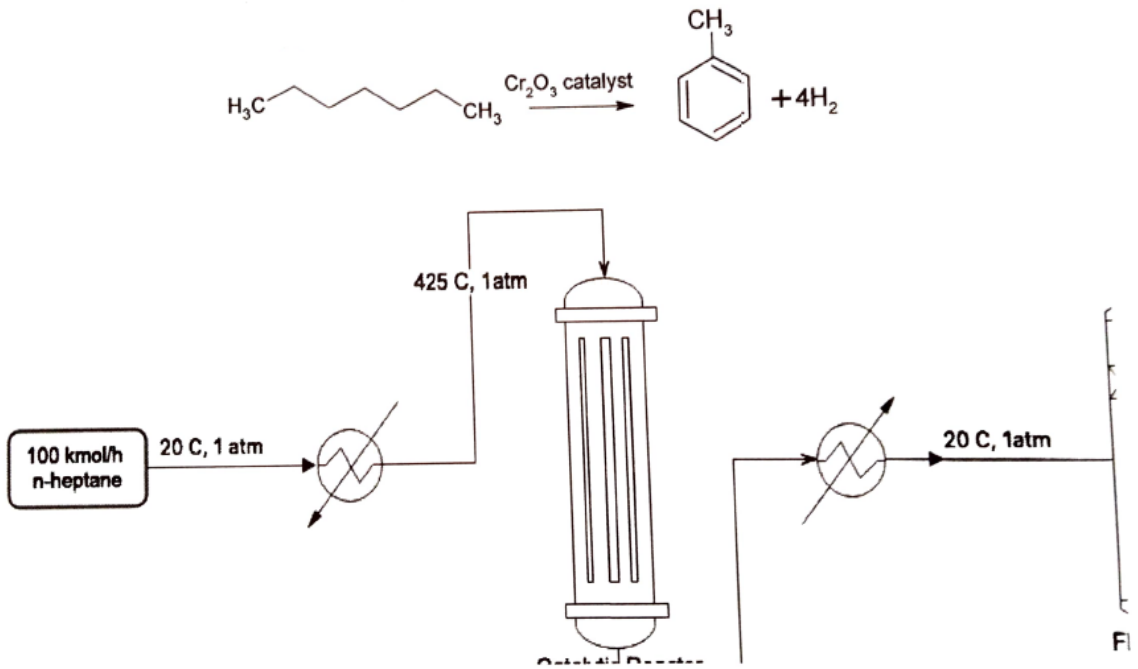
Question 1

Toluene is produced from n-heptane by dehydrogenation over Cr_2O_3 catalyst. The toluene production process requires heating 100 $kmol/h$ of n-heptane at atmospheric pressure from 20 ℃ to 425 ℃ in a heater. The preheated feed enters a catalytic reactor, which operates at 425 ℃ and atmospheric pressure and converts 15 % of the n-heptane to toluene. The reactor effluent is cooled to 20 ℃ and subsequently enters a flesh separator. Assuming that all units are operated at atmospheric pressure, determine the species flow rates, temperature and composition of each stream. Use Peng-Robinson EOS.



Now modify the process described in Problem by preheating the feed stream to 315 °c with hot reactor product before entering the reactor. Assume negligible pressure drop in both the tube and shell side of the preheater. Compare the energy requirements between the two.

Answer

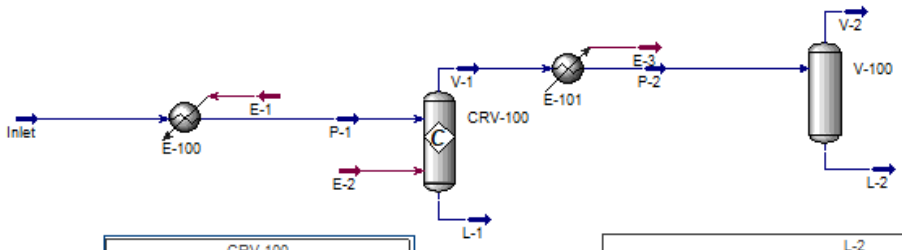
- Liquid Flowrate 97.05 $kmol/hr$
- Vapour Flowrate 62.95 $kmol/hr$
- Pressure 1 atm
- Product Composition—

Species	***Vapour Phase Composition***	***Liquid Phase Composition***
$\boldsymbol{n-heptane}$	0.0418	0.8487
Toluene	0.0063	0.1504
Hydrogen	0.9519	0.0009

E-100		
Duty	3766.1	kW
Feed Temperature	20.00	C
Product Temperature	425.0	C

E-101		
DUTY	3795.5	kW
Feed Temperature	425.0	C
Product Temperature	20.00	C

V-2		
Molar Flow	62.95	kgmole/h
Phase Comp Mole Frac (Vapour Phase-Hydrogen)	0.9519	
Phase Comp Mole Frac (Vapour Phase-n-Heptane)	0.0418	
Phase Comp Mole Frac (Vapour Phase-Toluene)	0.0063	



