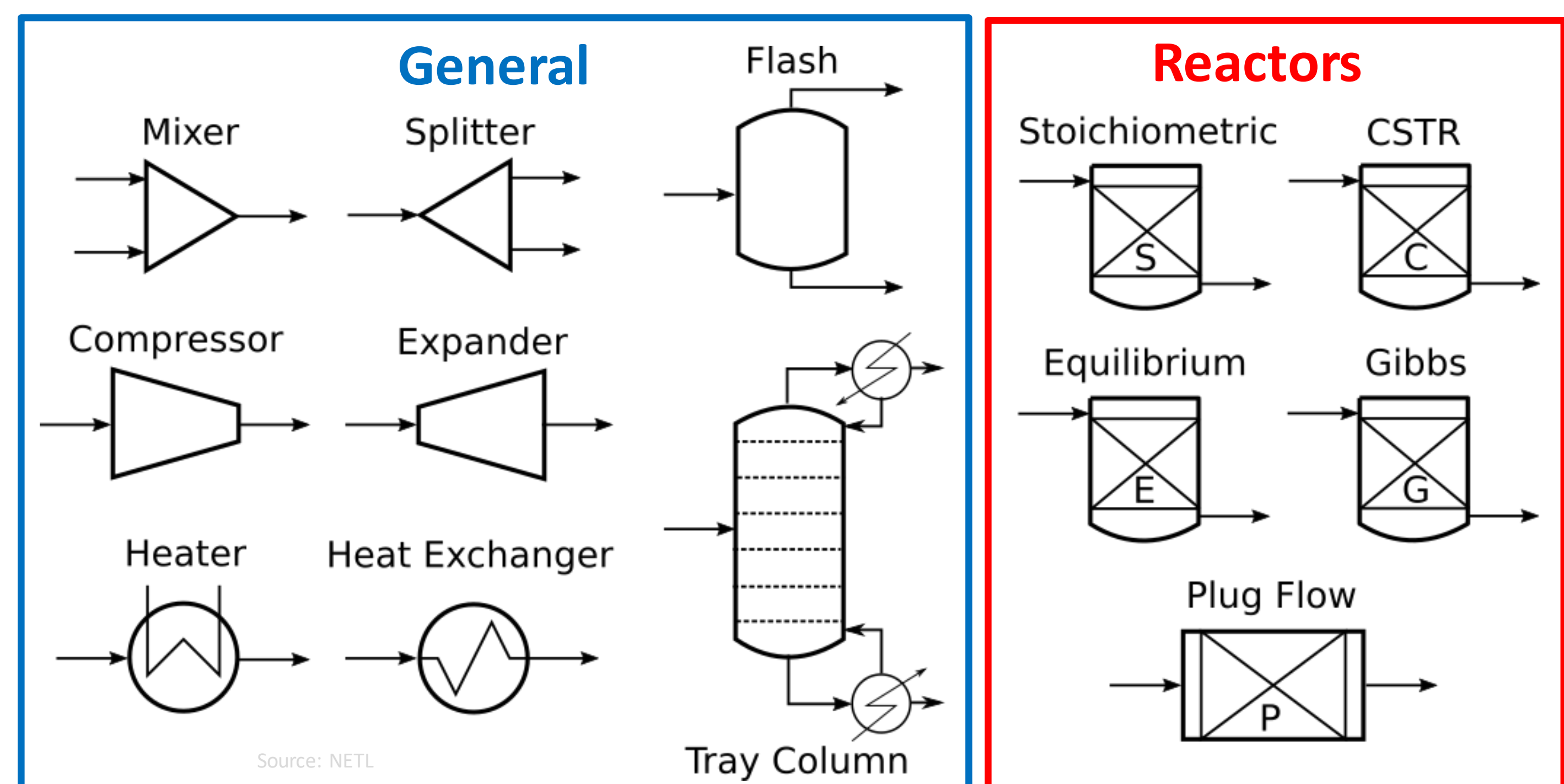




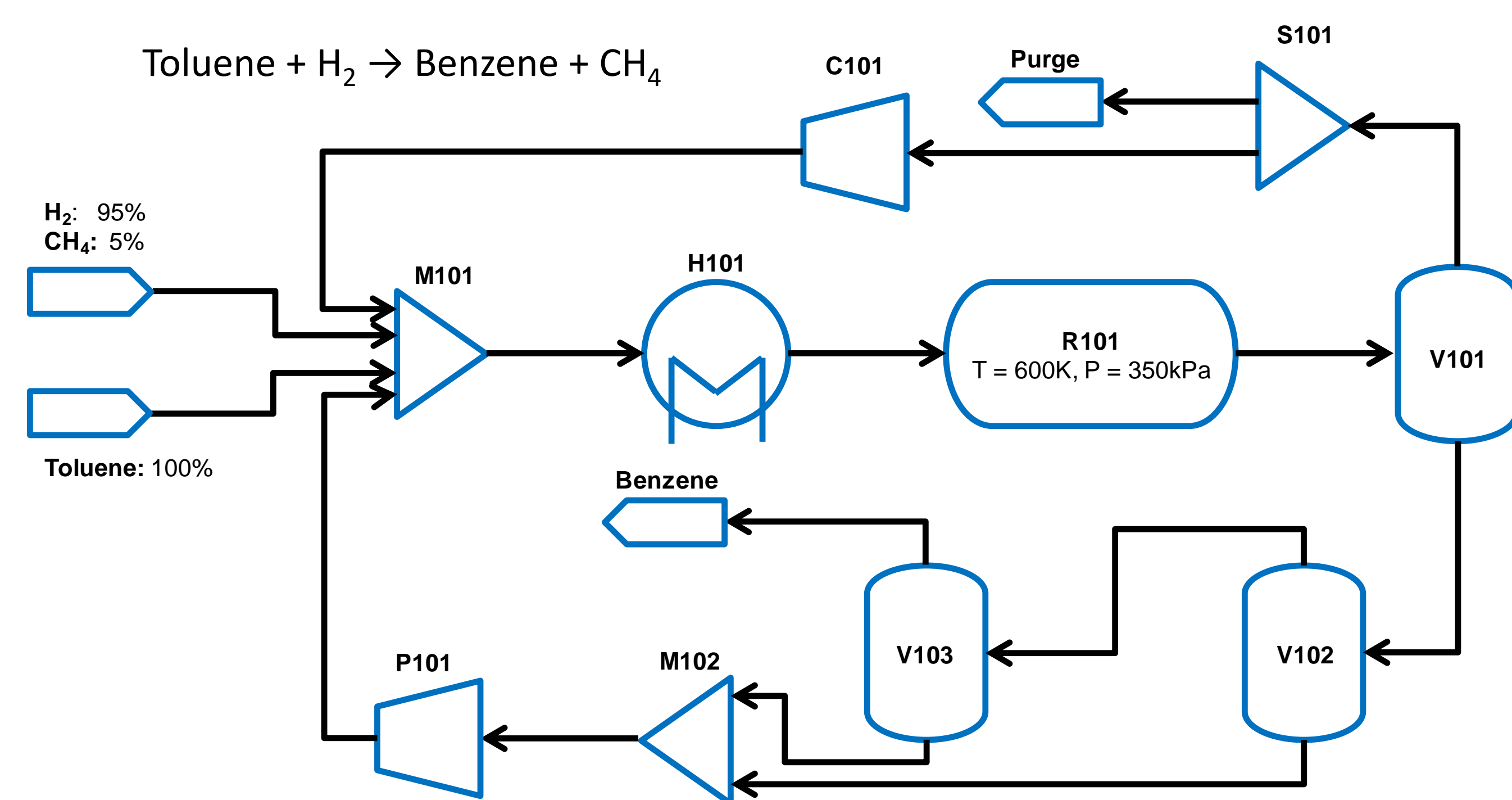
Unit Model Library and Process Flowsheeting

