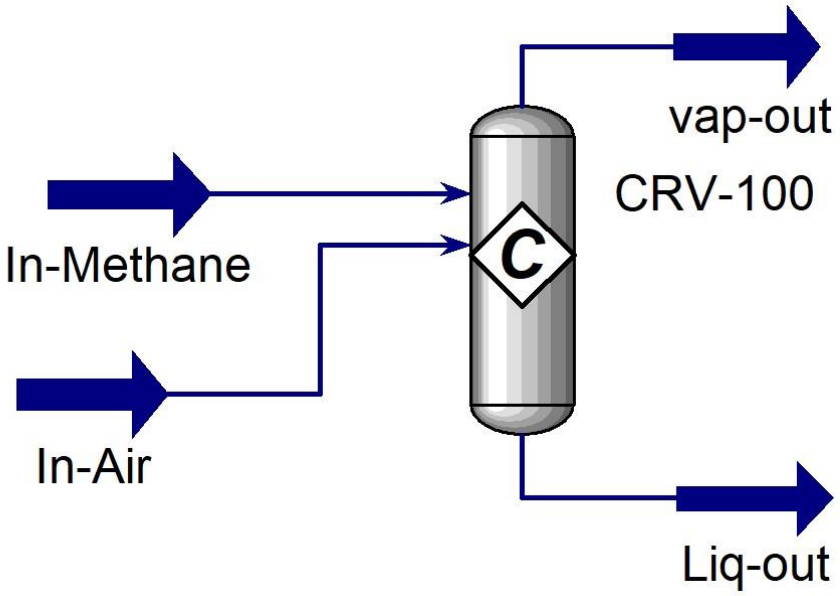
Conversion Reaction Using HYSYS V9

The reaction of methane with air producing hydrogen and carbon oxides is called the partial oxidation. Such kind of processes can be modeled using the conversion reaction in Aspen HYSYS V9. It is possible to perform more than one reaction in one group according to the given rank in order to operate them either sequentially or simultaneously. In this subject, it is intended to learn how to add and work with the reactors including setting up the reactions as well as giving the stoichiometry and the conversion of the basis reactant.



The figure above shows a simple model of the conversion reactor with its inlet, outlet streams using Aspen HYSYS V.9.

Example:

Hydrogyn production from hydrocarbon is an enabling technology. The fuel is converted to hydrogyn by the partial oxidation. The reaction of Methane with air producing the carbon oxides and the hydrogyn is an example of the partial oxidation.

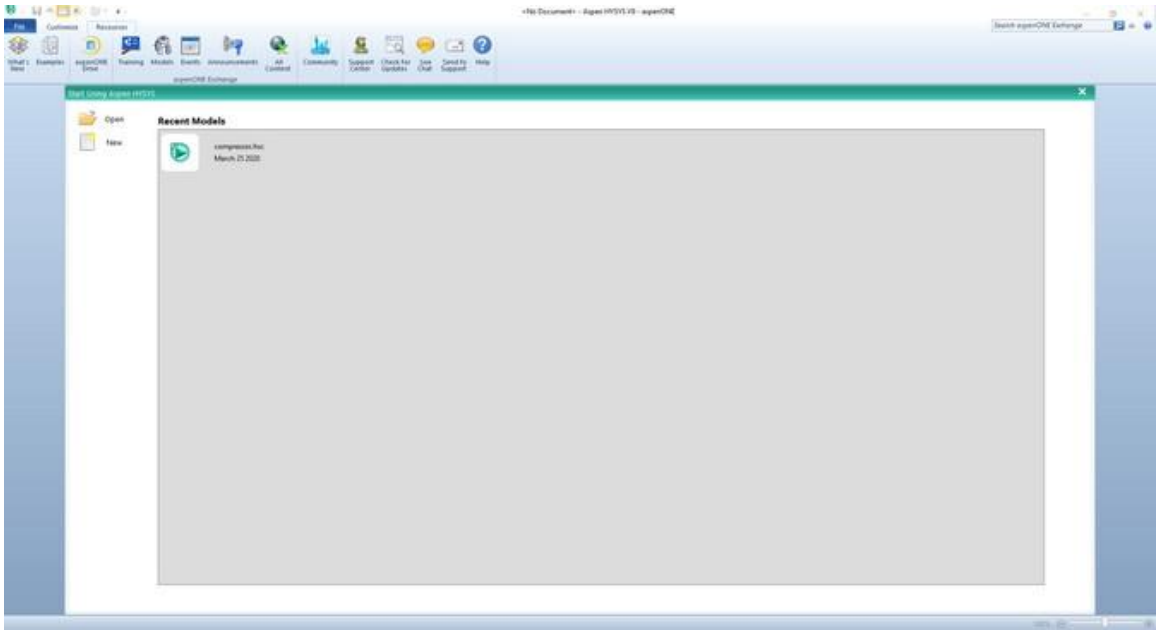
$$CH_4 + {}^1/_2\, O_2 \rightarrow CO + 2H_2$$

$$CH_4 + O_2 \rightarrow CO_2 + 2H_2$$

Model the partial oxidation of methane to produce hydrogyn [1].

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



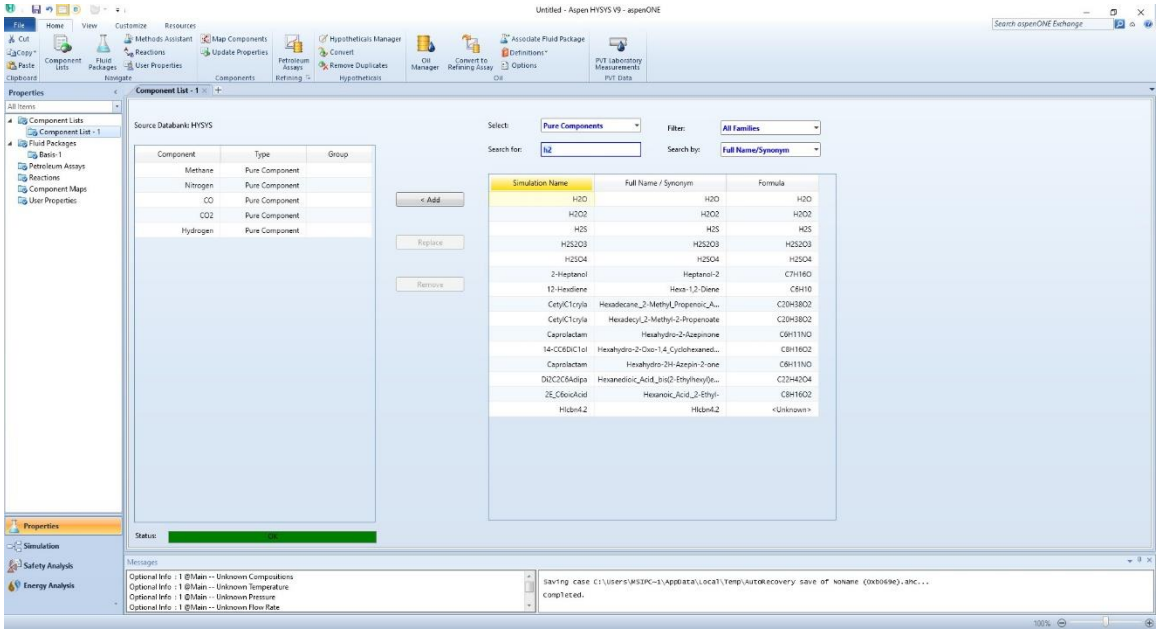
The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.

- Create a new case:

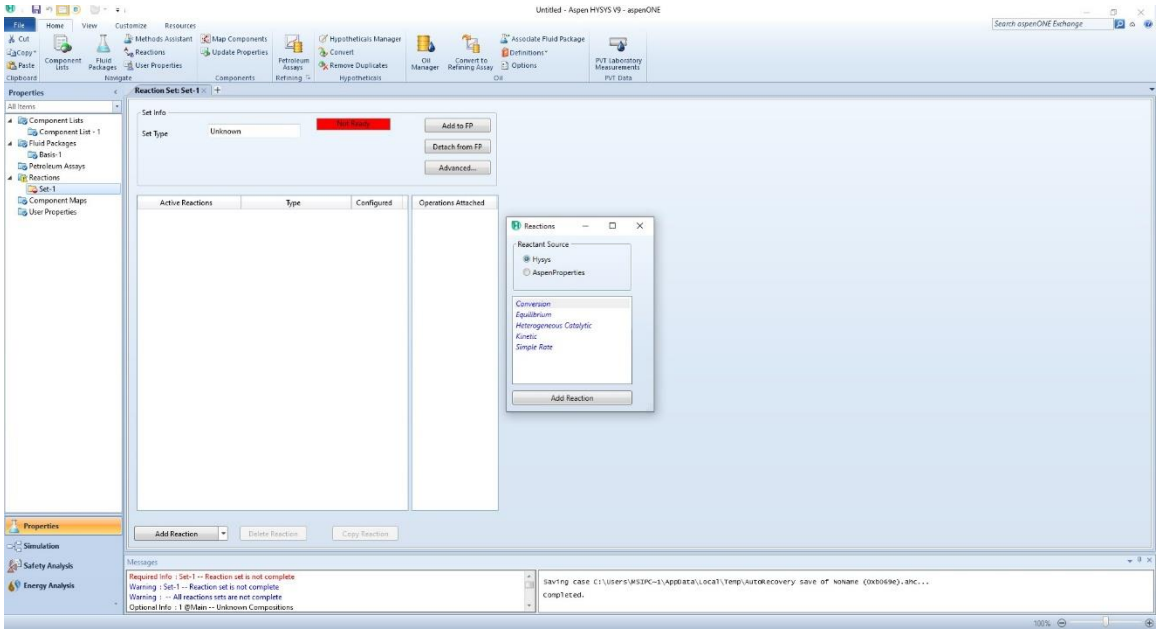
1. File menu
2. New \ case

- There are two main necessary information have to be given in the properties tab before starting the simulation:
    1. Property package : Peng-Robinson
    2. Components: CH_4, O_2, N_2 , CO, CO_2, H_2

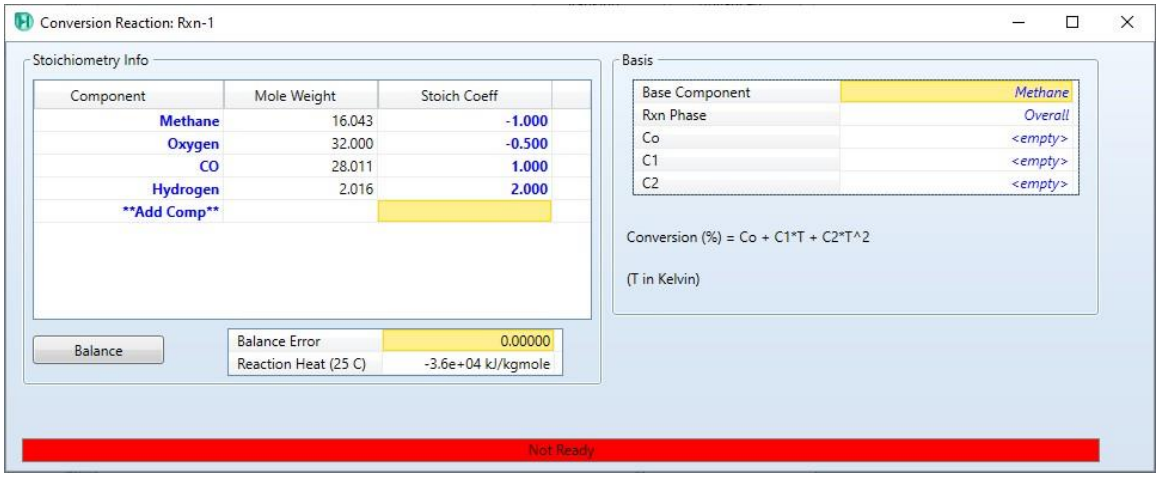
1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the serach field Ch_4
5. Select Ch_4 \ add
6. Repeat the steps (4,5) for N_2 , CO, CO_2, O_2 and H_2