CRV-100		
Vessel Temperature	425.00	C
Vessel Pressure	101.3	kPa
Vapour Molar Flow	160.0	kgmole/h
Liquid Molar Flow	0.0000	kgmole/h
Heat Flow	1051	kW

L-2		
Molar Flow	97.05	kgmole/h
Phase Comp Mole Frac (Liquid Phase-Hydrogen)	0.0009	
Phase Comp Mole Frac (Liquid Phase-n-Heptane)	0.8487	
Phase Comp Mole Frac (Liquid Phase-Toluene)	0.1504	

Case I:

Utilities Requirements are—

Heater Input, $Q_H = 3766.1\ kW$

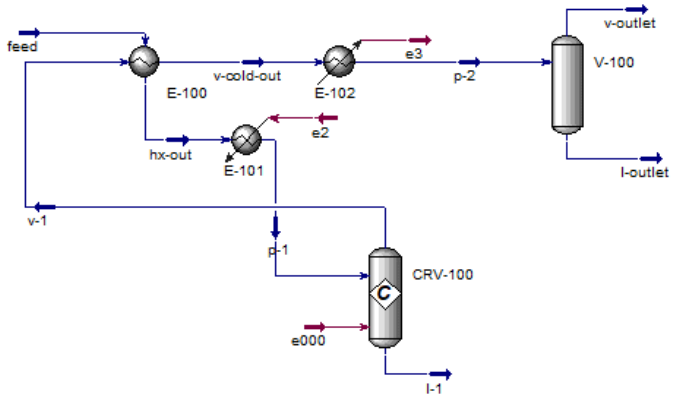
Cooler Output, $Q_C = 3795.5\ kW$

Energy Supplied to the Reactor $= 1051\ kW$

E-101		
Duty	913.1	kW
Feed Temperature	315.0	C
Product Temperature	425.0	C

E-102		
DUTY	942.5	kW
Feed Temperature	77.69	C
Product Temperature	20.00	C

v-outlet		
Molar Flow	62.95	kgmole/h
Phase Comp Mole Frac (Vapour Phase-Hydrogen)	0.9519	
Phase Comp Mole Frac (Vapour Phase-n-Heptane)	0.0418	
Phase Comp Mole Frac (Vapour Phase-Toluene)	0.0063	



l-outlet		
Molar Flow	97.05	kgmole/h
Phase Comp Mole Frac (Liquid Phase-Hydrogen)	0.0009	
Phase Comp Mole Frac (Liquid Phase-n-Heptane)	0.8487	
Phase Comp Mole Frac (Liquid Phase-Toluene)	0.1504	

CRV-100		
Vessel Temperature	425.0	C
Vessel Pressure	101.3	kPa
Vapour Molar Flow	160.0	kgmole/h
Liquid Molar Flow	0.0000	kgmole/h
Heat Flow	1051	kW

Case II:

Utilities Requirements are—

Heater Input, $Q_H = 913.1\ kW$

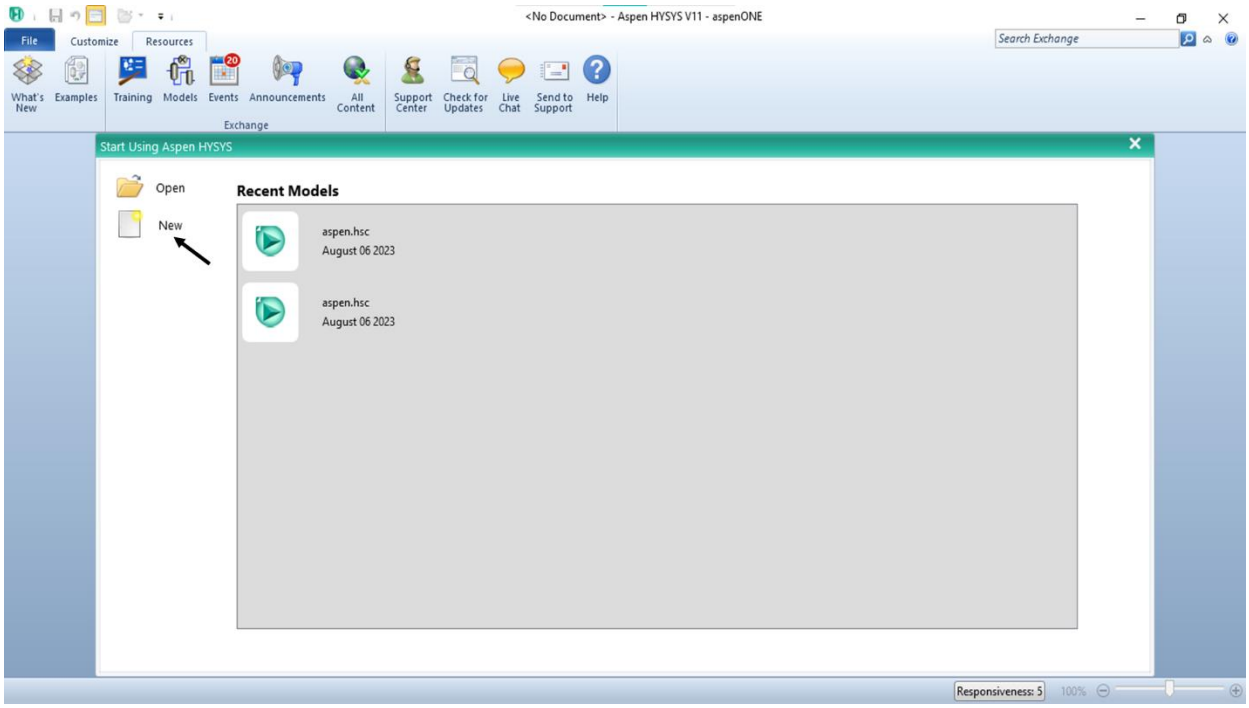
Cooler Output, $Q_C = 942.5\ kW$

Energy Supplied to the Reactor $= 1051\ kW$

So, the energy requirements in the utilities decreases and it decreases by $3766.1 - 913.1 = 3795.5 - 942.5 = 2853\ kW$.

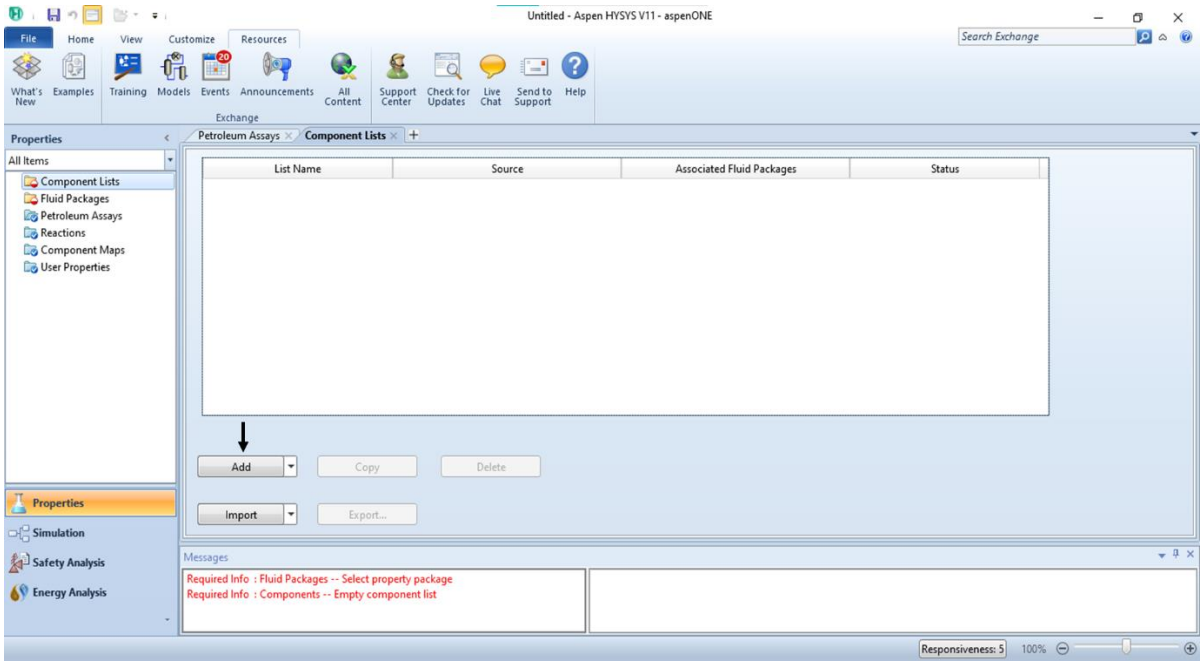
Step 1:

At first, we ASPEN HYSYS software by clicking on the shortcut icon from the desktop. The Initial Layout looks like the following. From the New menu we clicked on button to create a blank Simulation Workbook page.



