Conversion Reaction Simulation

Example: ATR technologies play a crucial role in hydrogen, ammonia and methanol plants. In ATR reactors simply oxygen and natural gas, mainly methane react in a burner and as a result, produce heat required for catalytic zone in the reactor. The reaction is fast and all oxygen reacts with methane without any exception. This means a conversion reaction and reactor are enough to simulate the burner in Aspen Hysys. Here is a summary of operating condition:

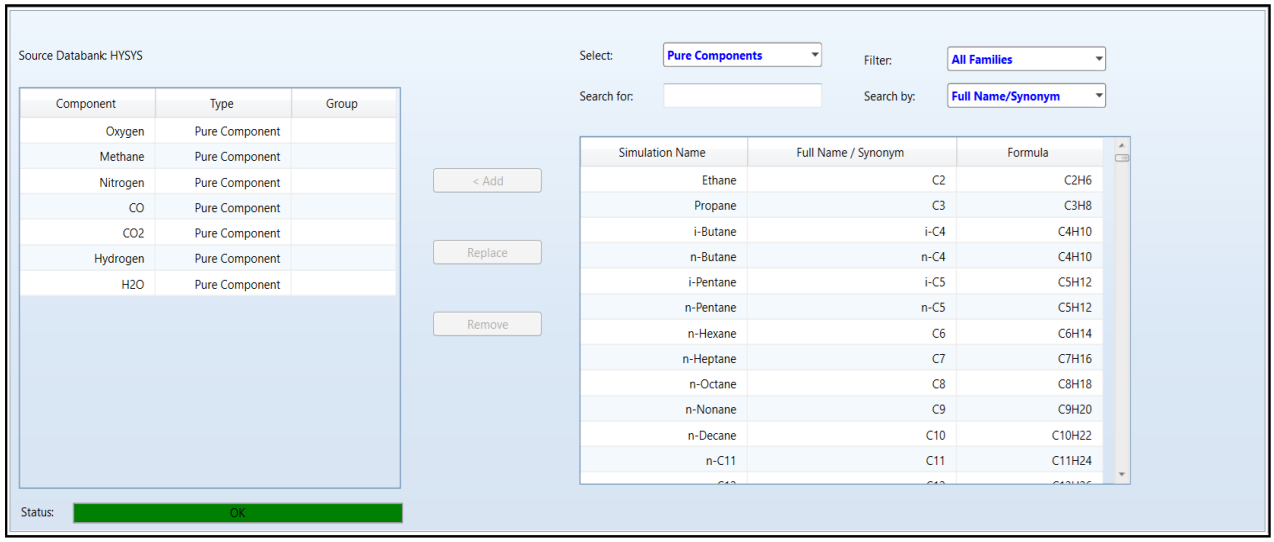
Operating Conditions	Oxygen	Reformer Outlet
Flowrate	82700 kg/hr.	365500 kg/hr.
Temperature	230 C	738 C
Pressure	34barg	31.4barg
Composition		
Methane	-	0.17
CO	-	0.043
CO_2	-	0.058
H_2	-	0.3629
N_2	-	0.0111
H_2O	-	0.3528
O_2	1	-

Here is the reaction:

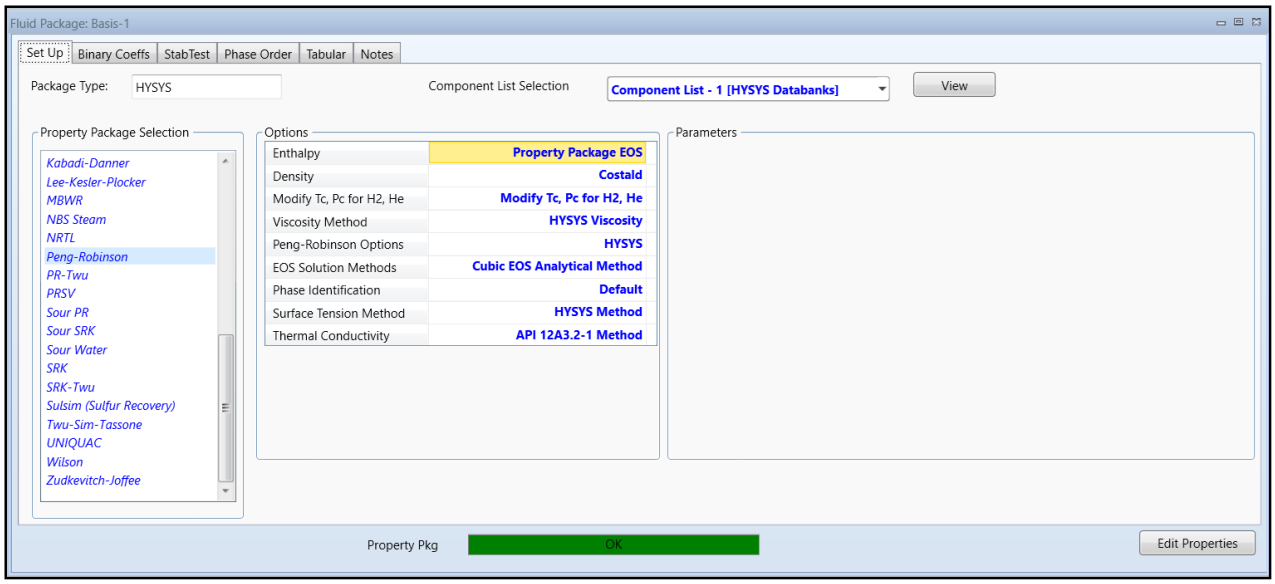
$$1.5\ O_2 + 1\ CH_4 = 1\ CO + H_2O$$

How to simulate:

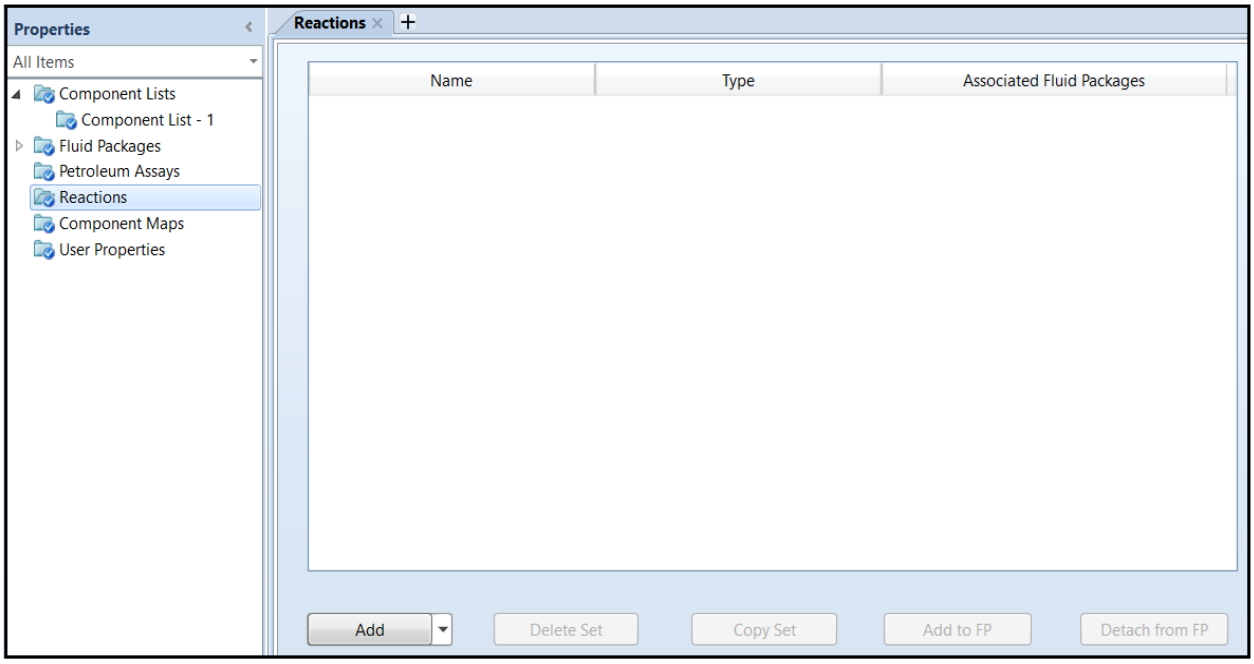
1.Add all components like below to component list.

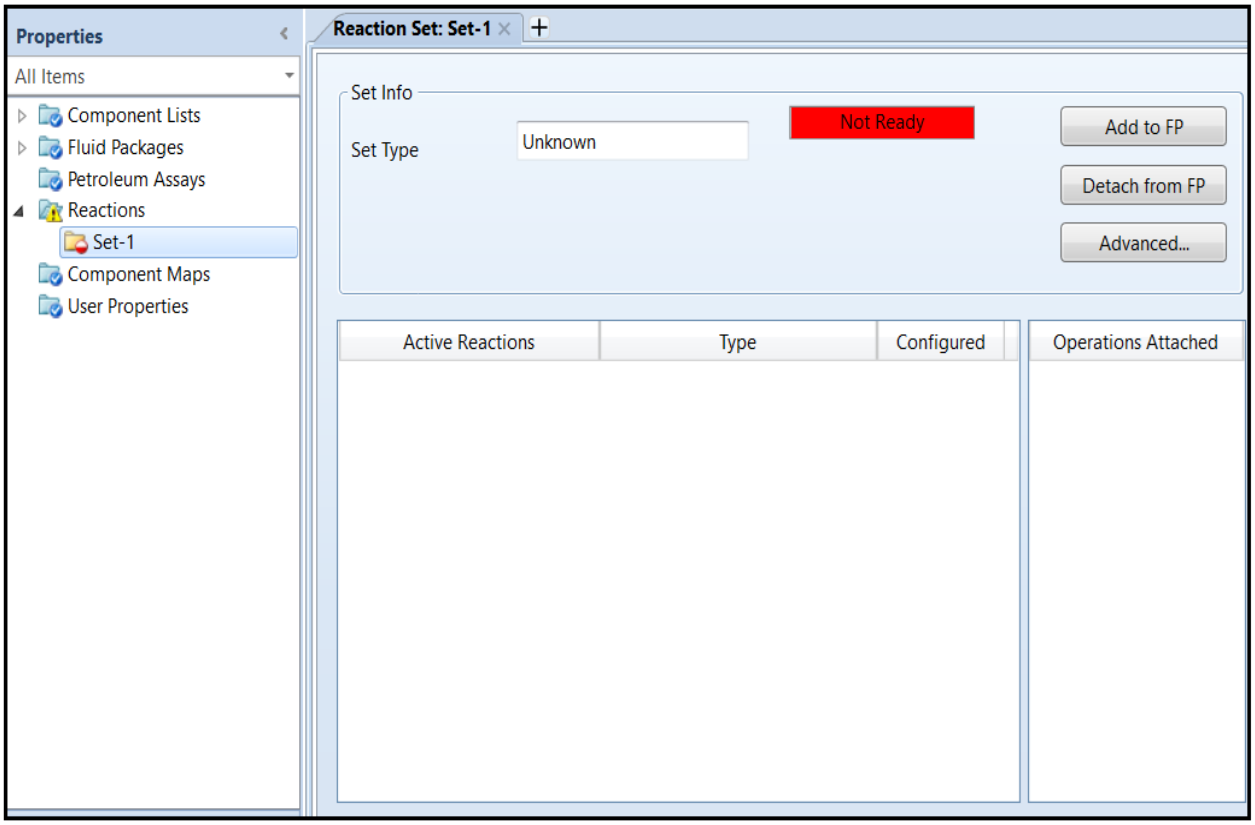


2.Select Peng-Robinson as the Fluid Package.