- Add fluid package:
  1. Select Fluid package
  2. Click Add
  3. Select (Peng-Robinson)
- Adding reactions
  1. Properties \ Reactions \ add
  2. Add Reaction \ conversion \ Add reaction

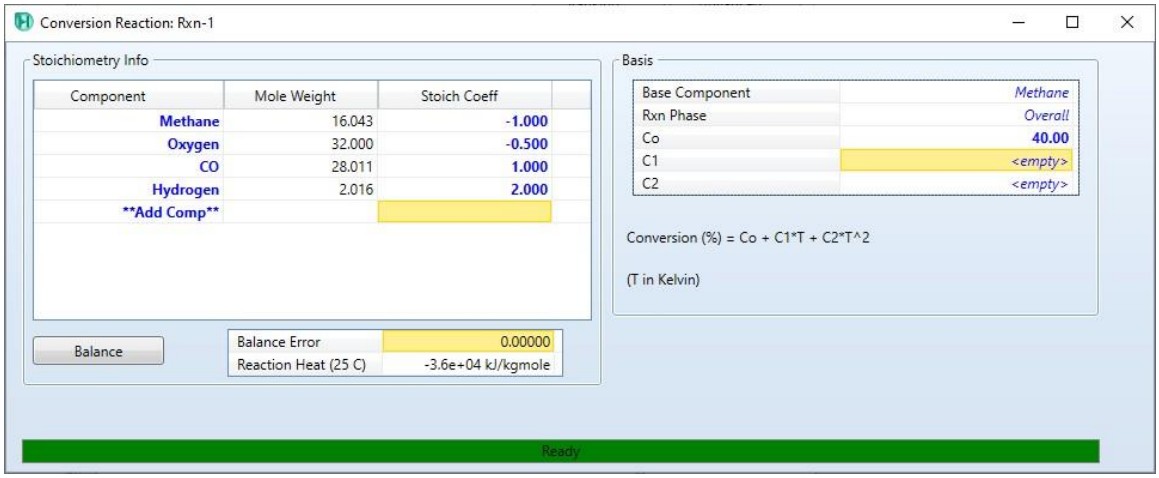


3. Double click on the added (Rxn-1)
4. Enter the related information according to what are given in the example.

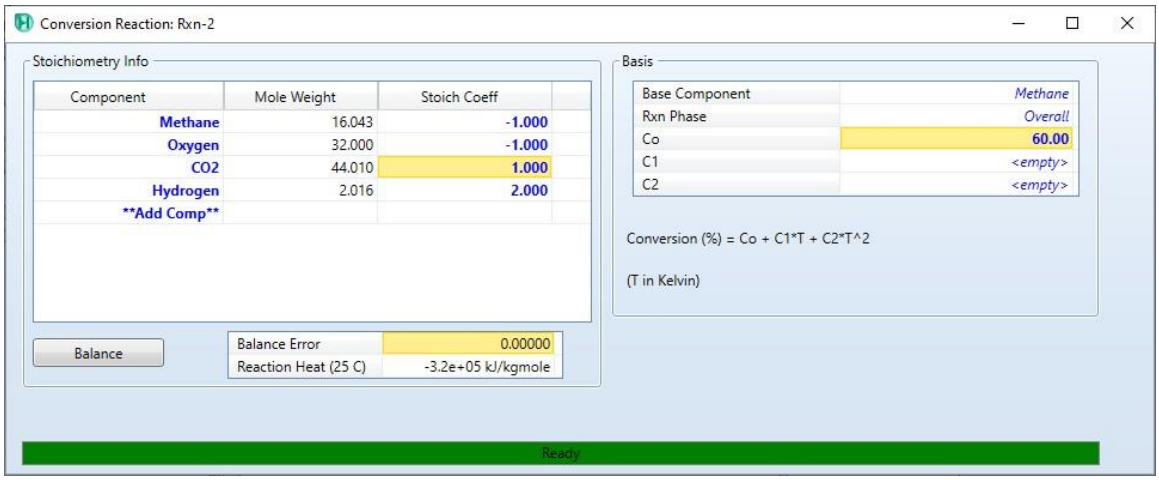


5. Basis

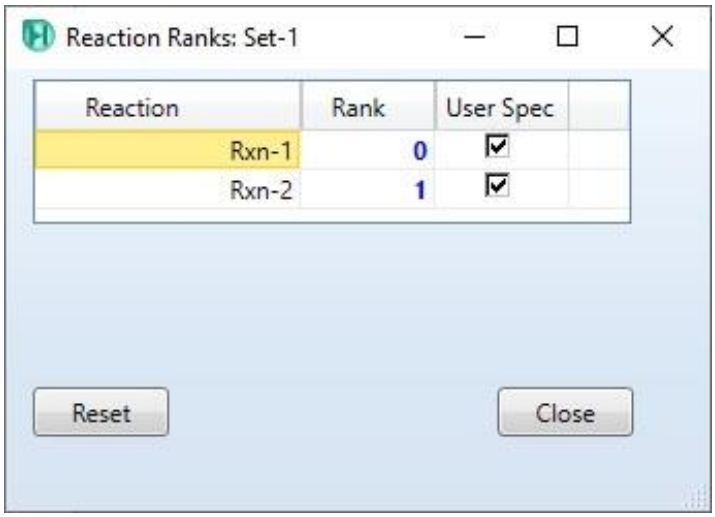
6. Enter the information as shown below:



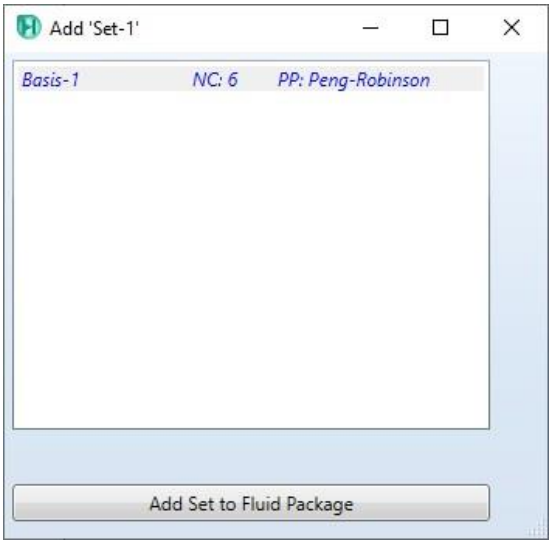
7. Enter the below information regarding the second reaction:



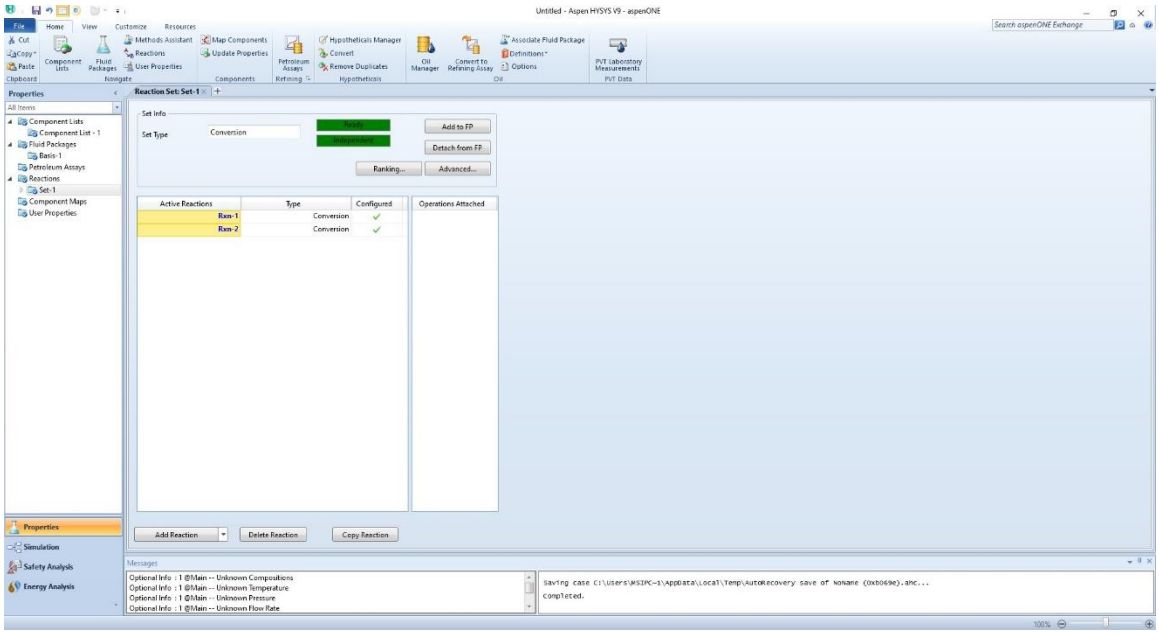
8. Click on Ranking and make the sequential as shown below:



- Attach the reaction set to a fluid package:
  1. Click (Add to FP)
  2. Select the desired fluid package
  3. Click (Add Set to fluid package)



Now we are ready to enter the simulation environment.



- Create new material stream:
  1. Select simulation.
  2. Object palette.
  3. Select the material stream icon.

Alternatively, you can add new material stream by pressing F11.

4. Double click on the added material stream
5. Give the below information:

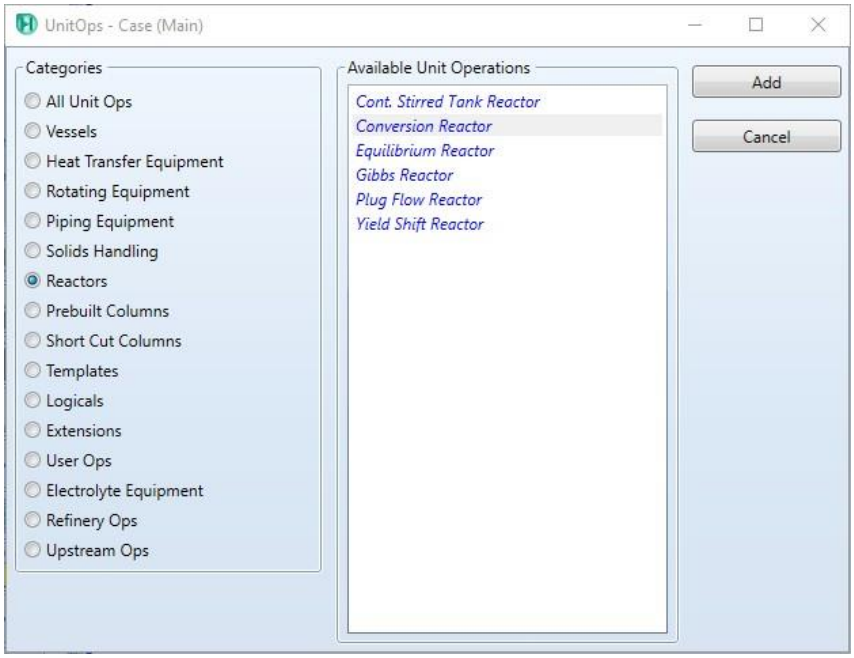
Name	In-Methane
Conditions	
Temperature	20^{O} C
Pressure	3 bar
Molar flow	100 kgmole/h
Composition	
C1	1

1. Add second material stream:

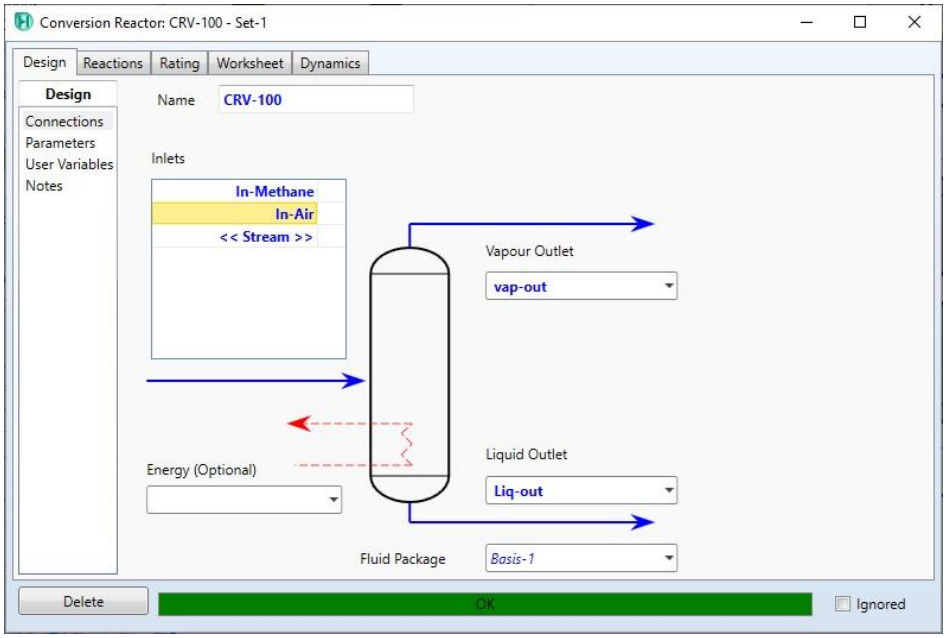
Name	In-Air
Conditions	
Temperature	20^{O} C
Pressure	3 bar
Molar flow	250 kgmole/h
Composition	
N_2	0.79
O_2	0.21

The above information should be given according to the application or example.