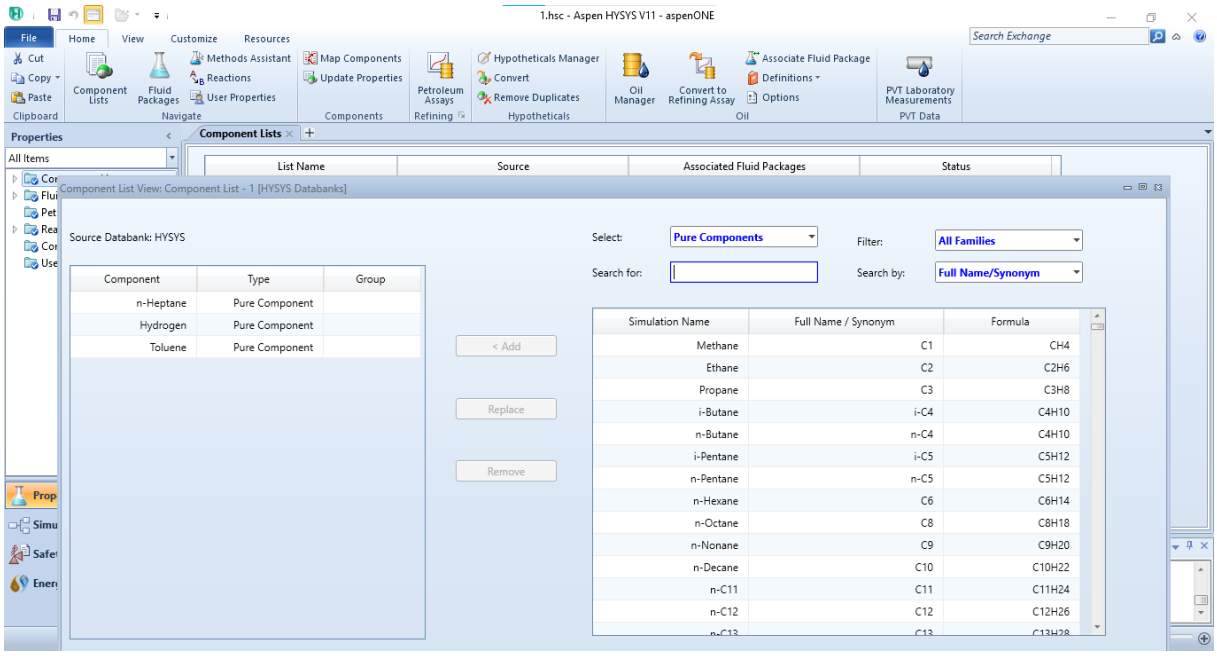
Step 2:

Now in the next page we will click on Add icon to select the components required for our simulation. Here we are dealing only with water we will add only water.



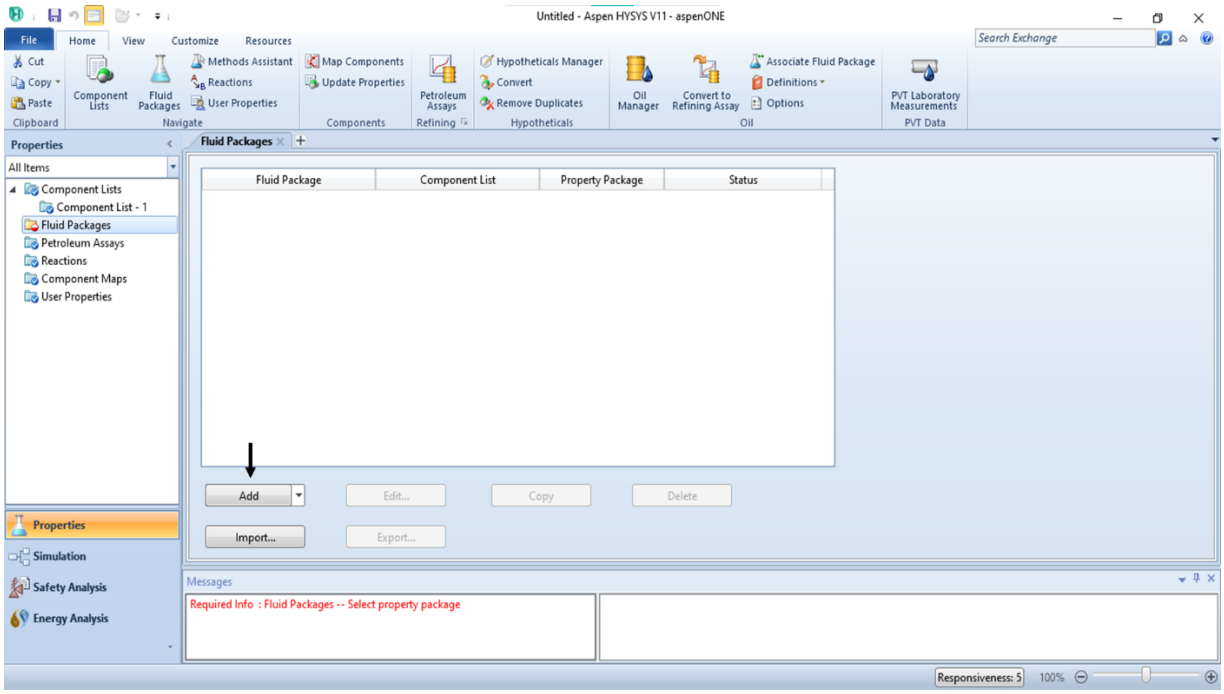
Step 4:

Now in the Component list page we will search for in Search for: box. Then we will select the components and click. < Add This will add the components in the component list. Now we will choose the desired fluid packages by clicking on Fluid Packages icon.