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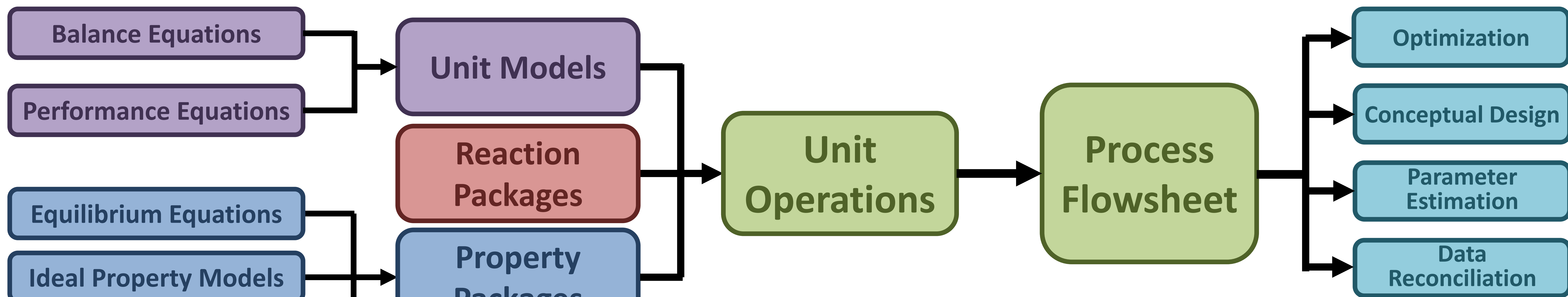
Optimization Ready Unit Model Library