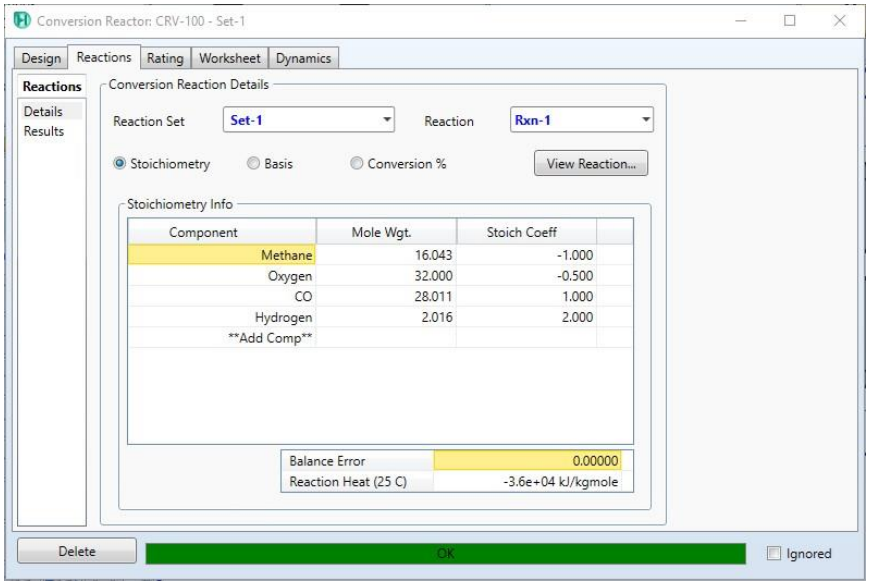
- Adding Conversion reactor:
    1. Press F12
    2. Select reactors
    3. Select conversion reactor
    4. Click (Add)



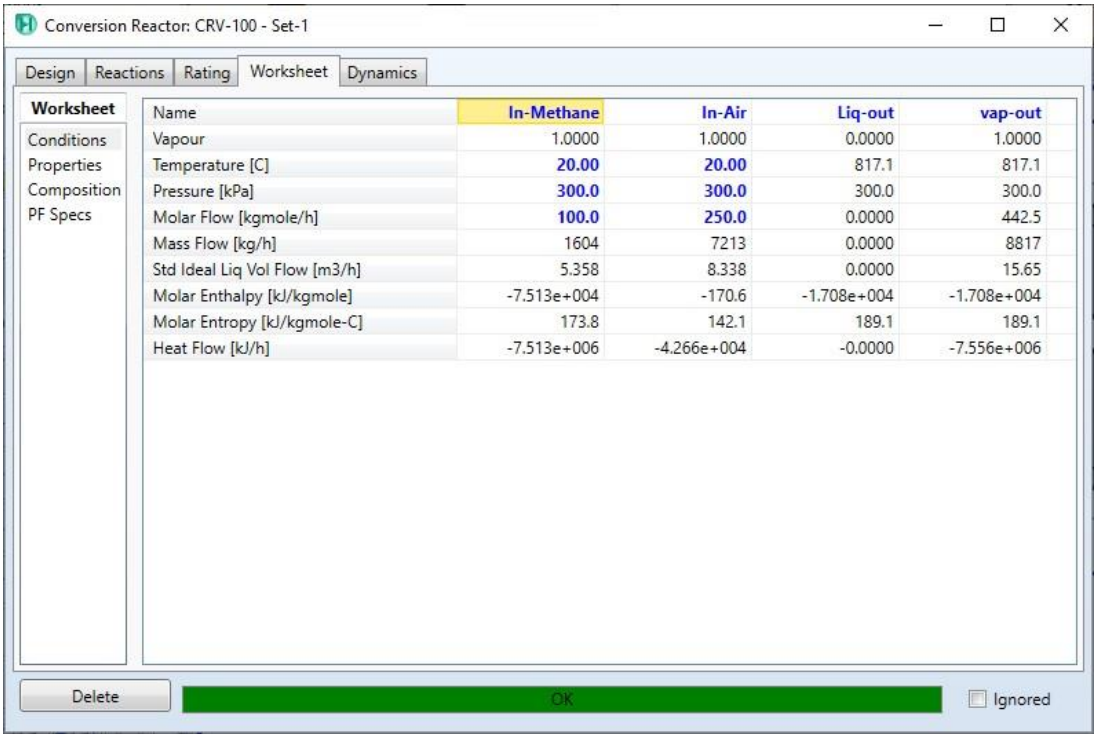
5. Place the selected unit in the desired position.
6. Double click on the added conversion reaction.
7. Design \ Connection
8. In the Inlets field select (In-Methane, In-Air)
9. In the field of Vapour outlet type (Vap-out) [a new material stream will be created and connected to the reactor]
10. In the field of Liquid outlet type (Liq-out) [a new material stream will be created and connected to the reactor]

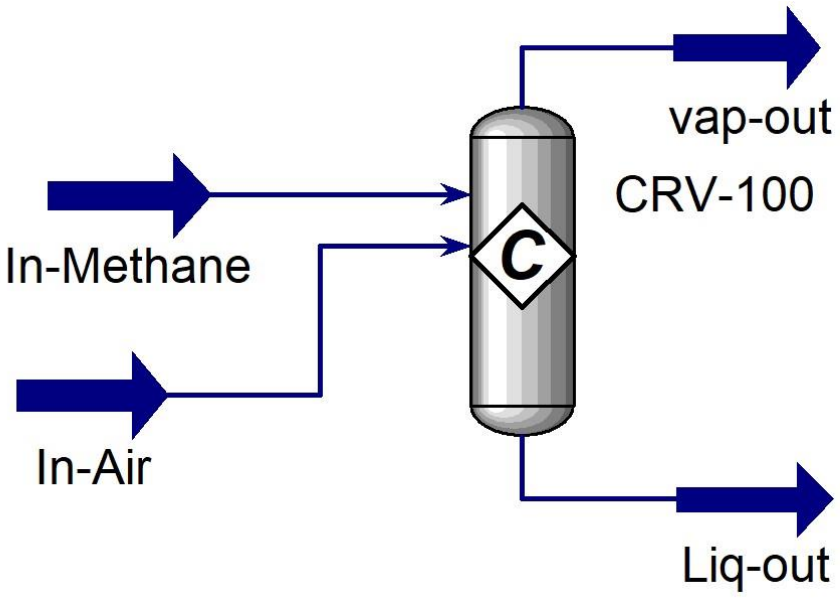


11. Reactions \ Reaction set
12. Select (Set-1)



13. Select Worksheet.
14. Read the desired results and compositions.
15. Select Reactions
16. Select the reaction (Rxn-2).
17. Repeat the steps (13,14).





- Save the case:

1. File menu
2. Select save as
3. Give the name (Conversion Reaction)

References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Equation Of State in HYSYS V9

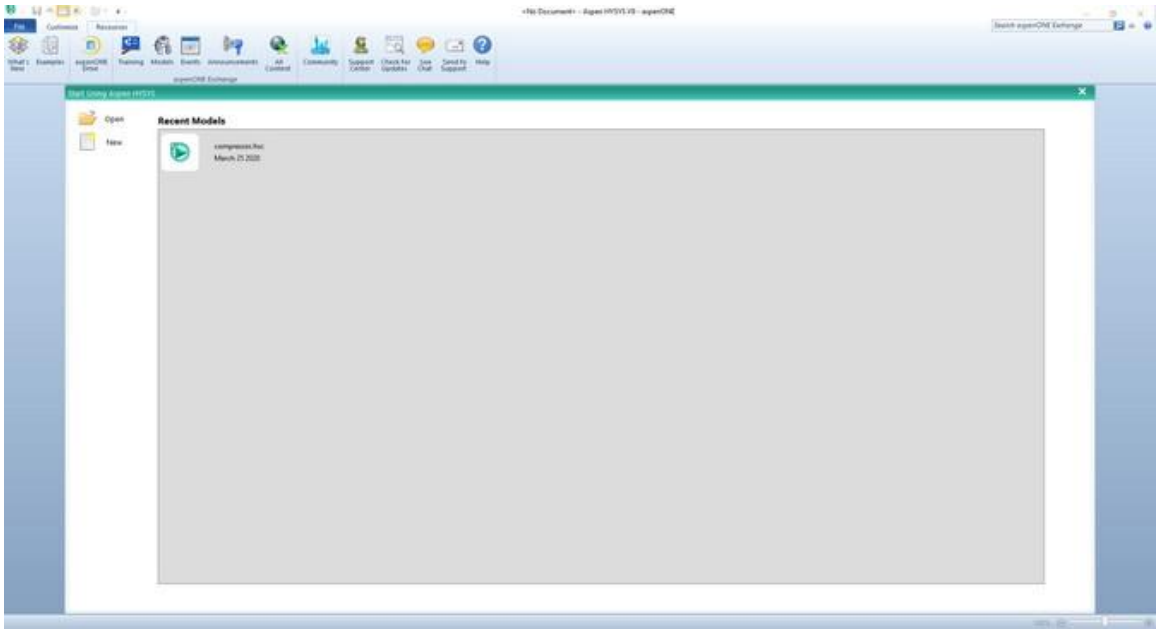
It is possible to find the molar volume of a mixture of material using an equation of state. Aspen HYSYS V9 give an access to several packages like Peng-Robinson (PR) equation of state which can fit with various operation processes. In this subject, it is intended to learn how to determine the specific volume of a mixture of materials at the given conditions and analyze a certain property with a range of independent values using Case Study utility in HYSYS V9.

Example:

A material stream of i-pentane with flow rate of 100kgmole\h. What is the molar volume at 300 K and 25 atm (use equation of state of Peng – Robinson) [1].