Step 5:

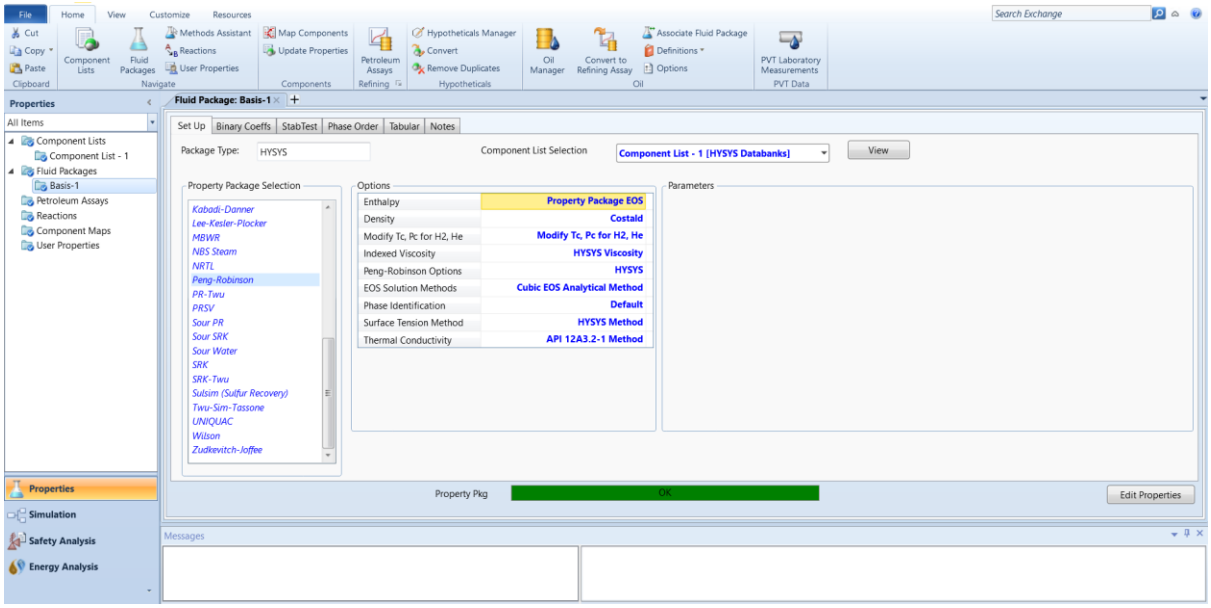
In the Fluid Packages tab, we will click Add to add new fluid packages.



Step 6:

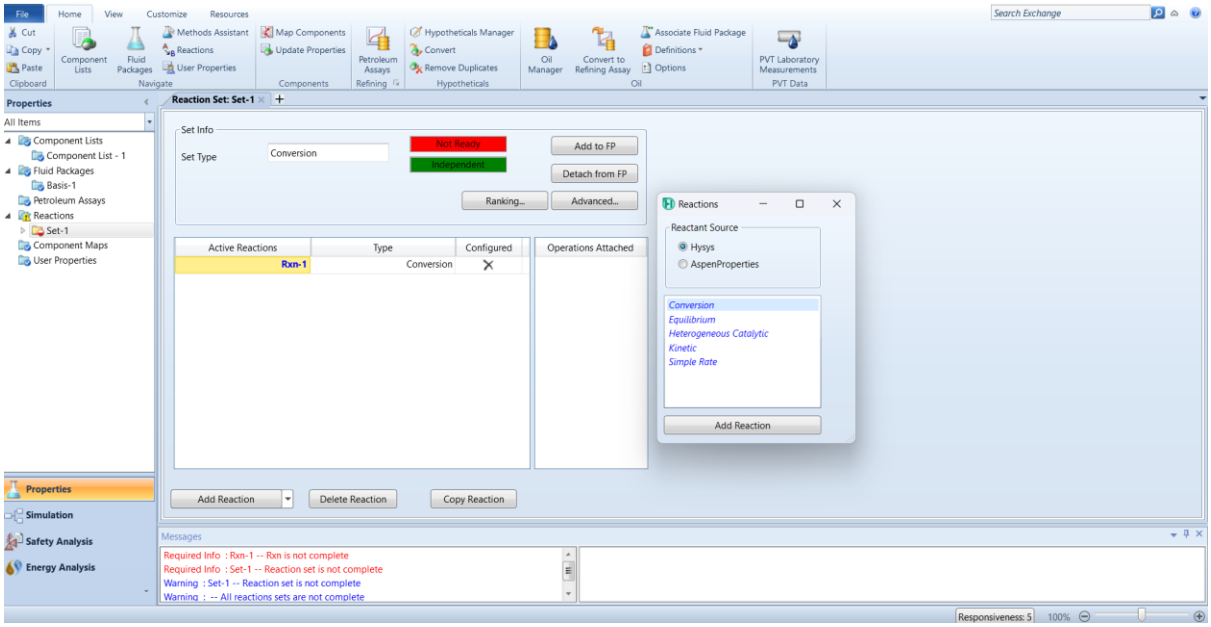
According to our given problem, we are supposed to use Peng-Robinson package for our problem. So, from the dropdown menu, we will select the Peng-Robinson option.

