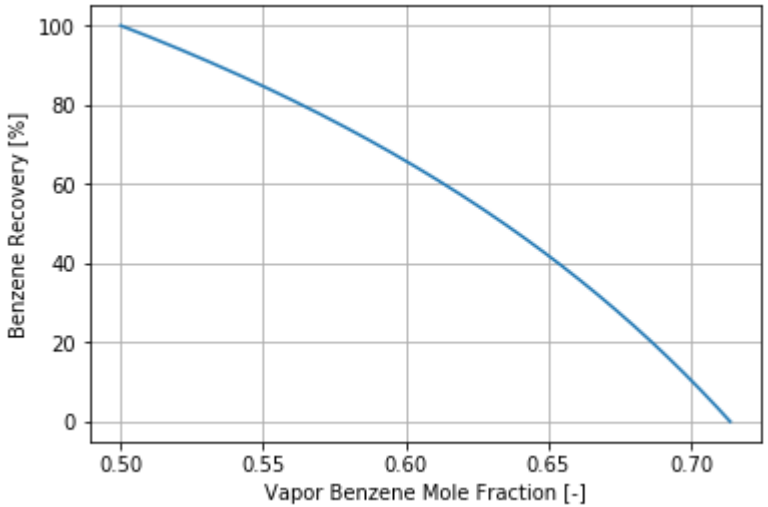
Property Models

- Optimization-ready unit models need optimization ready property packages
- Developing a limited library of standard property model forms
- Ideal-Ideal model for vapor-liquid equilibrium
  - Prototype for Ideal-NRTL and Ideal-Wilson
- Modular form allows different combinations of vapor and liquid phase properties

Vapor Fraction versus Heat Duty



Benzene Recovery versus Purity



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Integrating New Property Models

- Modular form allows for development of new property models
  - Add new component and parameters to existing models
  - Develop new correlations

- Models for each physical quantity are modular
  - Can model each property separately
  - Mix-and-match models for different properties

- IDAES tools for creating new property models

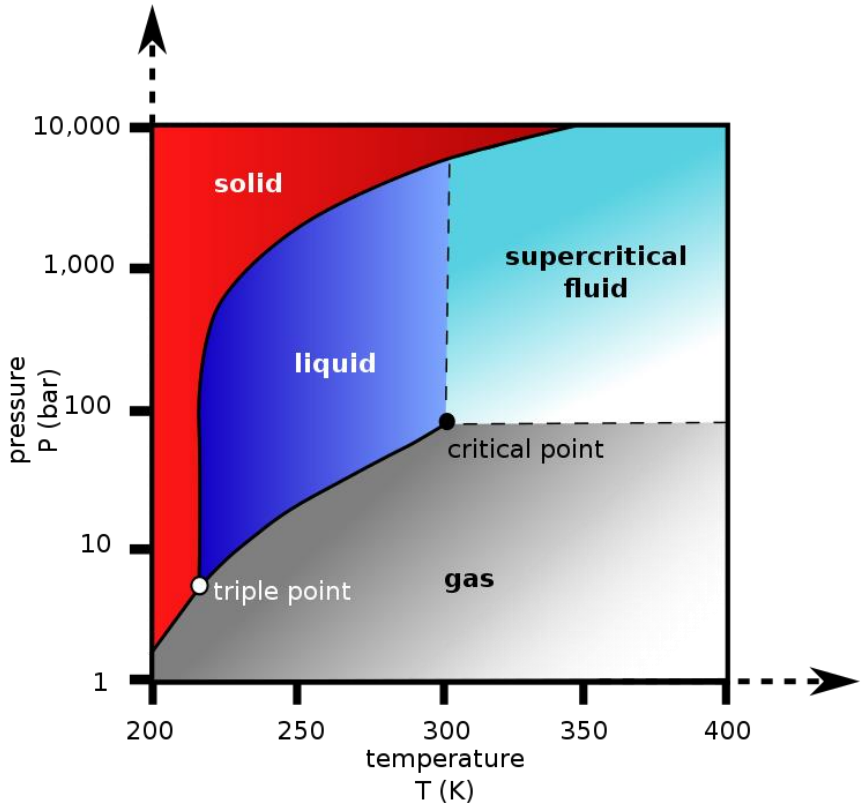

Image from
https://en.wikipedia.org/wiki/Supercritical_carbon_dioxide

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Using Model Libraries

Import desired models

```
from idaes.unit_models import CSTR
from idaes.properties import Ideal
```