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



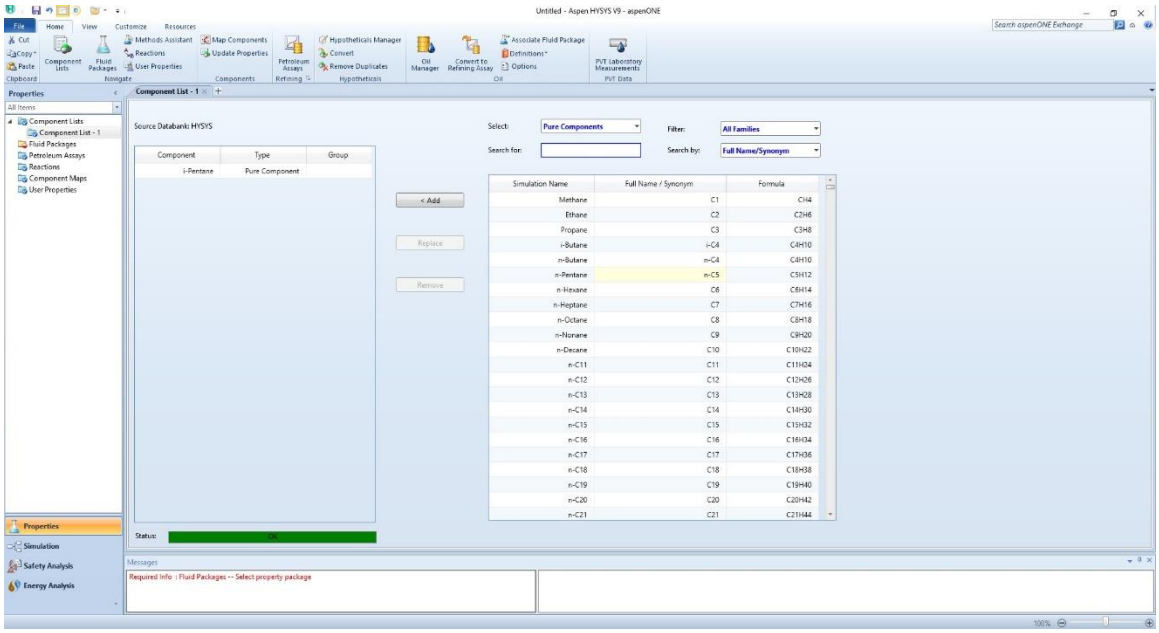
The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.

- Create a new case:

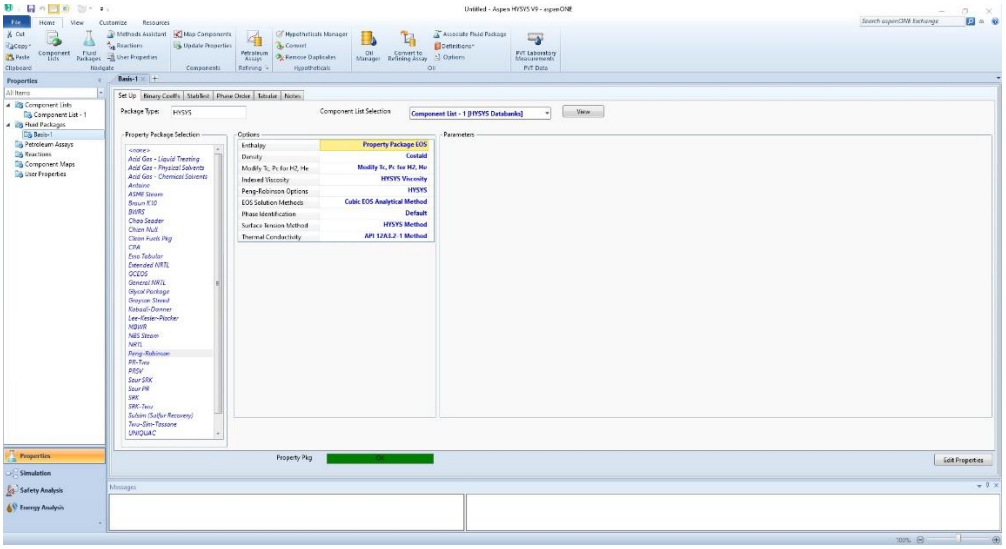
1. File menu
2. New \ case

- There are two main necessary information have to be given in the properties tab before starting the simulation:
    1. Property package : Peng-Robinson
    2. Components: i-pentane

1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the serach field i-pentane



- Add fluid package:
  1. Select Fluid package
  2. Click Add
  3. Select (Peng-Robinson)



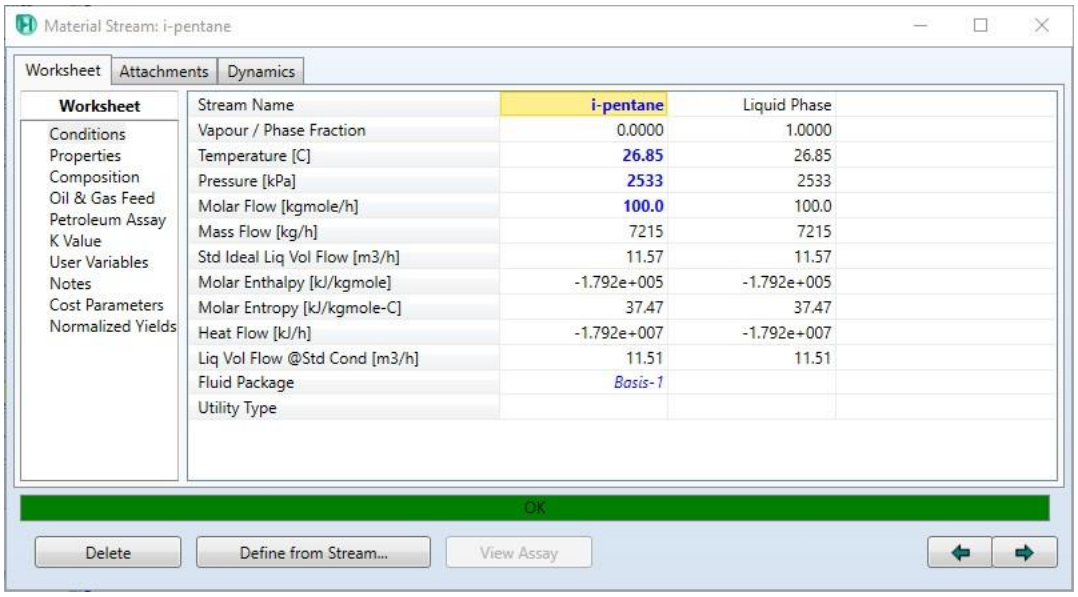
- Create new material stream:
  1. Select simulation.
  2. Object palette.
  3. Select the material stream icon.

Alternatively, you can add new material stream by pressing F11.

4. Double click on the added material stream
5. Give the below information:

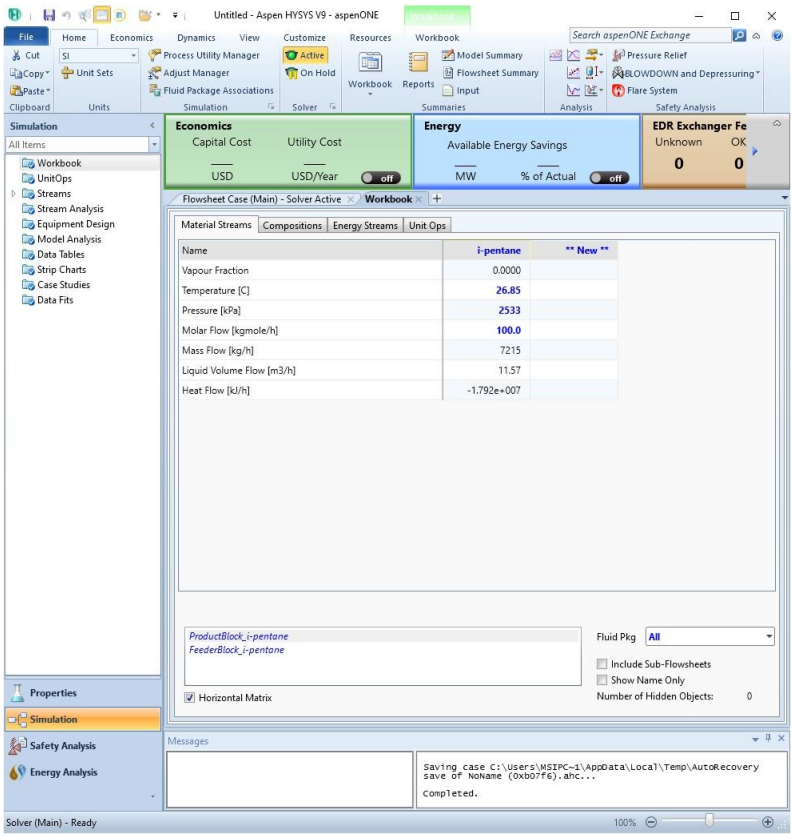
Name	i-pentane
Conditions	
Temperature	300 k
Pressure	25 atm
Molar flow	100 kgmole/h
Composition	
i-pentane	1

The above information should be given according to the application or example.



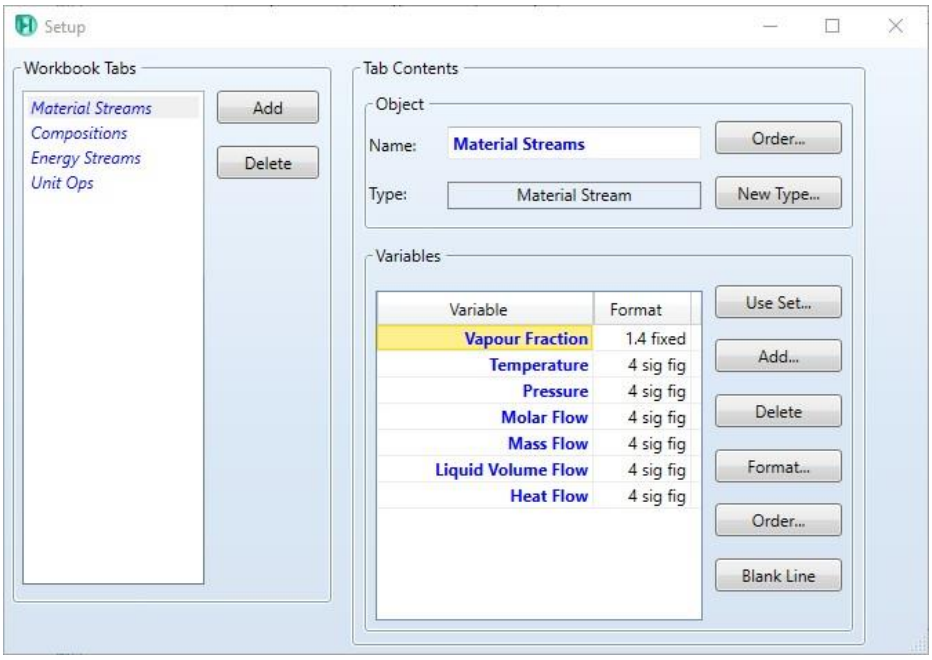
- Working with Workbook:
    1. From the Home toolbar, click on workbook

Alternatively, press Ctrl+w

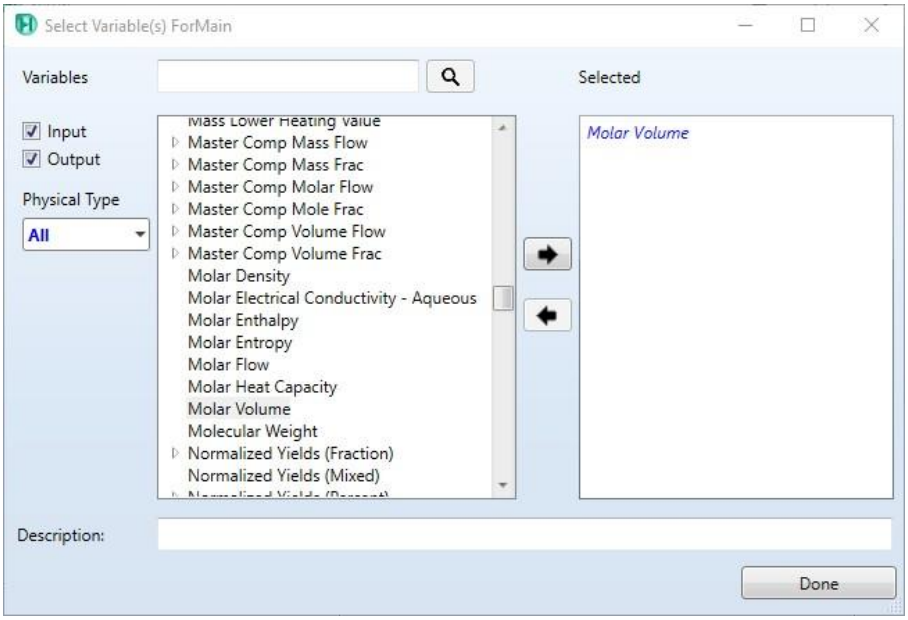


There is no molar volume in the workbook.

