13.1   Example 1: Process Involving Reaction and Separation

Toluene is produced from n-heptane by dehydrogenation over a Cr_2O_3 catalyst:

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_3 \rightarrow C_6H_5CH_3 + 4H_2$$

The toluene production process is started by heating n-heptane from 65 to 800 ^oF in a heater. It is fed to a catalytic reactor, which operates isothermally and converts 15 mol% of the n-heptane to toluene. Its effluent is cooled to 65 ^oF and fed to a separator (flash). Assuming that all of the units operated at atmospheric pressure, determine the species flow rates in every stream.

Solution

1. Start HYSYS and File/New/Case.
2. *Simulation Basis Manager* will pop up. Click **Add**. *Fluid Package* window will be opened. Choose **Peng Robinson** as Base Property Package.
3. Open **Component** page of *Fluid Package* window and add components (toluene, *n-heptane*, and hydrogen) and close the *Fluid Package.*
4. Click **Enter Simulation Environment** at the bottom of *Simulation Basis Manager*.
5. Click **Heater** in the *Object Palette* and click it on *Process Flow Diagram (PFD)*. Click General Reactor, three different reactors will pop up, click **conversion** reactor and click it on *PFD*. Do the same for the **Cooler** and **Separator**.
6. Name inlets and outlets of all process units as shown in *PFD* diagram on the Figure 13.1.
7. You will notice that the reactor is colored red with the error message, "Need a reaction set." Now we need to input what the reaction is. Click Flowsheet/Reaction Package. Add Global Rxn Set. Then, click Add Rxn at the lower right side of the window and choose Conversion. Add three components (n-Heptane, Toluene, Hydrogen) and Stoich Coeff (-1, 1, 4). Click Basis page, and type 15 for Co (this is the conversion). Close windows until you see *PFD*.
8. Double click reactor. Choose Global Rxn Set as Reaction set and close the window.
9. Now, open worksheet, and type in all the known conditions for the streams. Note that only blue colored fonts are the values that you specified. If you more information than the degree of freedom allows, it will give you error messages.
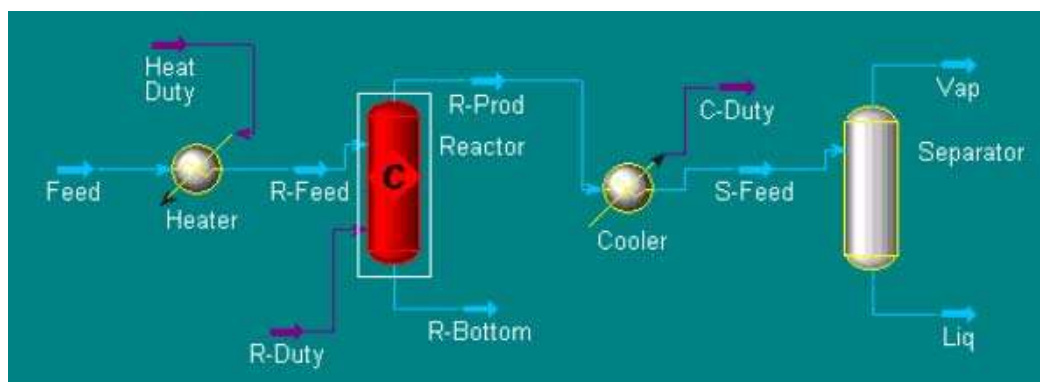

Figure 13-1