Now our components and property databases are ready. We are ready to add the necessary reactions.

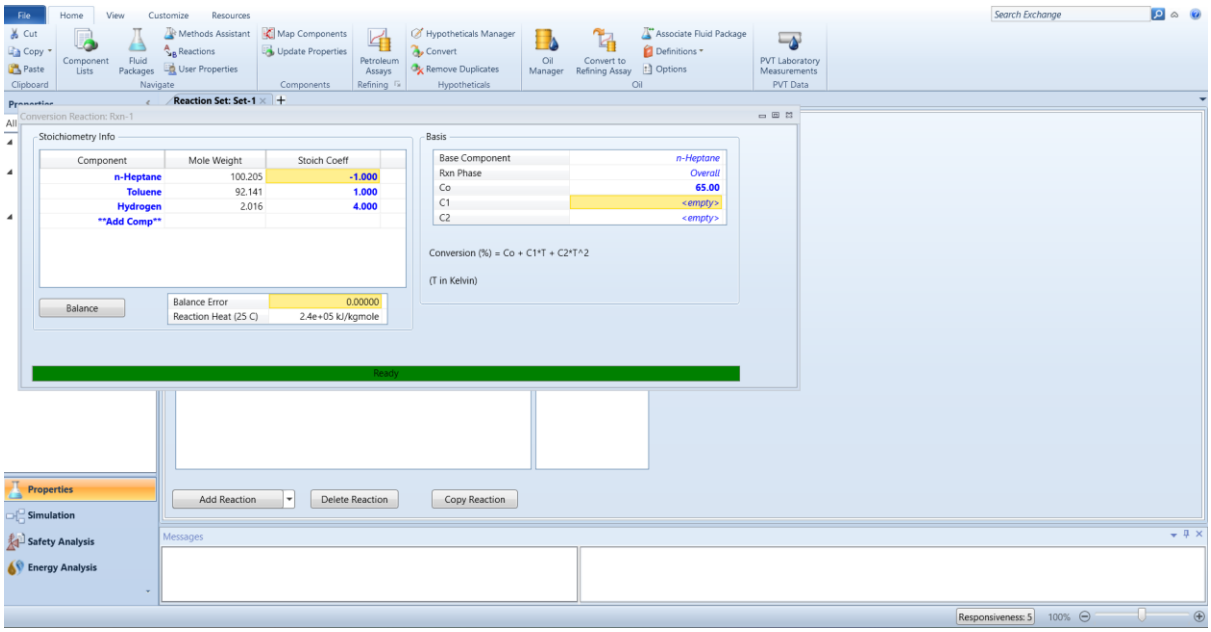


Step 7:

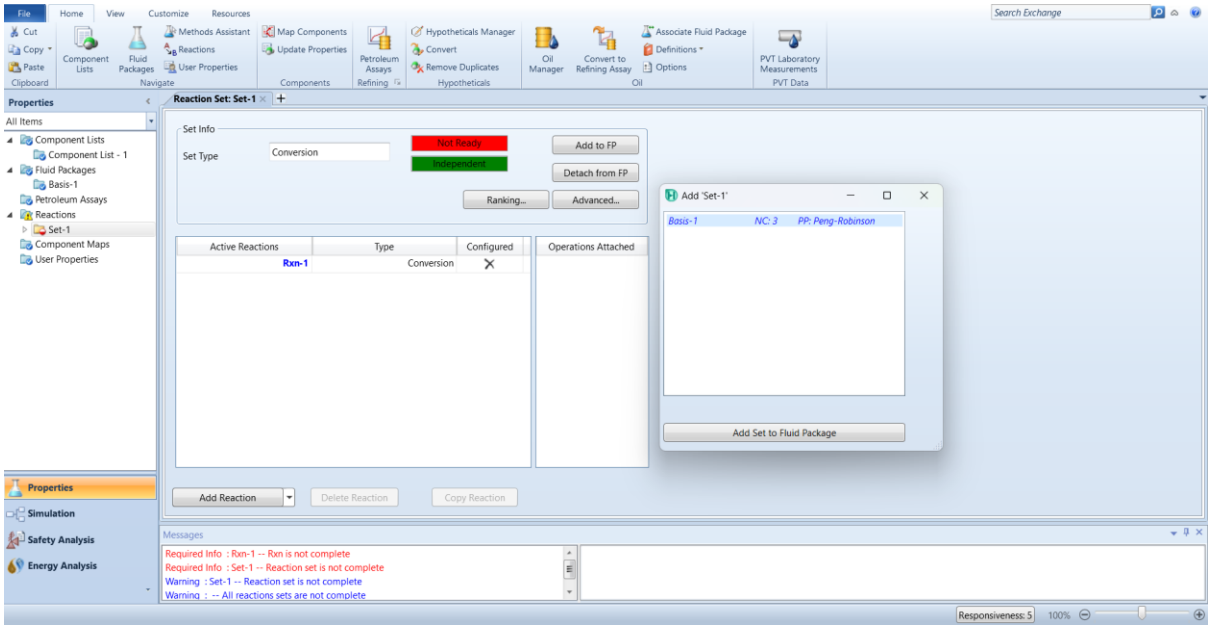
In this step we need to add the conversion reaction. we will click on the Reaction button then click add to add a new reaction. Here the type of reaction will be conversion reaction.