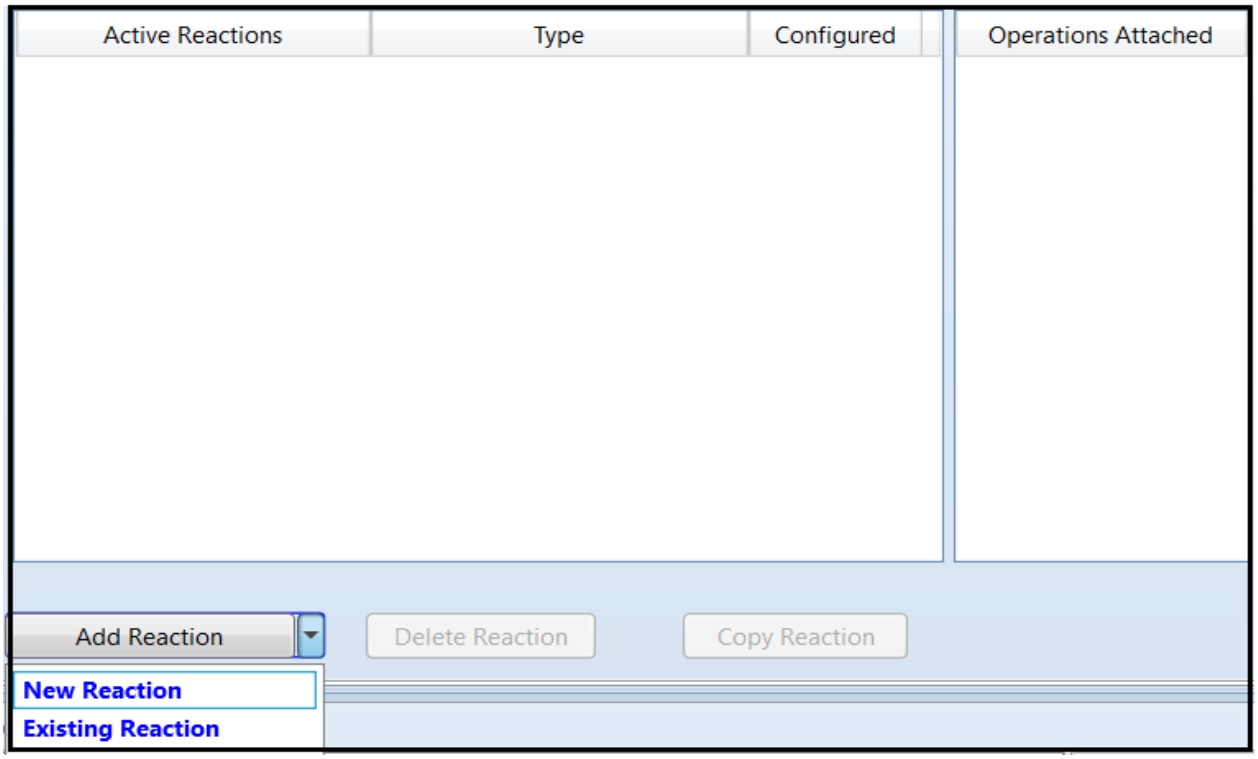


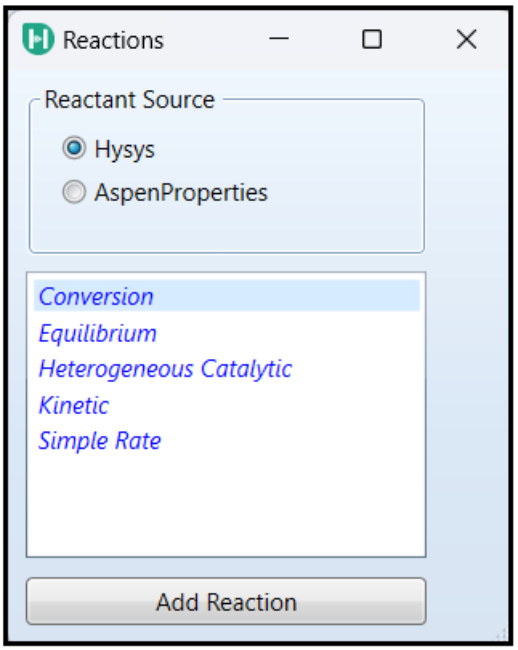
3.Under Properties/Reaction, add a set.

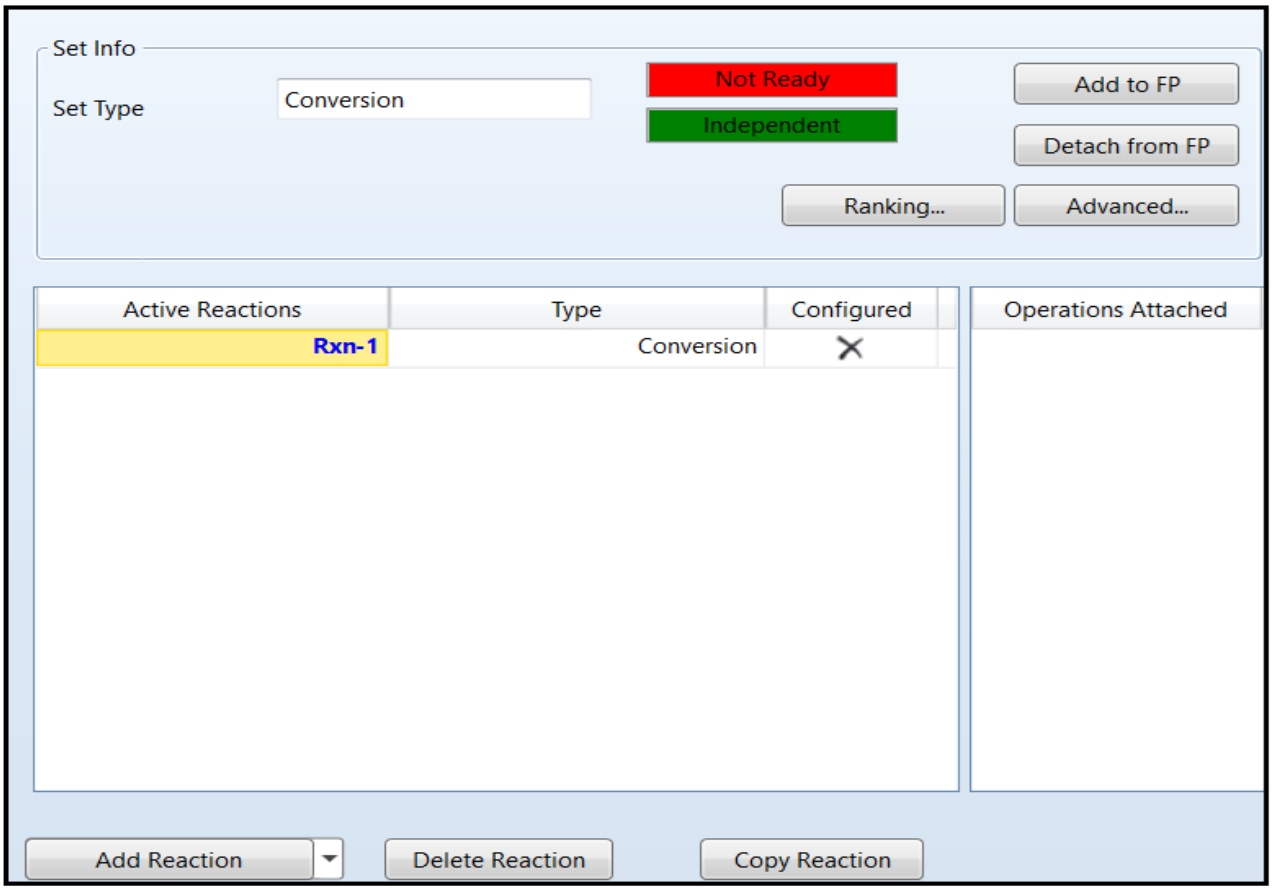

Properties
All Items
Component Lists
Component List - 1
Fluid Packages
Petroleum Assays
Reactions
Component Maps
User Properties
Reactions
Name
Type
Associated Fluid Packages
Add
Delete Set
Copy Set
Add to FP
Detach from FP