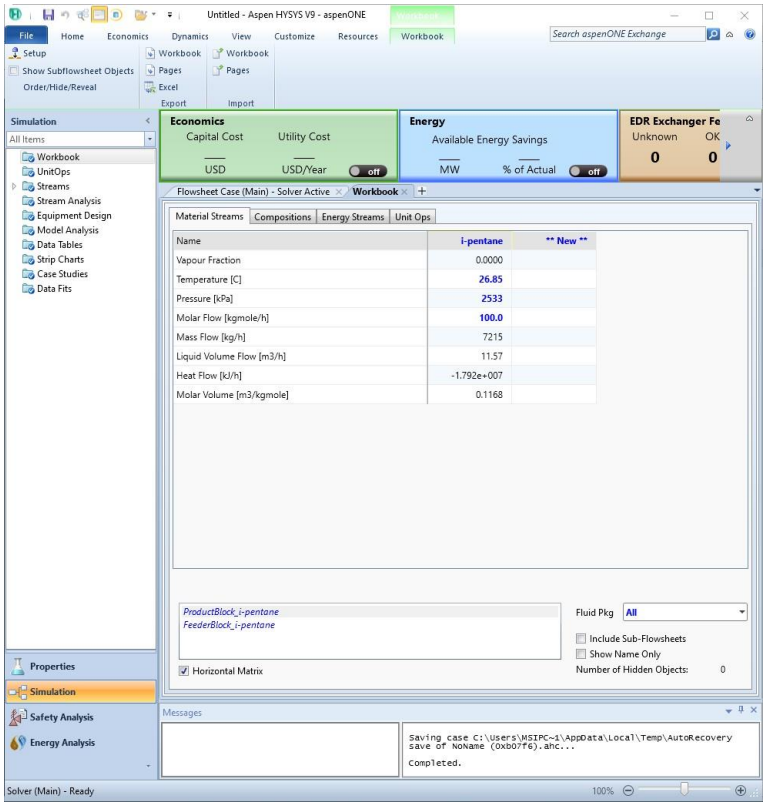
2. From the workbook toolbar, click on Setup



3. Highlight Material streams
4. Variables \ Add
5. Select Molar volume \ Add \ Done



6. Close the setup window.
7. Read the Molar volume



- Save the case:

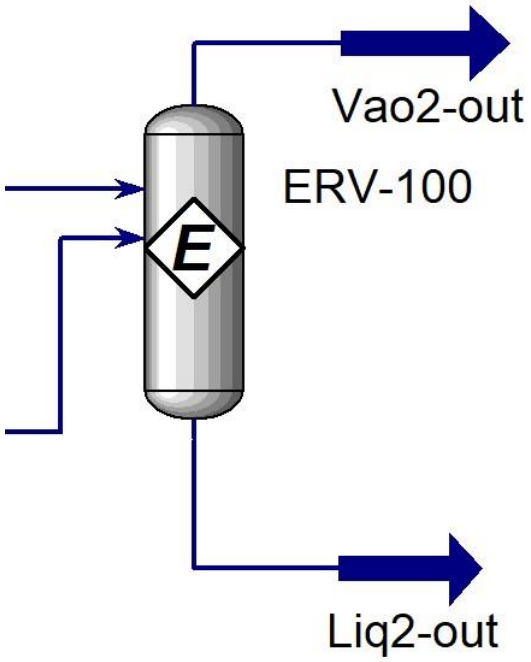
1. File menu
2. Select save as
3. Give the name (equation of State)

References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Equilibrium Reaction Using HYSYS V9

The Water gas shift reaction increases the H2 and decrease the CO concentrations. Such kind of processes can be modeled using equilibrium reactors in HYSYS V9. It is possible to perform more than one equilibrium reaction in one group according to the given rank to operate them either sequentially or simultaneously. In this subject, it is intended to learn how to add and work with the equilibrium..



The figure above shows a simple model of the Eqiulibirium reactor with its inlet and outlet streams using Aspen HYSYS V.9.

Example:

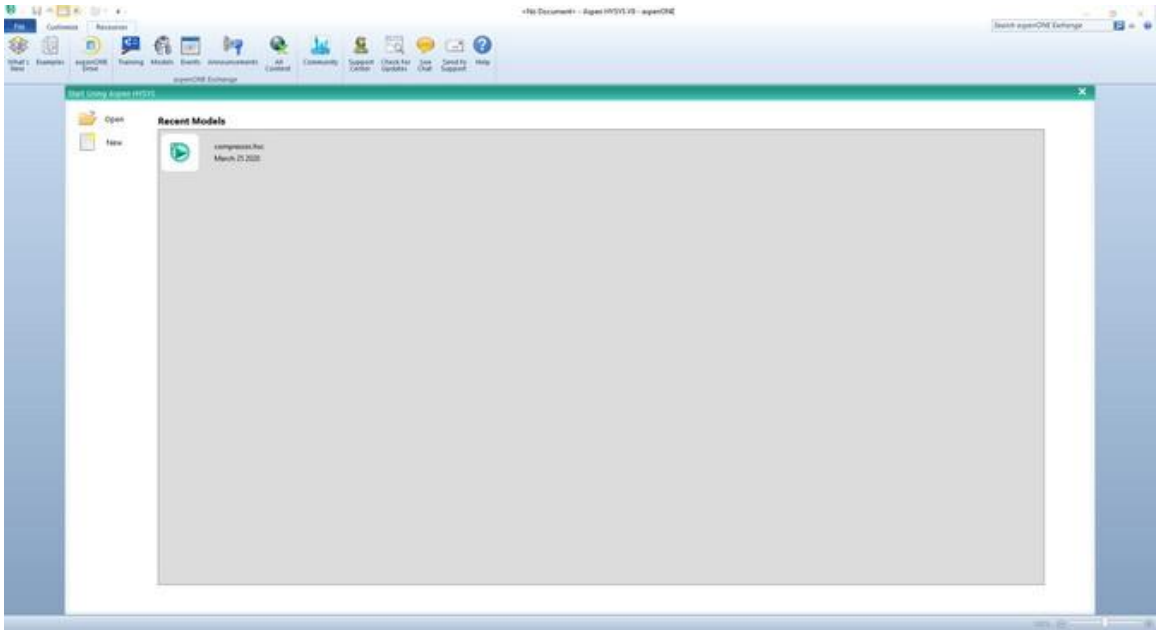
It is possible to improve the efficiency of Hydrogen production by reducing the CO levels. Water Gas Shift (WGS) reaction is an optimum purification process for increasing H2 yield and decreasing CO concentration. The following reaction:

$$CO + H_2 \leftrightarrow CO_2 + H_2$$

is an example of WGS. Model the equilibrium reaction in WGS [1].

Solution:

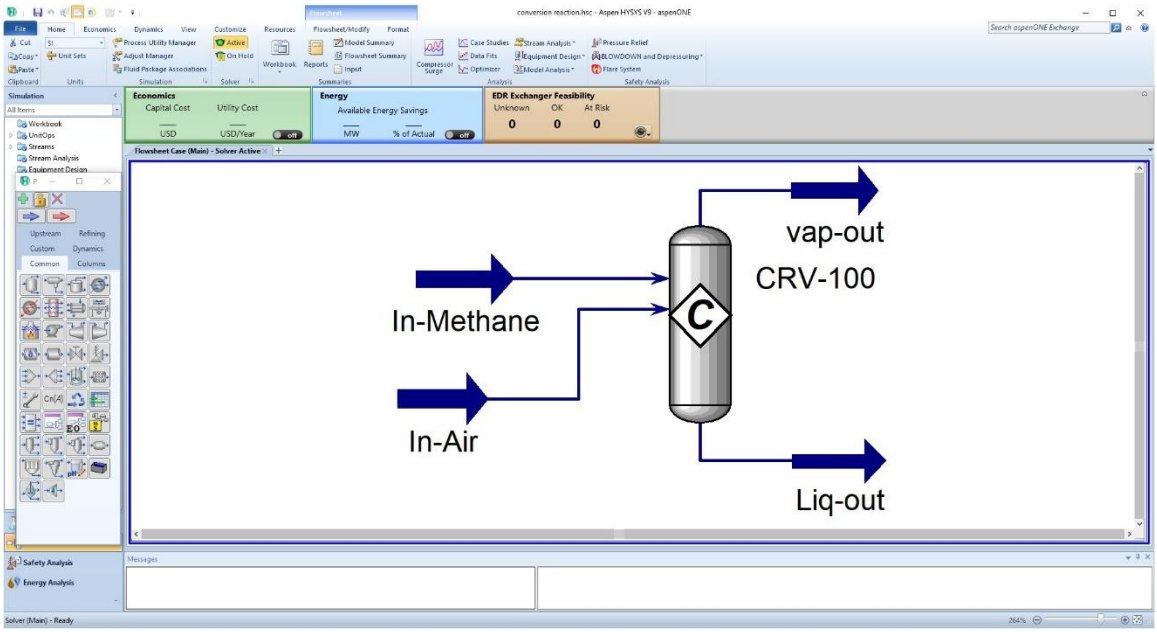
- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



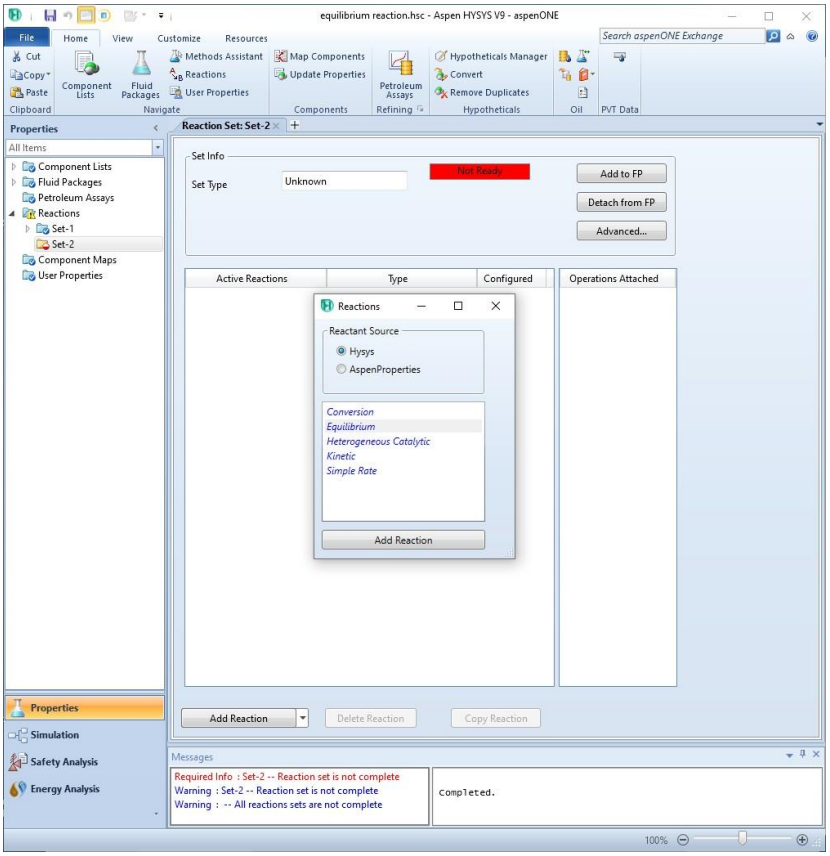
The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.