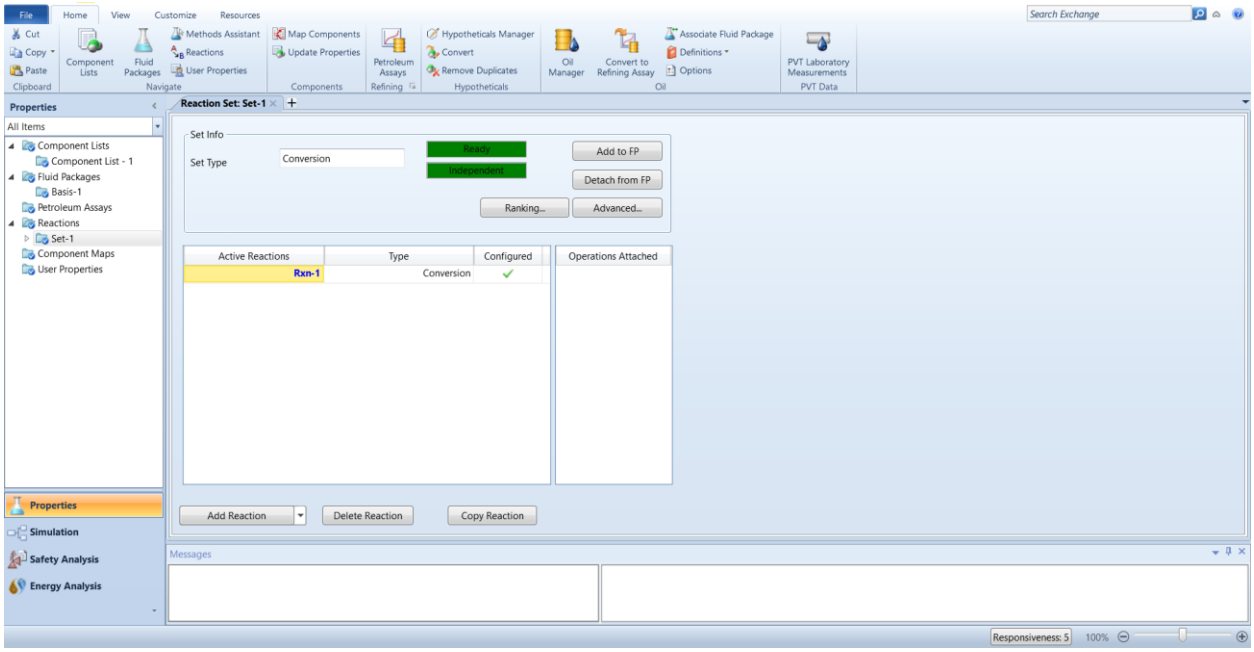


Now we will click on the **Rxn-1** to customise the reaction. Our reactants and products are $n-Heptane, H_2$ & $Toluene$. Respective Stoichiometric Coefficient and conversion are also entered.



When the set of reaction is ready we will close the window and click the **Add to FP** button.Now we will go to the simulation environment.