Properties
All Items
Component Lists
Fluid Packages
Petroleum Assays
Reactions
Set-1
Component Maps
User Properties
Reaction Set: Set-1
Set Info
Set Type
Unknown
Not Ready
Add to FP
Detach from FP
Advanced...
Active Reactions
Type
Configured
Operations Attached

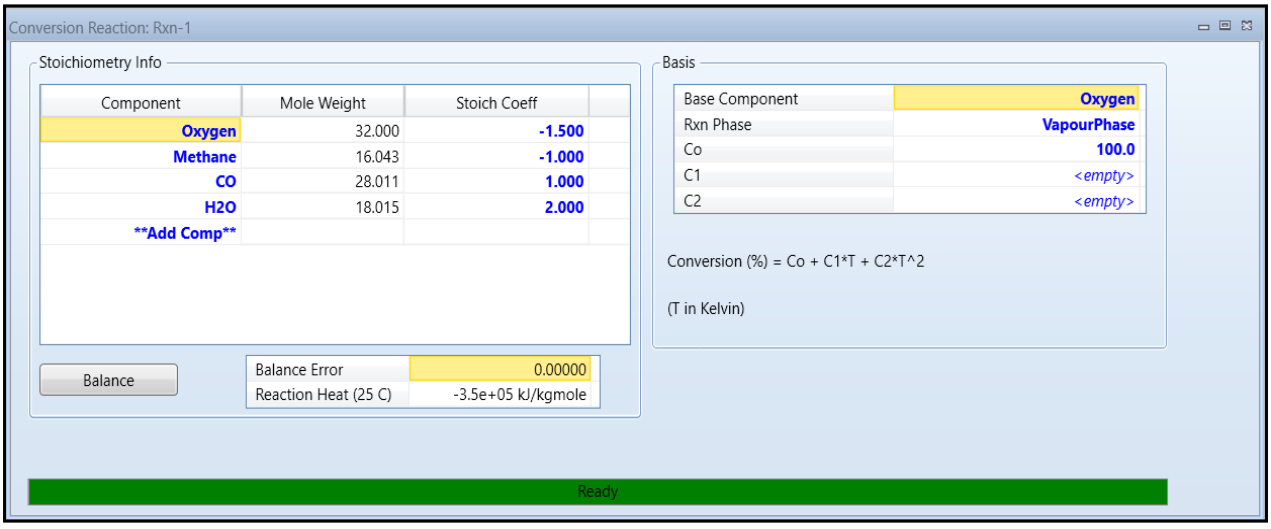
4.Add a new reaction and select conversion.



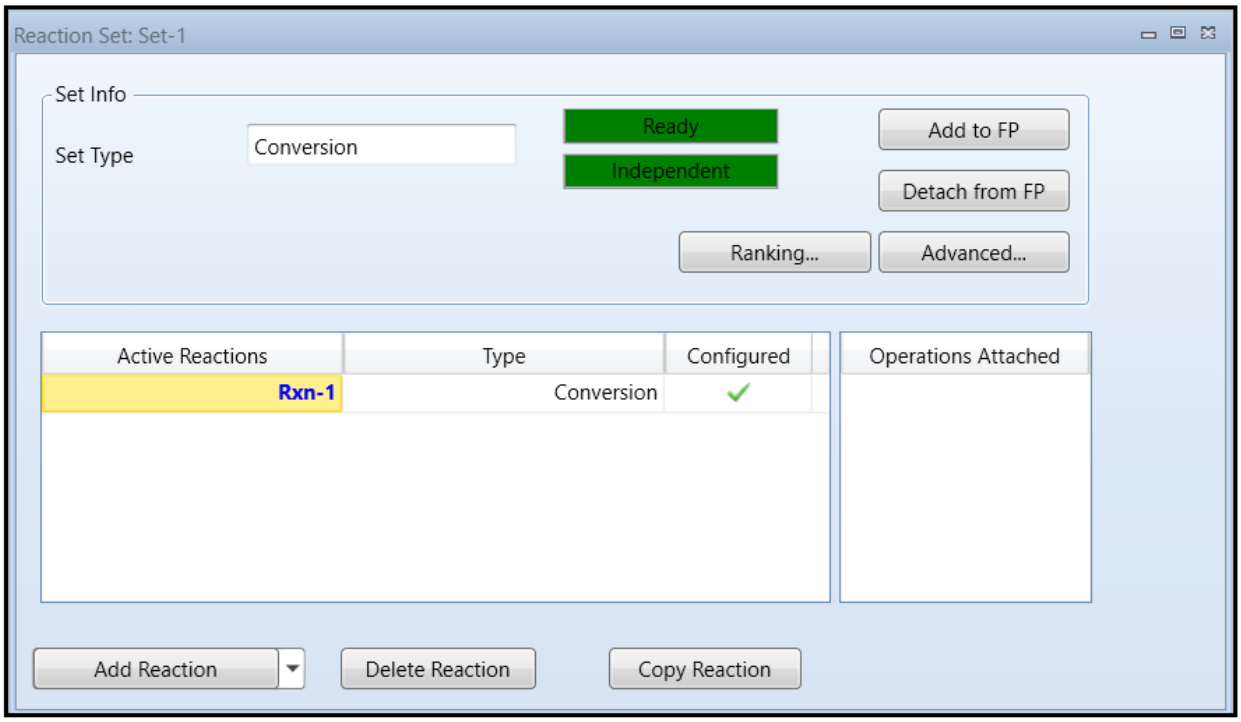


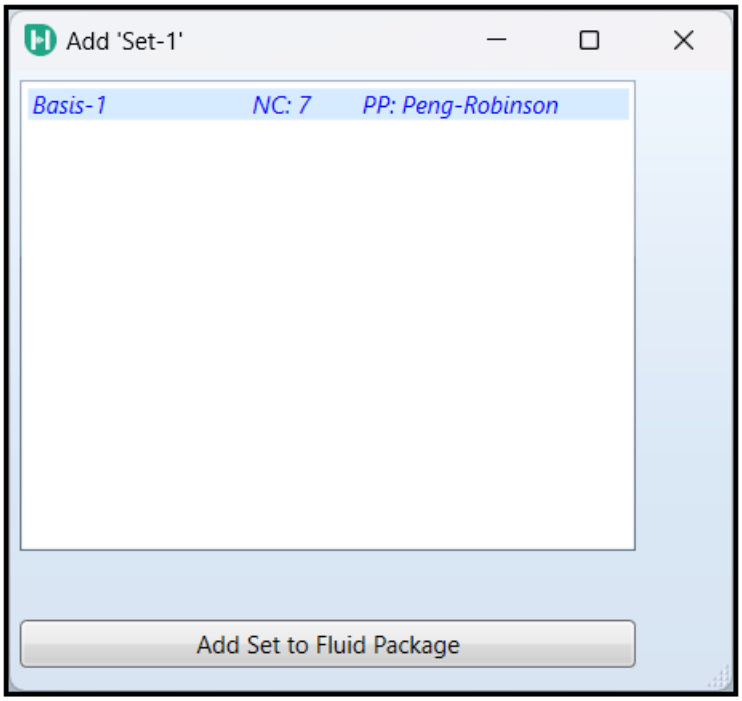


5.Double-click on the Rxn-1 and add reactants and their corresponding coefficients.

