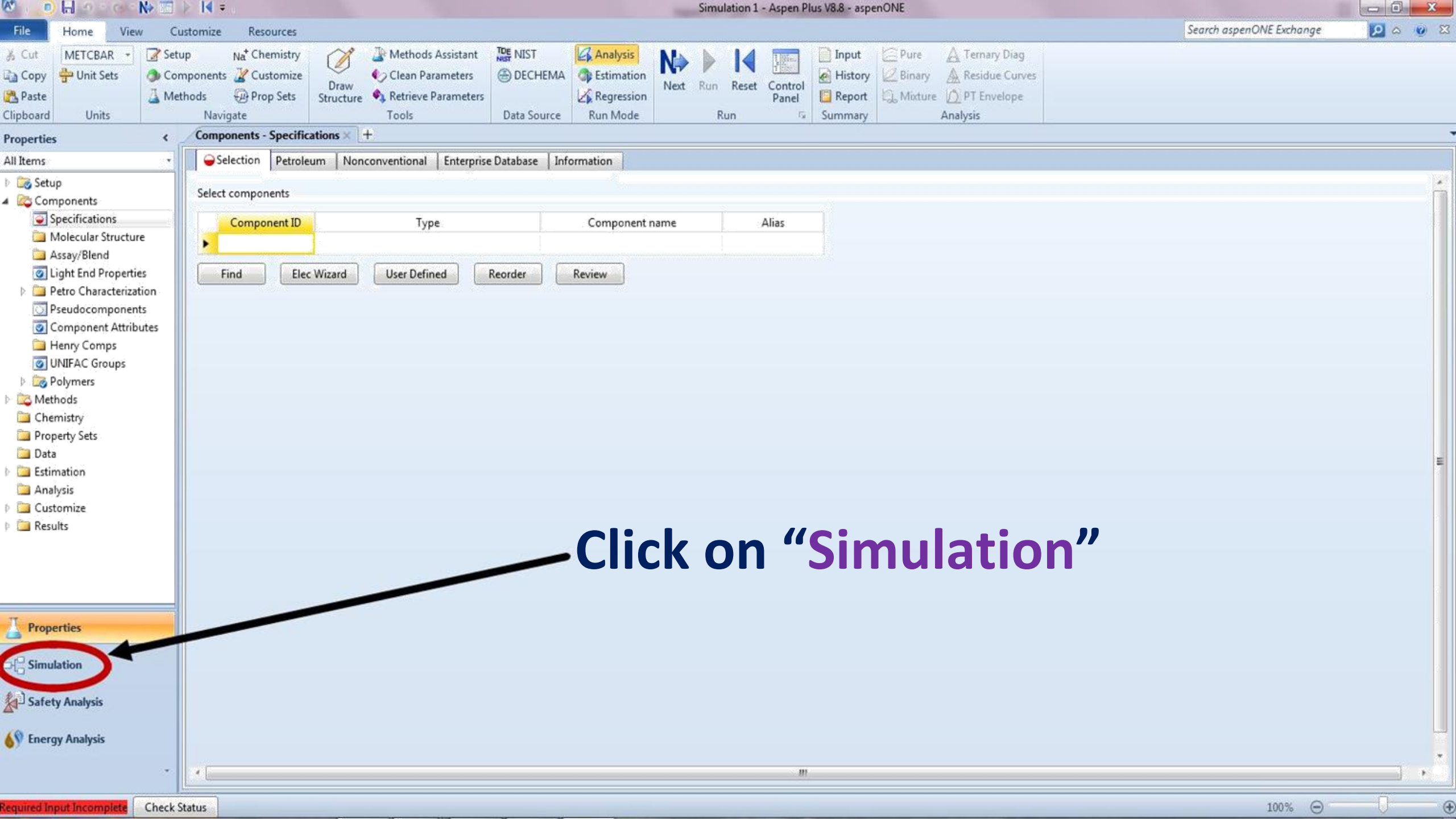
CL-402: Chemical Process Technology

July-November Session, 2018

7^{th} semester, Department Of Chemical Engineering

Indian Institute Of Technology Guwahati, Guwahati

Reactor Models
in
Aspen Plus V8.8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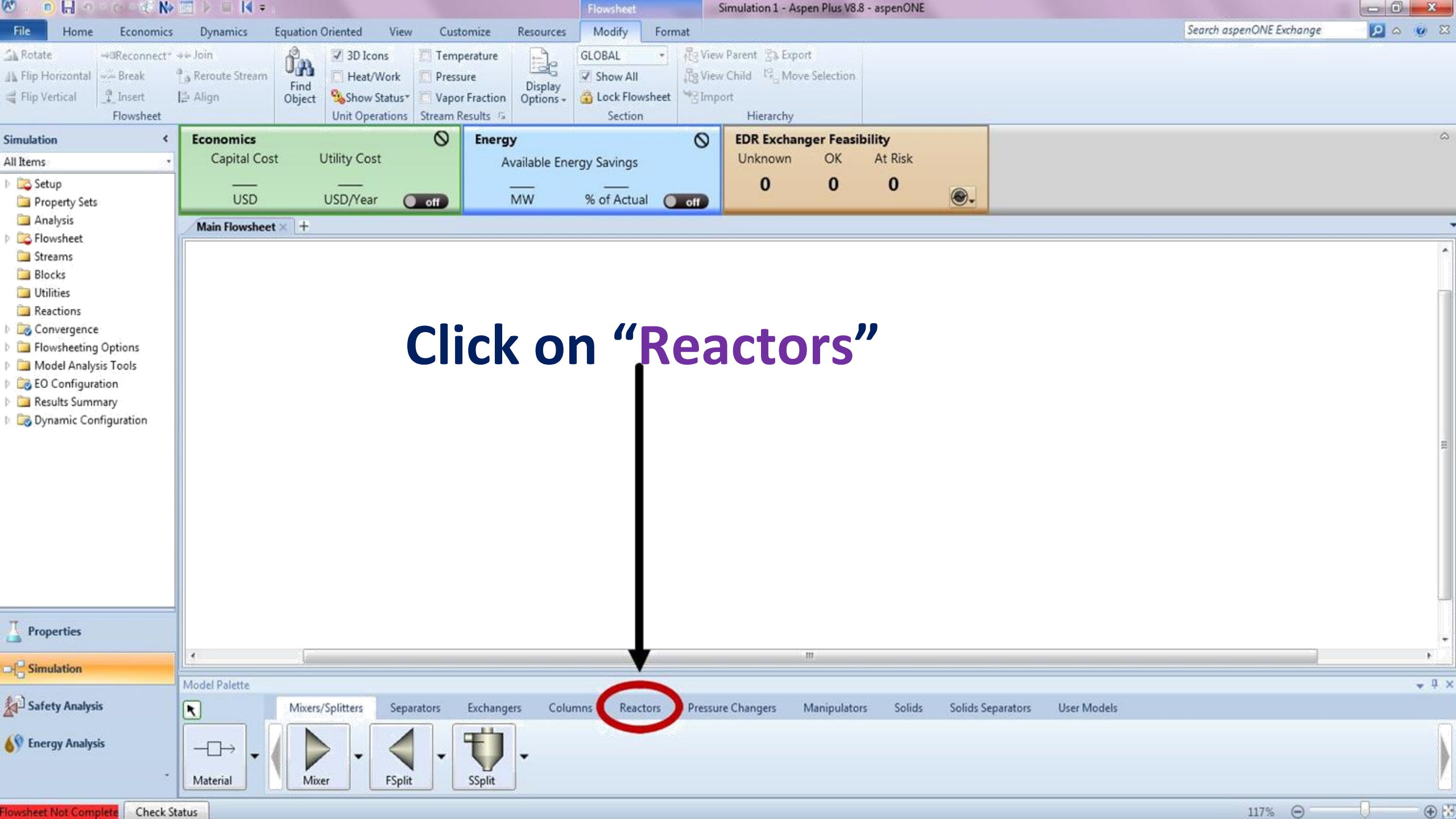
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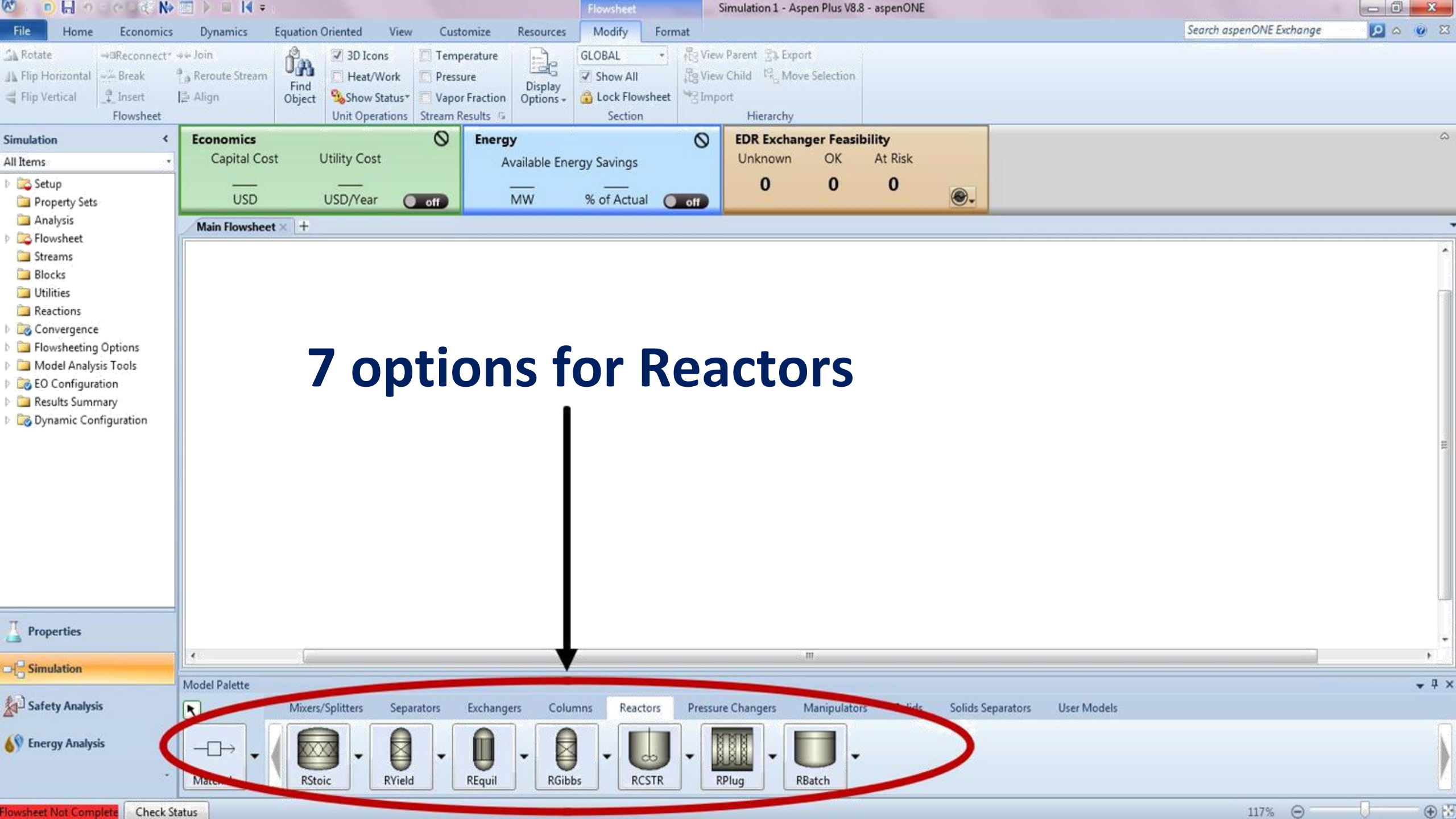
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RCSTR
RPlug
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Model	Description	Purpose	Use For
RStoic	Stoichiometric reactor	**Models stoichiometric reactor with specified reaction extent or conversion.**	Reactors where reaction kinetics are unknown or unimportant but stoichiometry and extent or conversion of reaction are known.
RYield	Yield reactor	**Models reactor with specified yield.**	Reactors where stoichiometry and kinetics are unknown or unimportant but a yield distribution is known. **Can model one-, two-, and three-phase reactors.**