Create a flowsheet

```
fs = Flowsheet(default={“dynamic”=False))
```

Create a property instance

```
fs.ideal_props = Ideal.Parameters()
```

Create a model instance

```
fs.reactor = CSTR(default={
    “property_package”: fs.ideal_props})
```

Connect units

```
fs.stream = Arc(source=fs.reactor.outlet,
                destination=fs.unit2.inlet)
```

Fix conditions

```
fs.reactor.volume.fix(10)
```

Initialization of Models

- All IDAES models contain initialization methods
  - unit models
  - control volumes
  - property packages

```
fs.reactor.initialize(initial_guesses)
```

- Facilitates a hierarchical, modular approach to initialization

- Developing tools to automate much of the process

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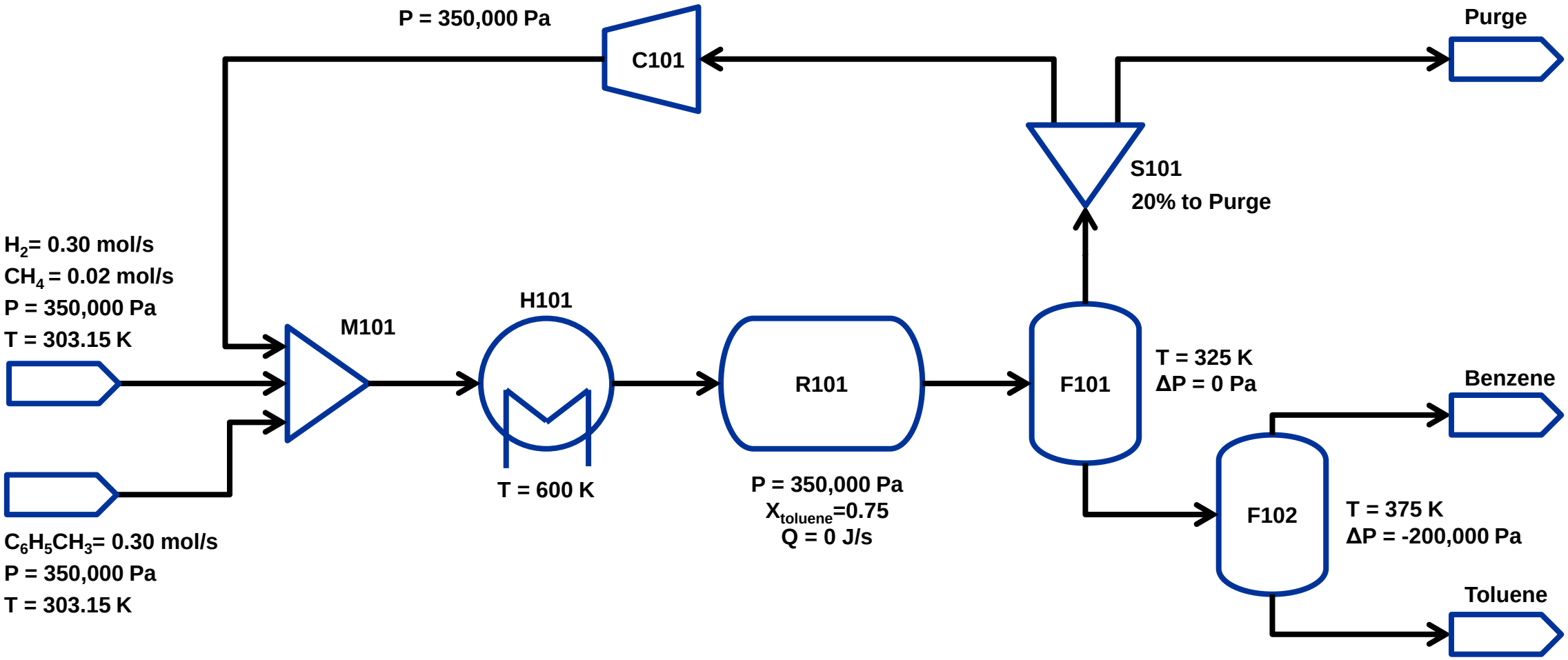
Workshop Flowsheet



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Summary

- Core libraries contain models for most common unit operations
- Library of basic property methods and tools for generating new models
- All models are optimization ready
- Modular structure designed for extensibility

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