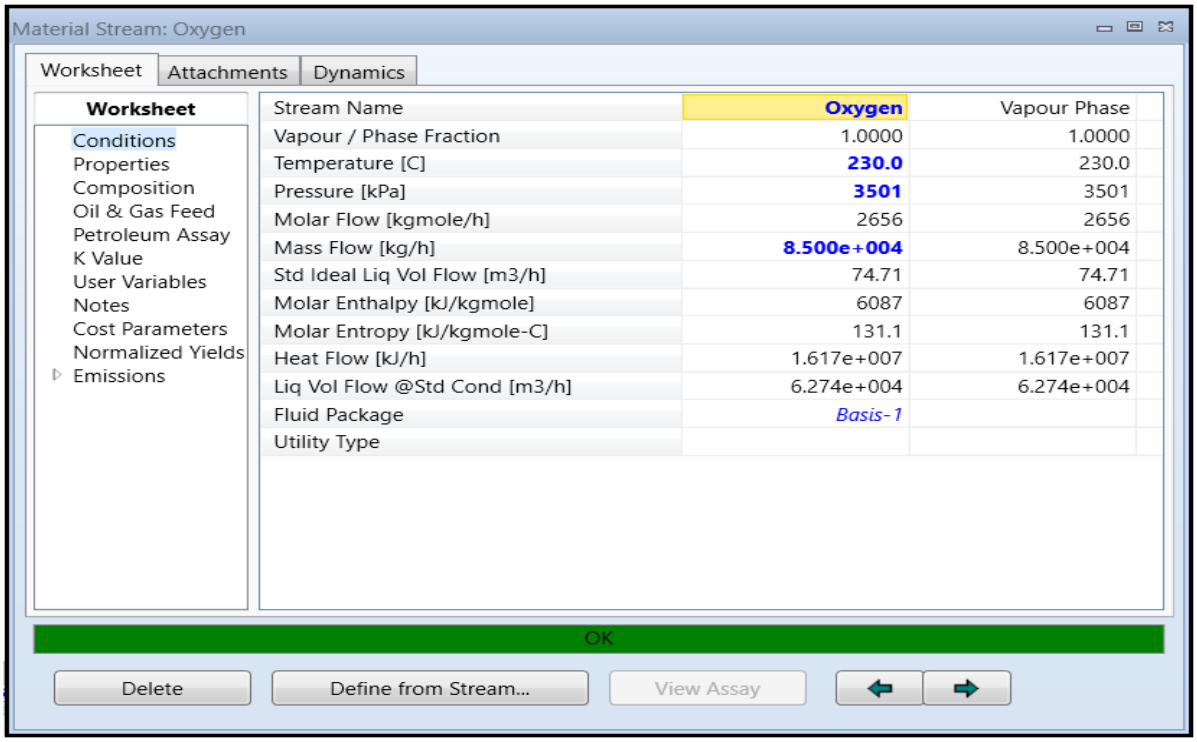


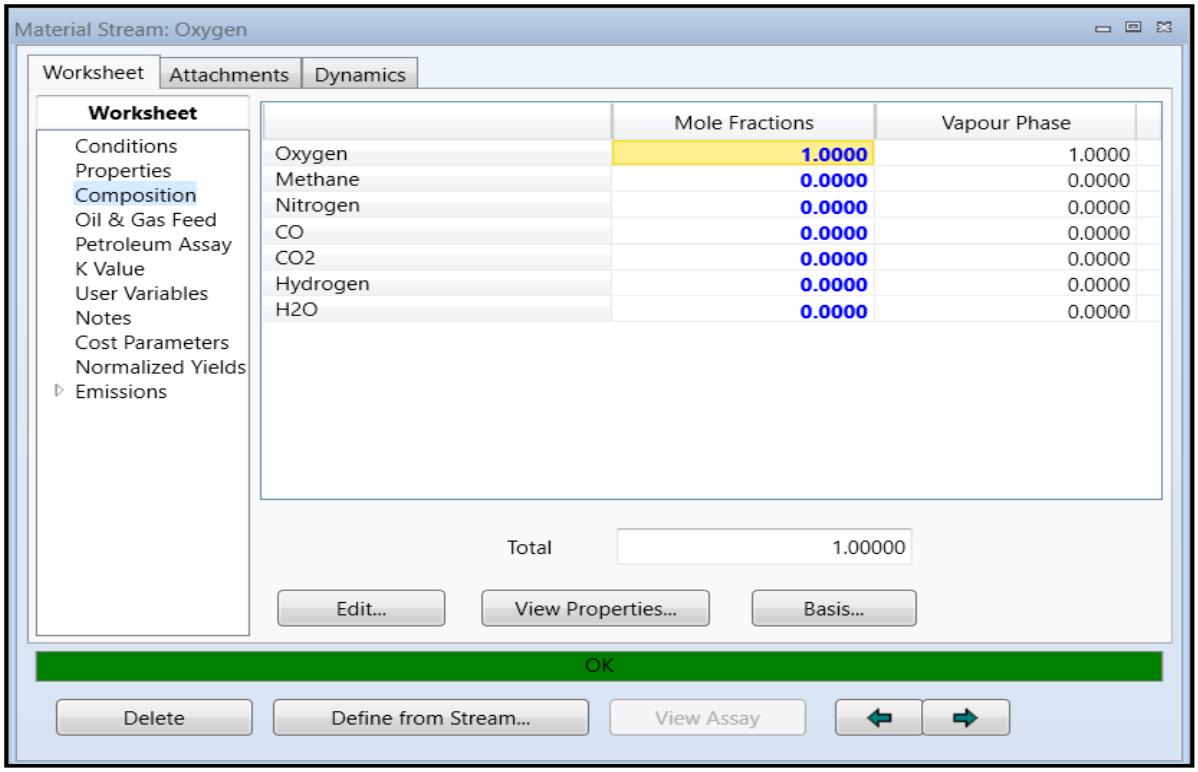
6. Finally add it to FP.