- Open the previous case of conversion reaction:

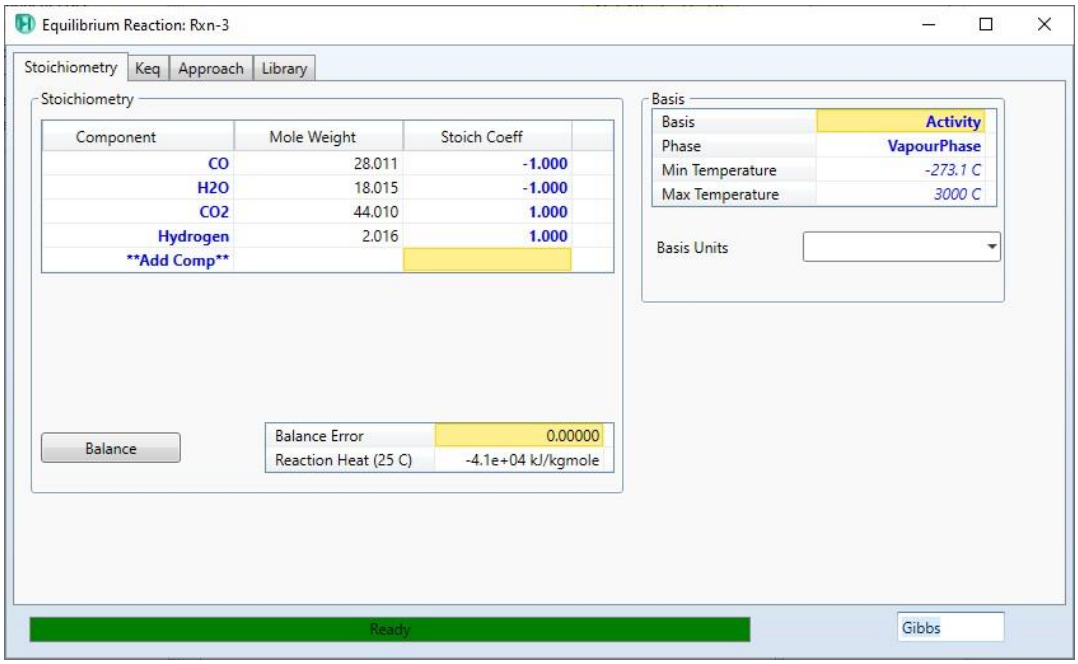
1. File menu
2. Open \ conversion reaction



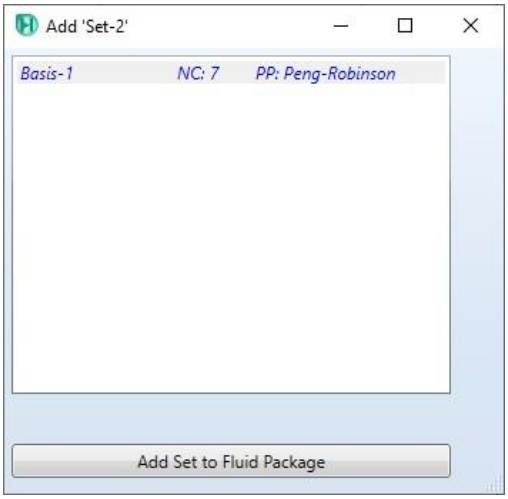
- Modify the component list:
    1. Propoerties
    2. Double click on (Component list)
    3. Component List-1
    4. Add H_2O to (Component List-1)
- Adding reaction set
    1. Properties \ Reactions \ add
    2. Add Reaction \ Equilibrium \ Add reaction



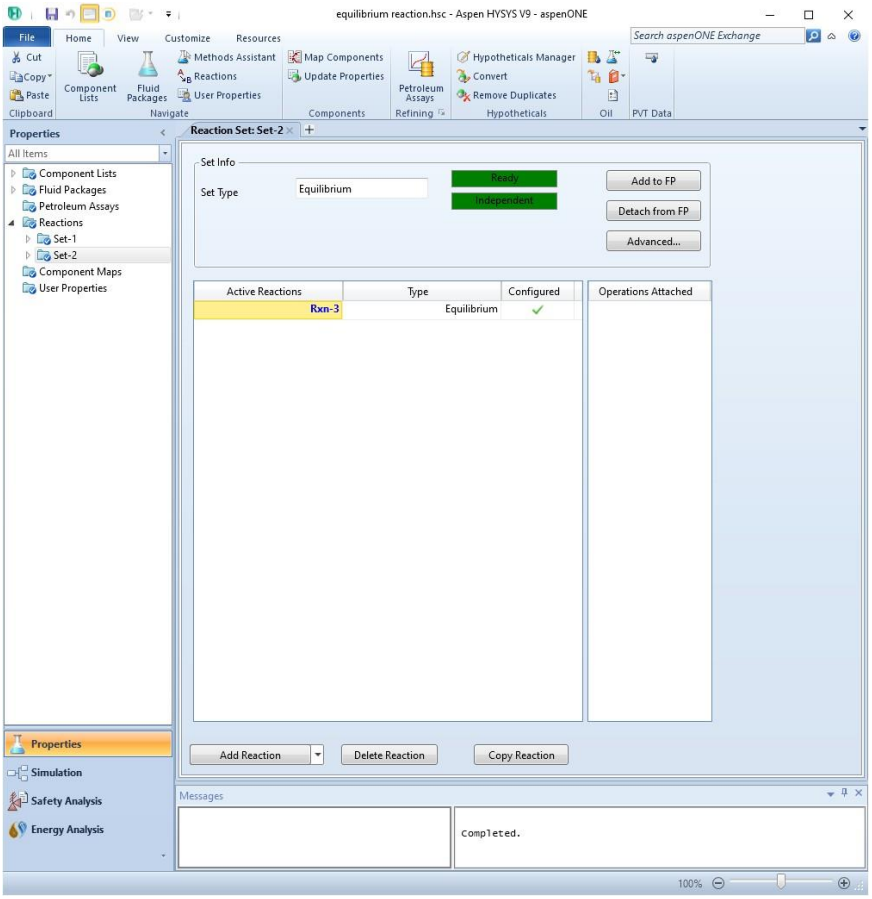
3. Double click on the added reaction
4. Enter the related information according to what is given in the example.



- Attach the reaction set to a fluid package:
  1. Click (Add to FP)
  2. Select the desired fluid package
  3. Click (Add Set to fluid package)



Now we are ready to enter the simulation environment.

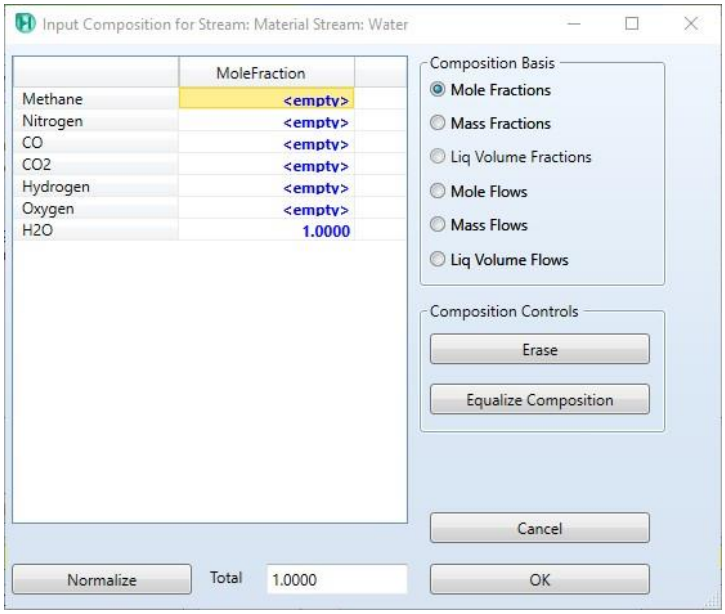


- Create new material stream:
  1. Select simulation.
  2. Object palette.
  3. Select the material stream icon.

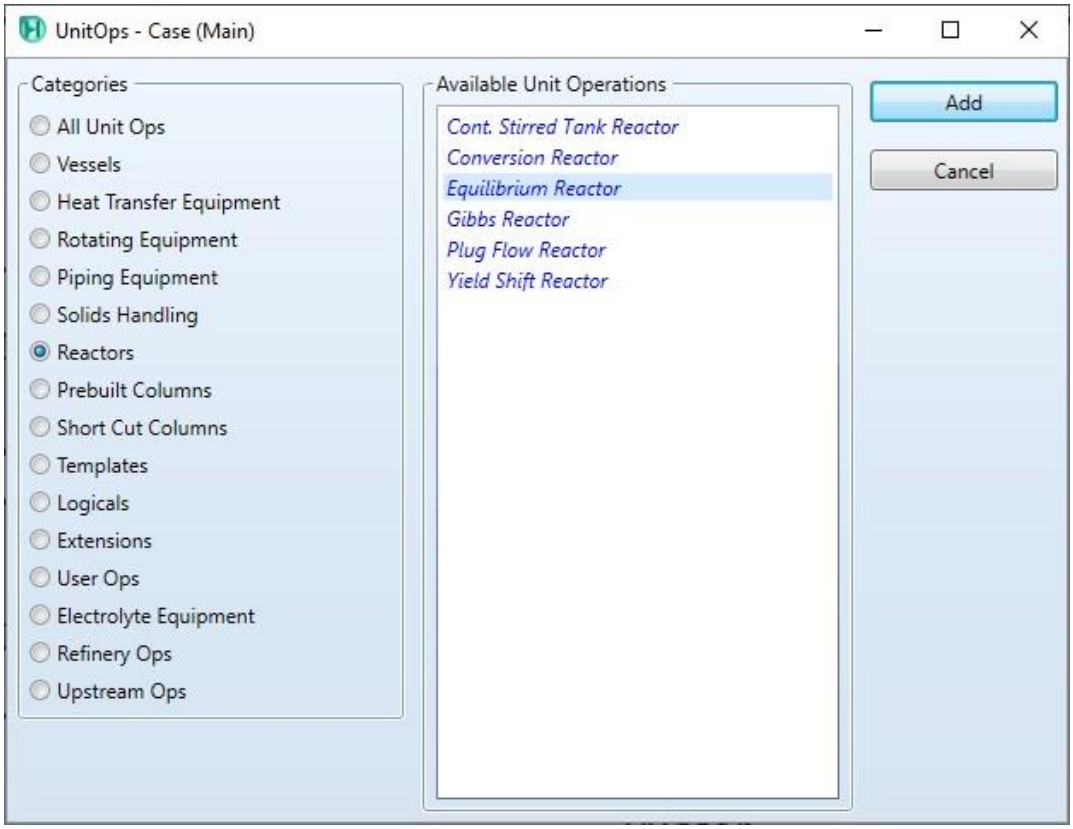
Alternatively, you can add new material stream by pressing F11.