Model	Description	Purpose	Use For
RCSTR	Continuous stirred tank reactor	Models continuous stirred tank reactor.	One-, two, or three-phase stirred tank reactors with rate-controlled and equilibrium reactions in any phase based on known stoichiometry and kinetics.
RPlug	Plug flow reactor	Models plug flow reactor.	One-, two-, or three-phase plug flow reactors with rate-controlled reactions in any phase based on known stoichiometry and kinetics.
RBatch	Batch reactor	Models batch or semi-batch reactor.	One-, two-, or three-phase batch and semi-batch reactors with rate-controlled reactions in any phase based on known stoichiometry and kinetics.

For RCSTR, RPlug, and RBatch, you must provide reaction kinetics information using: (rigorous models)

- The built in power law model.
- The built in generalized Langmuir Hinshelwood Hougen Watson (LHHW) model.
- A user written Fortran subroutine.

Model	Description	Purpose	Use For
REquil	Equilibrium reactor	Performs chemical and phase equilibrium by stoichiometric calculations.	Reactors with simultaneous chemical equilibrium and phase equilibrium. REquil can model one- and two-phase reactors.
RGibbs	Equilibrium reactor with Gibbs energy minimization	**Performs chemical and phase equilibrium by Gibbs energy minimization.**	Reactors with phase equilibrium or simultaneous phase and chemical equilibrium. Calculating phase equilibrium for solid solutions and vapor-liquid-solid systems.

How RGibbs block works?

- At equilibrium at constant temperature and pressure, the Gibbs energy should be a minimum.
- Aspen develop a general expression for the Gibbs energy of the system in terms of the number of moles of all species present, reactants, products, and inert species, and in all phases. The calculation then is to vary the number of moles of each species in each phase subject to the stoichiometric constraints and find a solution that minimizes the total Gibbs energy of the system. In this way, a general minimization algorithm can be used to solve all chemical reaction equilibrium problems.