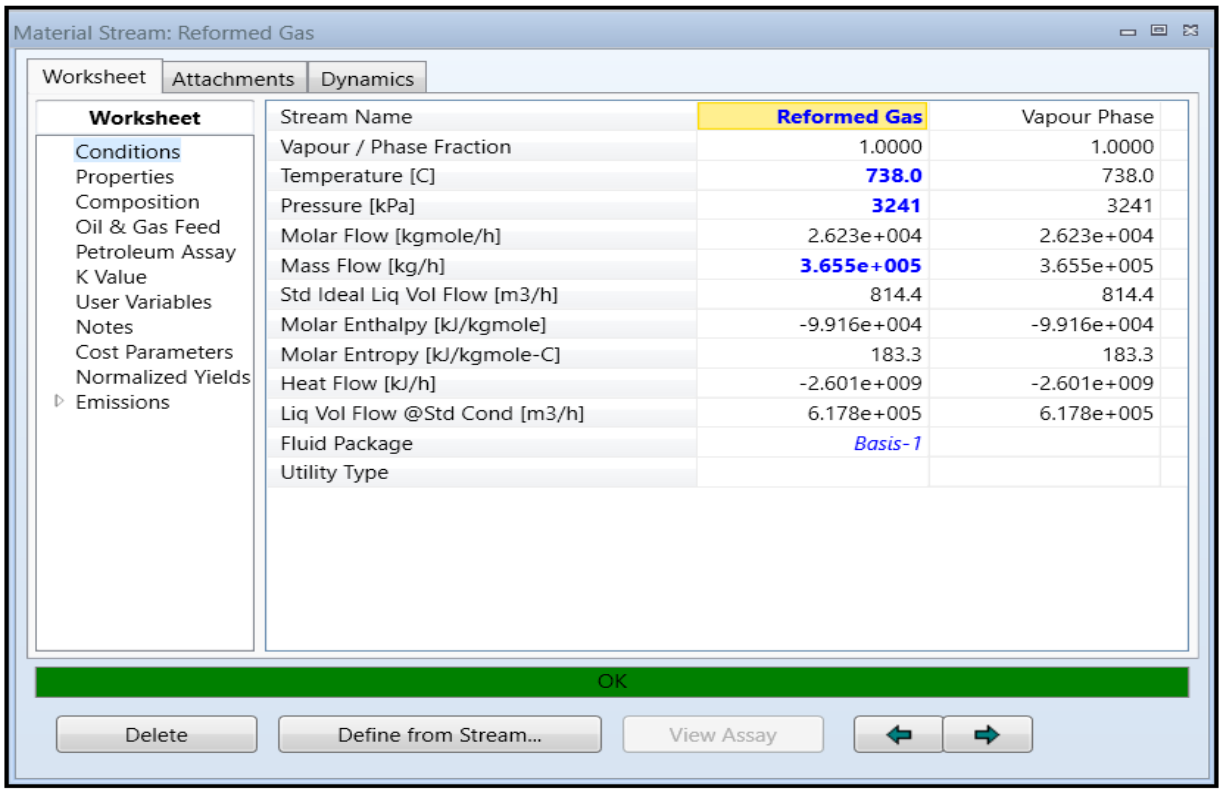


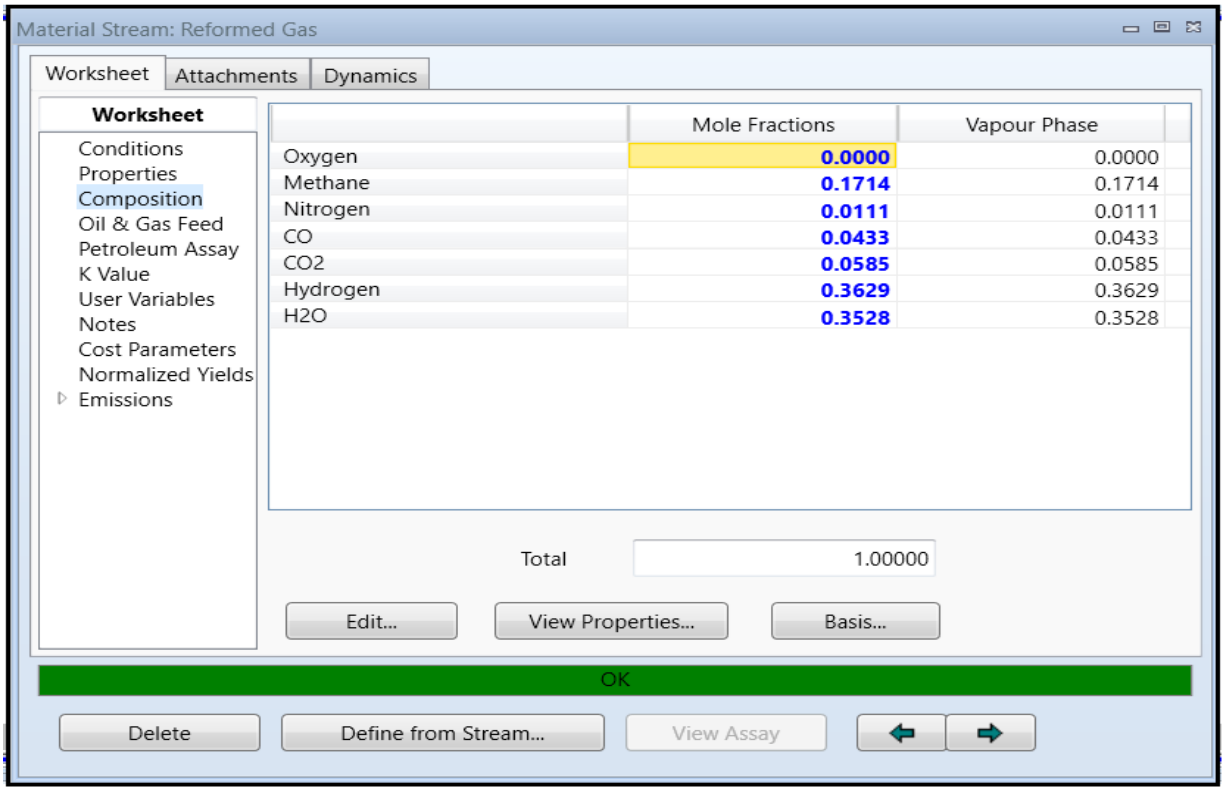


7.Enter Simulation Environment and streams like below:

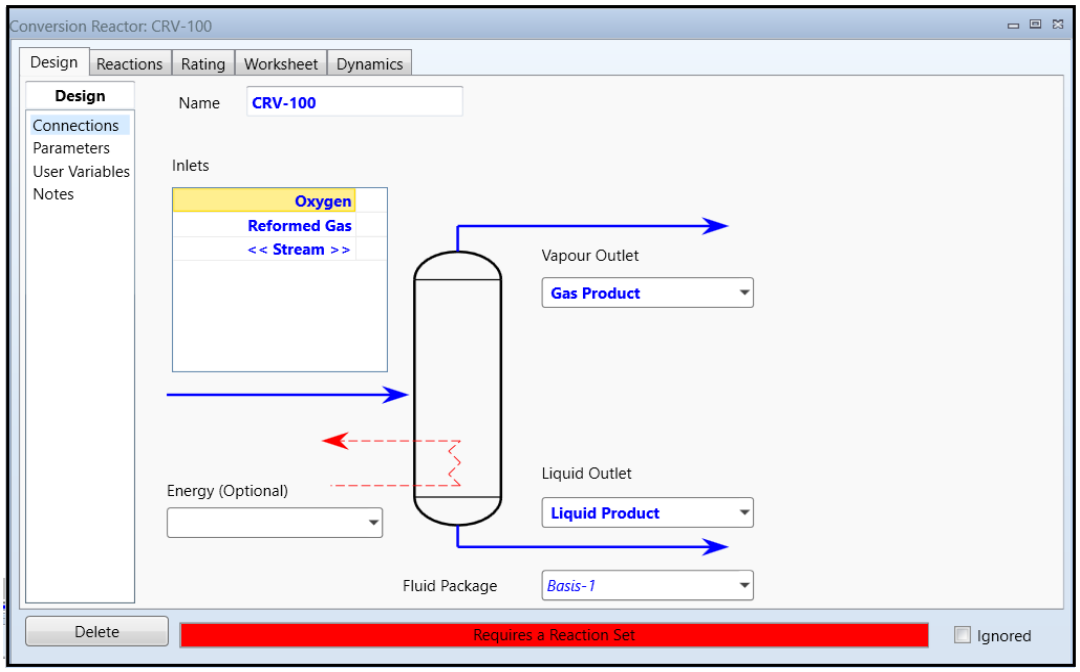




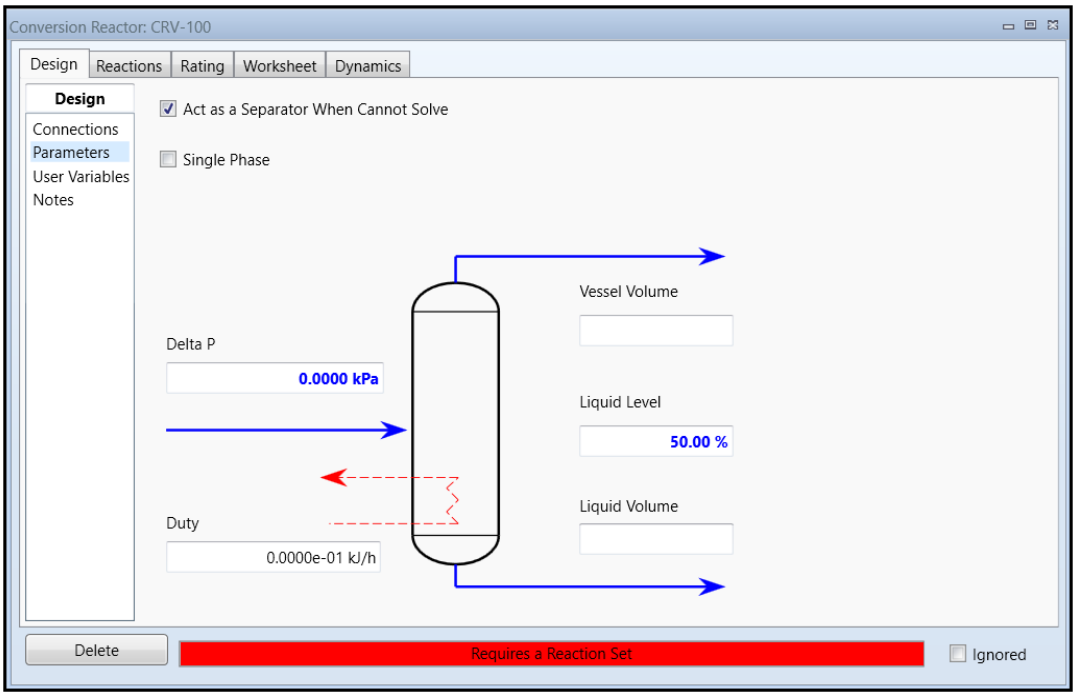

Material Stream: Reformed Gas
Worksheet
Attachments
Dynamics
Worksheet
Conditions
Properties
Composition
Oil & Gas Feed
Petroleum Assay
K Value
User Variables
Notes
Cost Parameters
Normalized Yields
Emissions
Stream Name
Reformed Gas
Vapour Phase
Vapour / Phase Fraction
1.0000
1.0000
Temperature [C]
738.0
738.0
Pressure [kPa]
3241
3241
Molar Flow [kgmole/h]
2.623e+004
2.623e+004
Mass Flow [kg/h]
3.655e+005
3.655e+005
Std Ideal Liq Vol Flow [m3/h]
814.4
814.4
Molar Enthalpy [kJ/kgmole]
-9.916e+004
-9.916e+004
Molar Entropy [kJ/kgmole-C]
183.3
183.3
Heat Flow [kJ/h]
-2.601e+009
-2.601e+009
Liq Vol Flow @Std Cond [m3/h]
6.178e+005
6.178e+005
Fluid Package
Basis-1
Utility Type
OK
Delete
Define from Stream...
View Assay


Material Stream: Reformed Gas
Worksheet
Attachments
Dynamics
Worksheet
Conditions
Properties
Composition
Oil & Gas Feed
Petroleum Assay
K Value
User Variables
Notes
Cost Parameters
Normalized Yields
Emissions
Mole Fractions
Vapour Phase
Oxygen
0.0000
0.0000
Methane
0.1714
0.1714
Nitrogen
0.0111
0.0111
CO
0.0433
0.0433
CO2
0.0585
0.0585
Hydrogen
0.3629
0.3629
H2O
0.3528
0.3528
Total
1.00000
Edit...
View Properties...
Basis...
OK
Delete
Define from Stream...
View Assay