4. Double click on the added material stream
5. Give the below information:

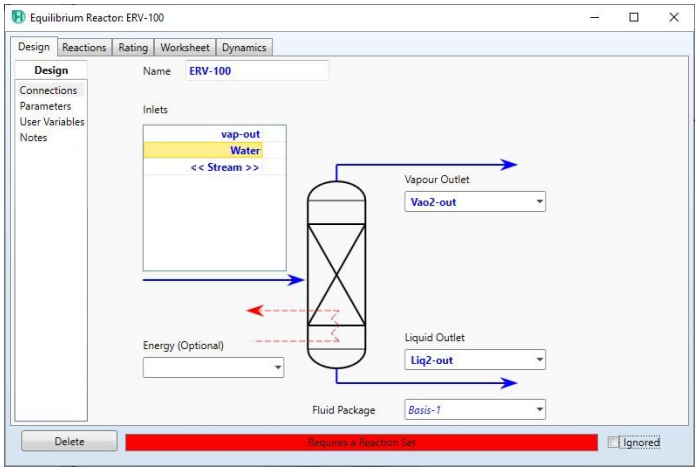
Name	Water
Conditions	
Temperature	110^{O} C
Pressure	3 bar
Molar flow	100 kgmole/h
Composition	
H_2O	1



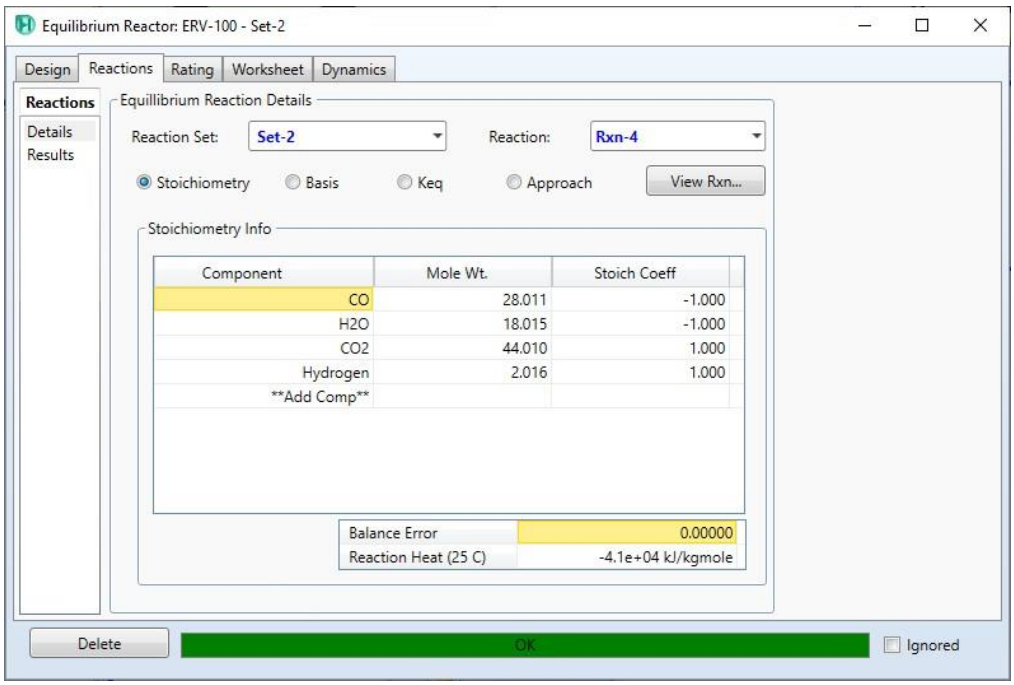
- Adding Equilibrium reactor:
  1. Press F12
  2. Select reactors
  3. Select Equilibrium reactor
  4. Click (Add)



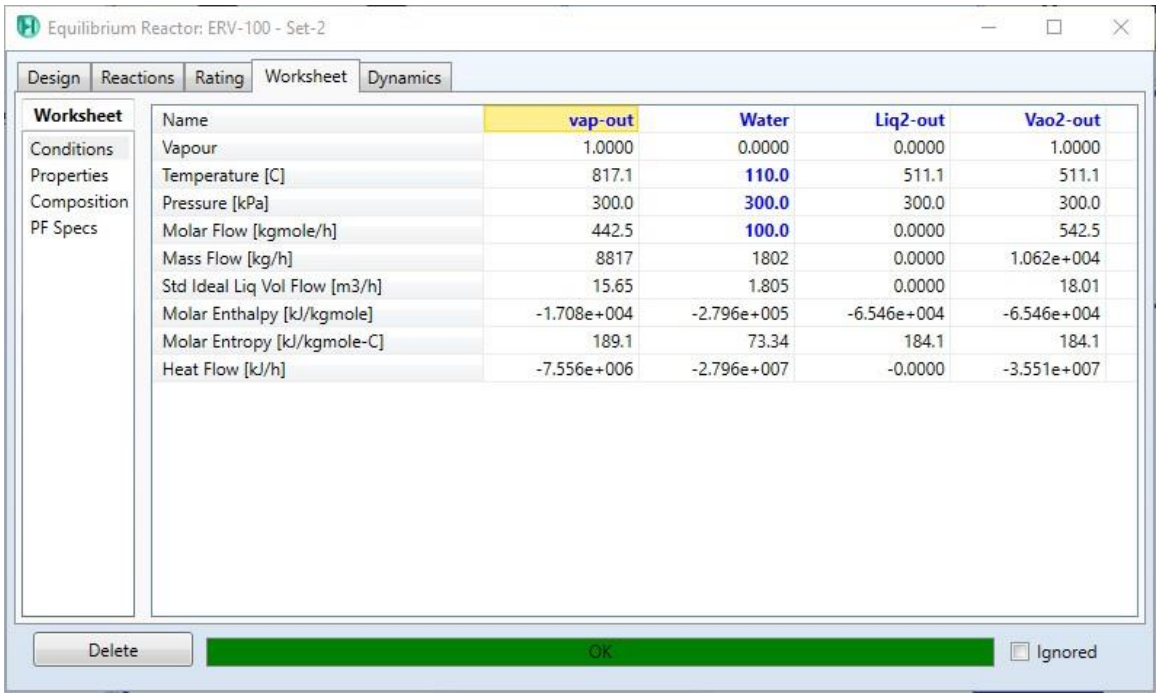
5. Place the selected unit in the desired position.
6. Double click on the added conversion reaction.
7. Design \ Connection
8. In the Inlets field select (Vap-out, water)
9. In the field of Vapour outlet type (Vap2-out) [a new material stream will be created and connected to the reactor]
10. In the field of Liquid outlet type (Liq2-out) [a new material stream will be created and connected to the reactor]

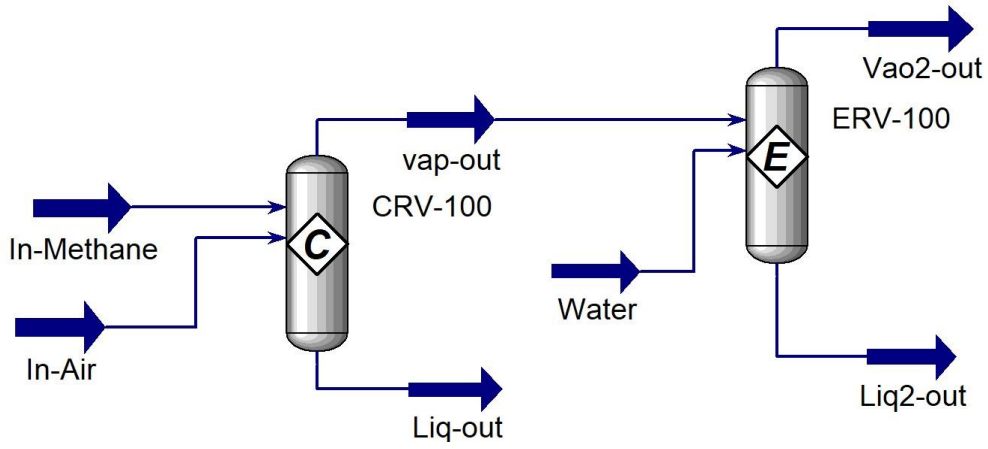


11. Reactions \ Reaction set
12. Select (Set-2)



13. Select Worksheet.
14. Composition
15. Read the compositions of the outlet streams.





- Save the case:

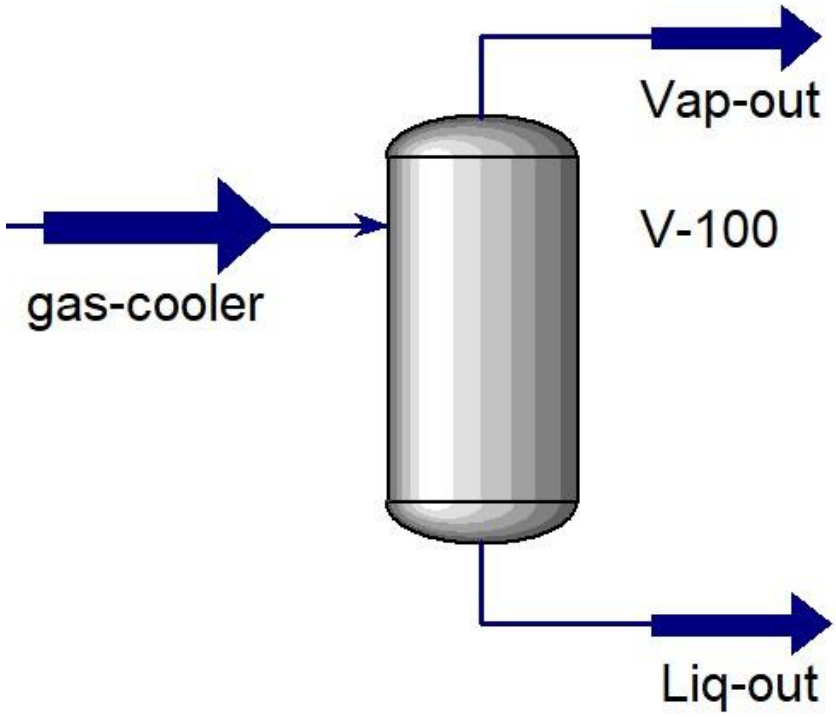
1. File menu
2. Select save as
3. Give the name (equilibrium Reaction)

References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Modeling of Flash Separator using HYSYS V9

The Flash separator is used to divide the inlet mixture into vapor and liquid phases. HYSYS V9 can model such process and determine the desired properties like the flowrates of the outlet streams at certain conditions. In this subject, it is intended to learn how to work with the flash separator unit and how to connect the right streams in their optimum directions as well as setting up the other related parameters.



The figure above shows a simple model containing the flash seperator with the inlet and outlet streams using Aspen HYSYS V.9.

Example:

Given that a mixture of 30% i-butan, 40% Ethane and 30% Propane at 40^{o} F and atmospheric pressure, and a flowrate of 100 lbmole/hr. The pressure of the mixture is to be raised to 60 psia and then, the temeprature is to be reduced to 35^{o} F. The resulting vapour and liquid are to be separated using a flash seprator. Determine the flow rates and compositions of these two streams. (use Peng-Robinson as a fluid package) [1].

Solution:

- Starting HYSYS:
    1. Start menu.
    2. Type in the search field: Aspen HYSYS V9.
    3. Select open.
- Create a new case:

1. File menu
2. New \ case

- There are two main necessary information have to be given in the properties tab before starting the simulation:
    1. Property package : Peng-Robinson
    2. Components: C2, C3 and i-C4
- Create list of components

1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the serach field C2
5. Select C2 \ add
6. Repeat steps (4,5) to add C3 and i-C4.

- Add fluid package:
    1. Select Fluid package.
    2. Click Add.
    3. Select (Peng-Robinson).
- Create new material stream:
    1. Select simulation.
    2. Object palette.
    3. Select the material stream icon.

Alternatively, you can add new material stream by pressing F11.