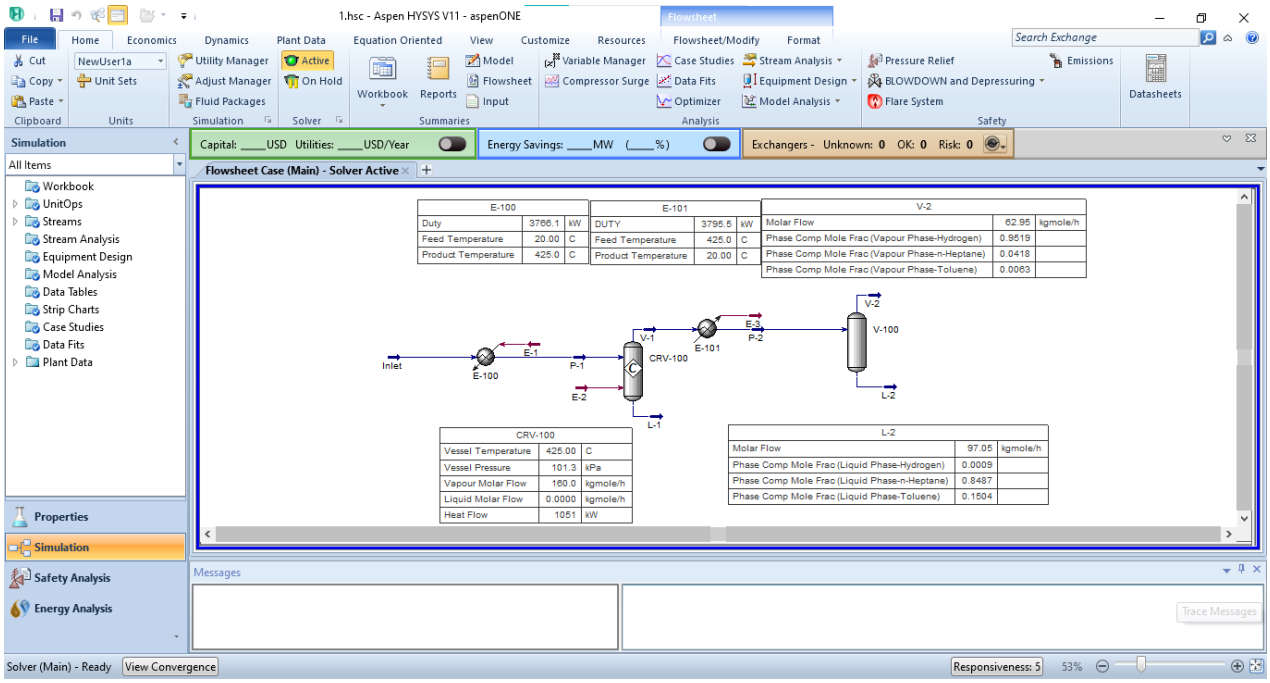




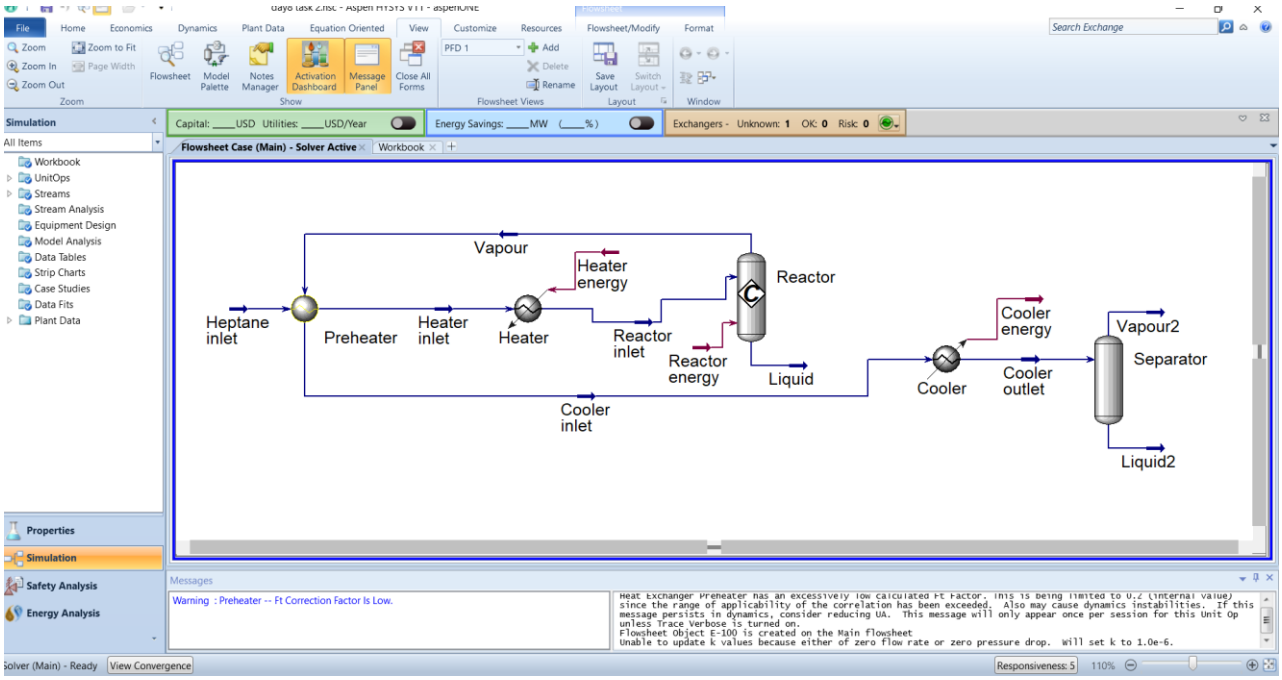
Step 8:

After bringing all the necessary unit operations and entering all the given condition we get the following results.

- **Case 1**: No Heat exchanger is used only hot and cold utilities are there.



- **Case 2**: Heat exchanger along with hot and cold utilities are used.


Vapour
Heater energy
Reactor
Heptane inlet
Preheater
Heater inlet
Heater
Reactor inlet
Reactor energy
Liquid
Cooler energy
Vapour2
Separator
Cooler
Cooler outlet
Cooler inlet
Liquid2