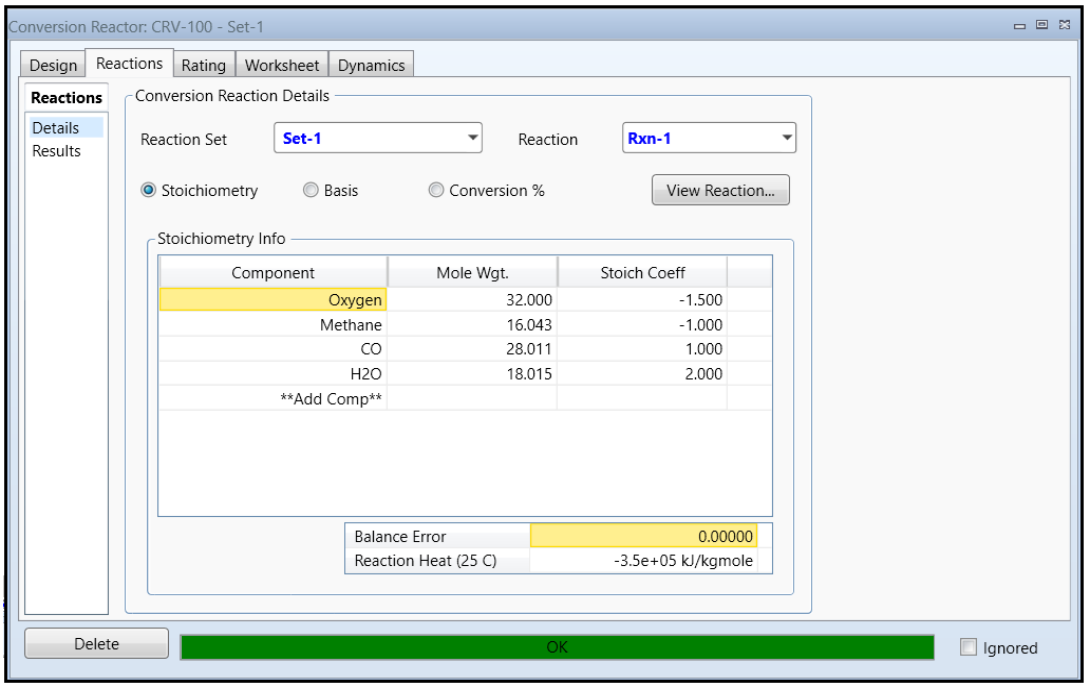
8.Now it is time to set-up the conversion reactor. Select conversion reactor from Model Pallete/Reactors. Select Oxygen and Reformed Gas stream as the inlet and define Gas Product and Liquid Product as the outlet streams.



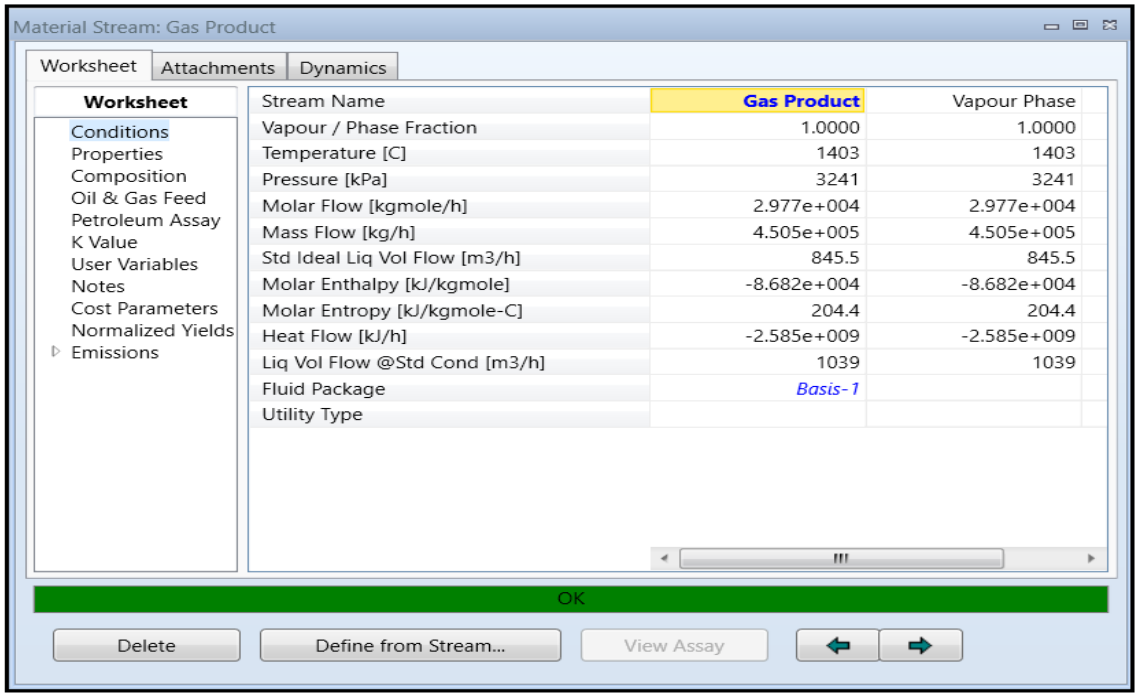
9.Under Design/Parameter sheet, set pressure drop to zero.



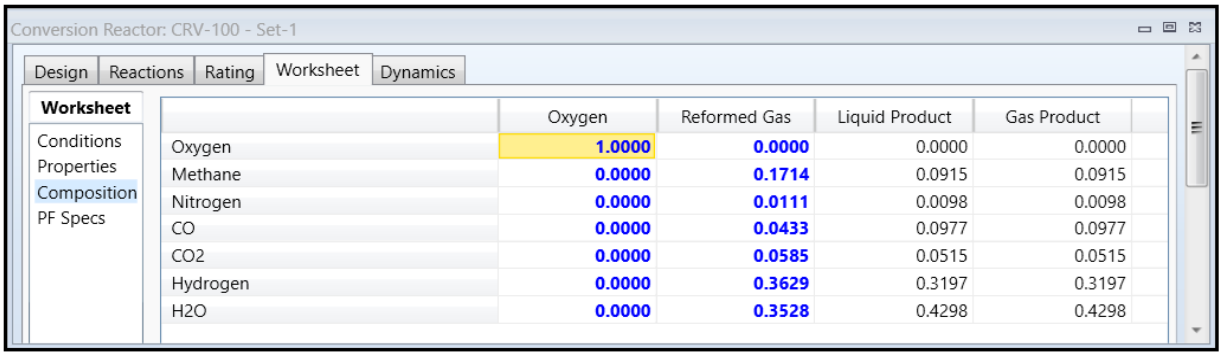
10.Under Reaction tab, select set-1 as the reaction set.



11.Based on the result, the mixture has a temperature of approximately 1400C and a Heat Flow of 2.585×10^9.



Also Under Worksheet tab, you can see changes in composition.



	Oxygen	Reformed Gas	Liquid Product	Gas Product
Oxygen	1.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.1714	0.0915	0.0915
Nitrogen	0.0000	0.0111	0.0098	0.0098
CO	0.0000	0.0433	0.0977	0.0977
CO2	0.0000	0.0585	0.0515	0.0515
Hydrogen	0.0000	0.3629	0.3197	0.3197
H2O	0.0000	0.3528	0.4298	0.4298