Hydroalkylation Process Flowsheet



```
m.fs = ConcreteModel()
m.fs.ideal_props = Ideal.Parameters()
m.fs.reactor = CSTR(default={
    "property_package": m.fs.ideal_props})
m.fs.stream = Arc(source=m.fs.R101.outlet,
    destination=m.fs.V101.inlet)
TransformationFactory("network.expand_arcs").apply_to(m)
seq = SequentialDecomposition()
seq.set_guesses_for(m.fs.H101.inlet, tear_guesses)
seq.run(m, function)
```



Structure of a Vapor-Liquid Equilibrium Property Package

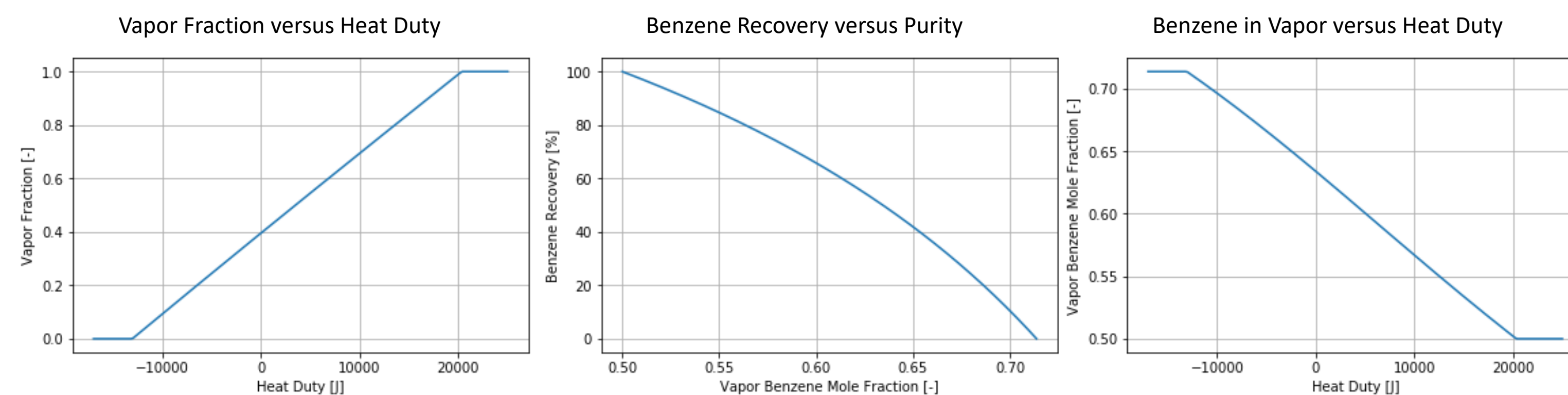
- State variables
- Vapor-Liquid Equilibrium model
 - Vapor phase fugacity model
 - Component fugacity coefficient models
 - Liquid phase fugacity model
 - Component activity coefficient models
- Mixture property model
 - Vapor phase property model
 - Vapor phase pure component property models
 - Liquid phase property model
 - Liquid phase pure component property models

Ideal Two Phase (Vapor-Liquid) Property Package

Smooth equilibrium formulation

$$T_1 = \max(T, T_{bub}) = 0.5 \cdot \left(T + T_{bub} + \sqrt{(T - T_{bub})^2 + \epsilon_1^2} \right) \quad \Phi_V(P, T_{eq}) = \Phi_L(P, T_{eq})$$

$$T_{eq} = \min(T_1, T_{dew}) = 0.5 \cdot \left(T_1 + T_{dew} - \sqrt{(T_1 - T_{dew})^2 + \epsilon_1^2} \right)$$



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