4. Double click on the added material stream.
5. Give the below information:

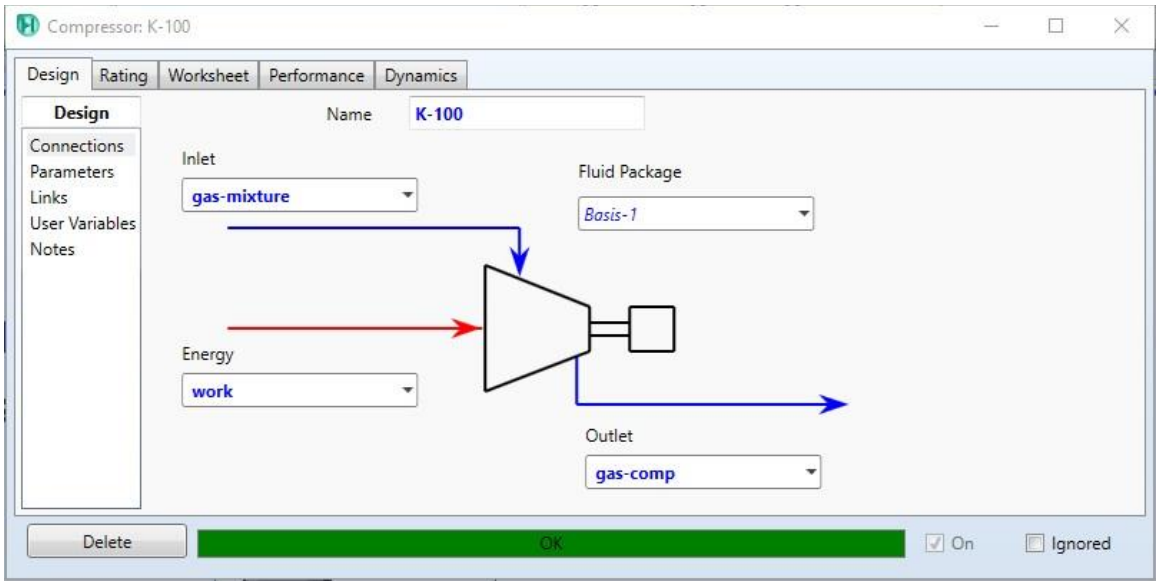
Name	Gas-Mixture
Conditions	
Temperature	40^{O} F
Pressure	1 atm
Molar flow	100 lbmole/hr
Composition	
i-C4, C2, C3	0.3, 0.4, 0.3

- Adding compressor:
    1. Object palette.
    2. Select compressor
    3. Place the selected unit in the desired position.

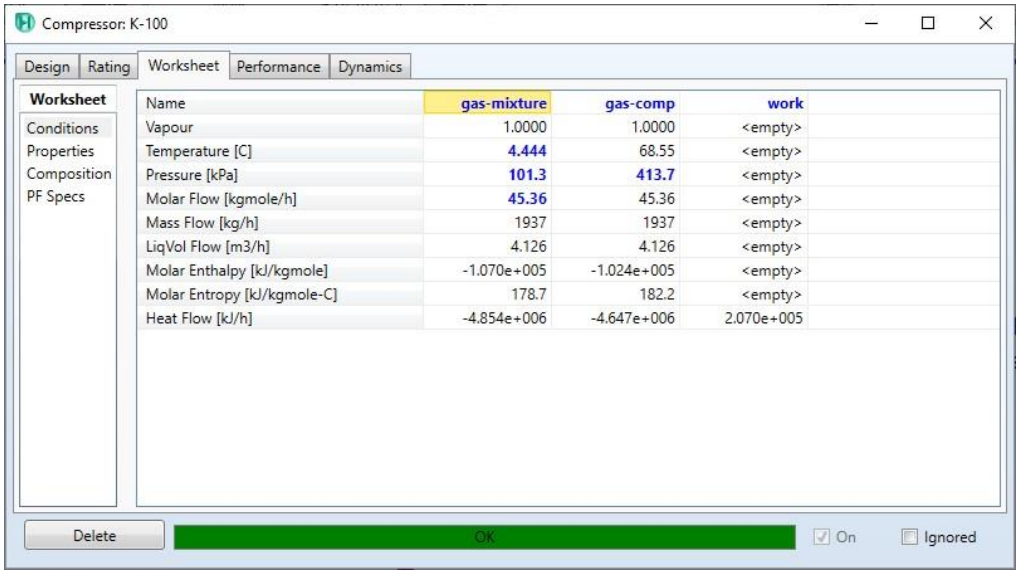
You can add a new unit by pressing F12 and select the desired unit.

4. Double click on the compressor
5. Select Design \ connections
6. In the Inlet field, select gas-mixture

7. In the outlet field, type (gas-comp). [a new material stream will be created and connected to the heat exchanger]
8. In the Energy field, type (work). [a new energy stream will be created and connected to the heat exchanger]

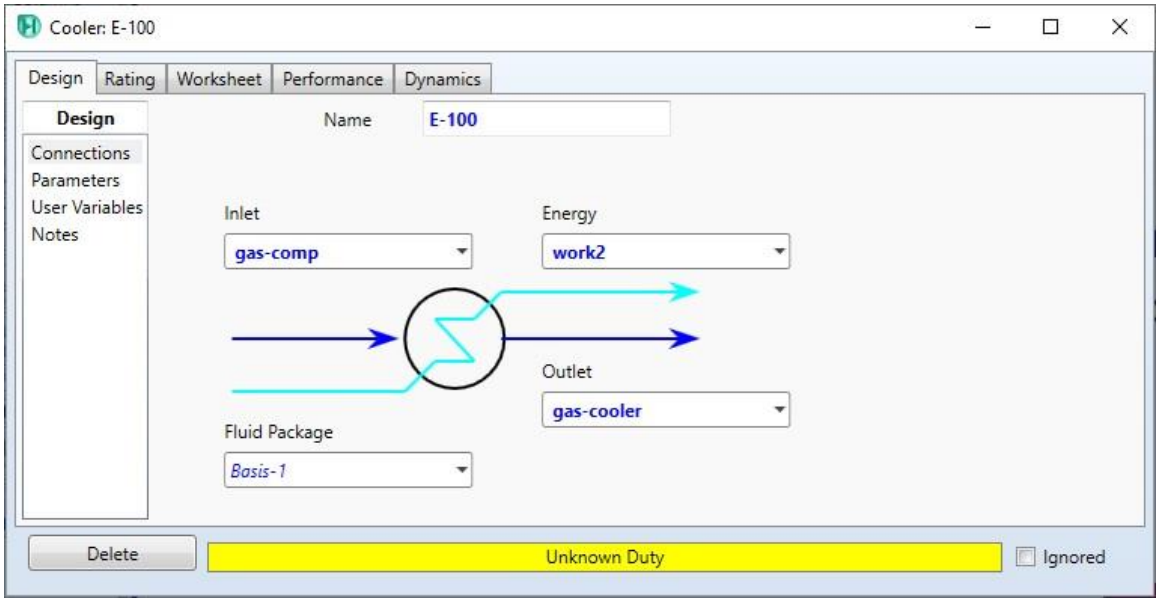


9. Worksheet\ gas-comp
10. Change the pressure to 60 psia

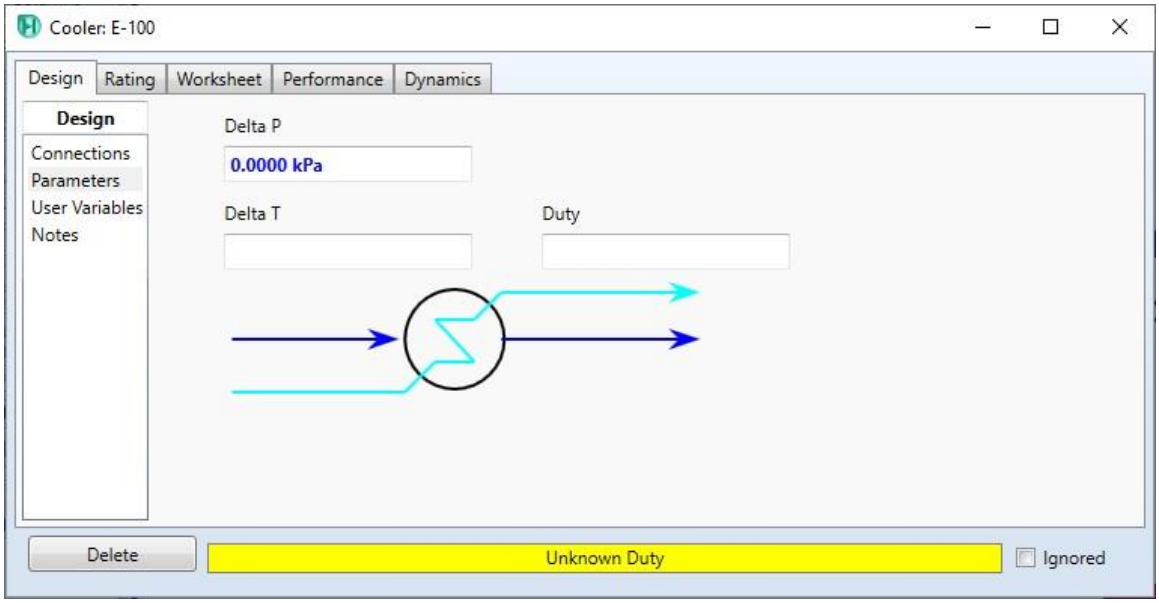


- Adding cooler:

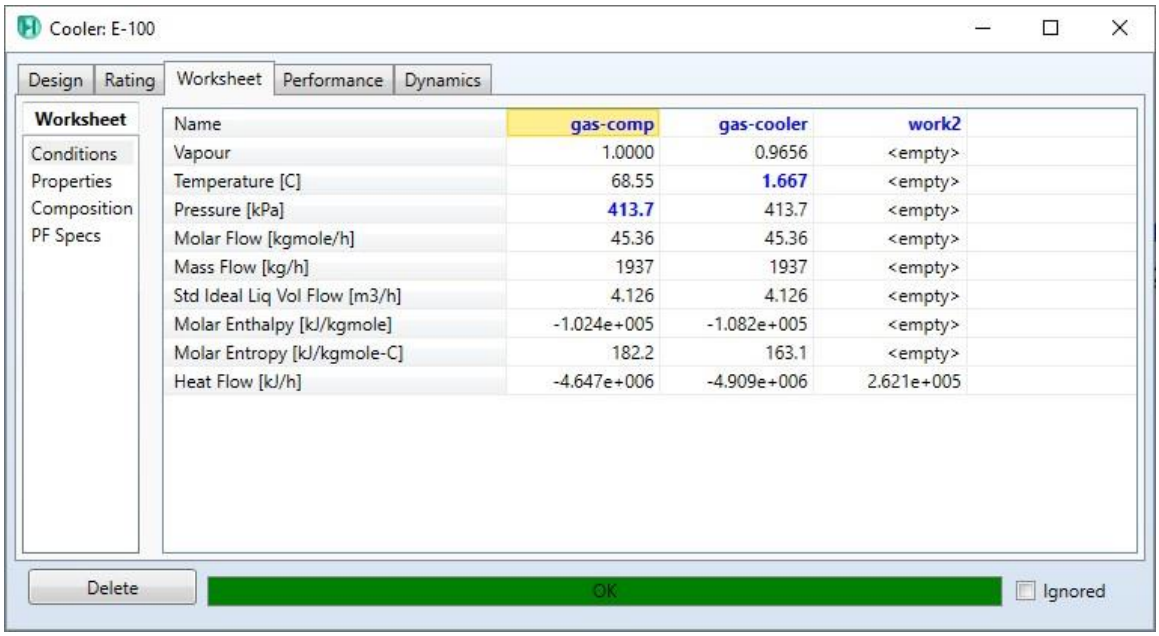
1. Object palette.
2. Select cooler.
3. Place the selected unit in the desired position.
4. Double click on the cooler
5. Select Design \ connections
6. In the Inlet field, select gas-comp.
7. In the outlet field, type (gas-cooler). [a new material stream will be created and connected to the cooler]
8. In the energy field, type (work2). [a new energy stream will be created and connected to the cooler]



9. Select parameters
10. Change the Delta P to (0).



11. Select worksheet
12. Change the temperature in gas-cooler to 35º F

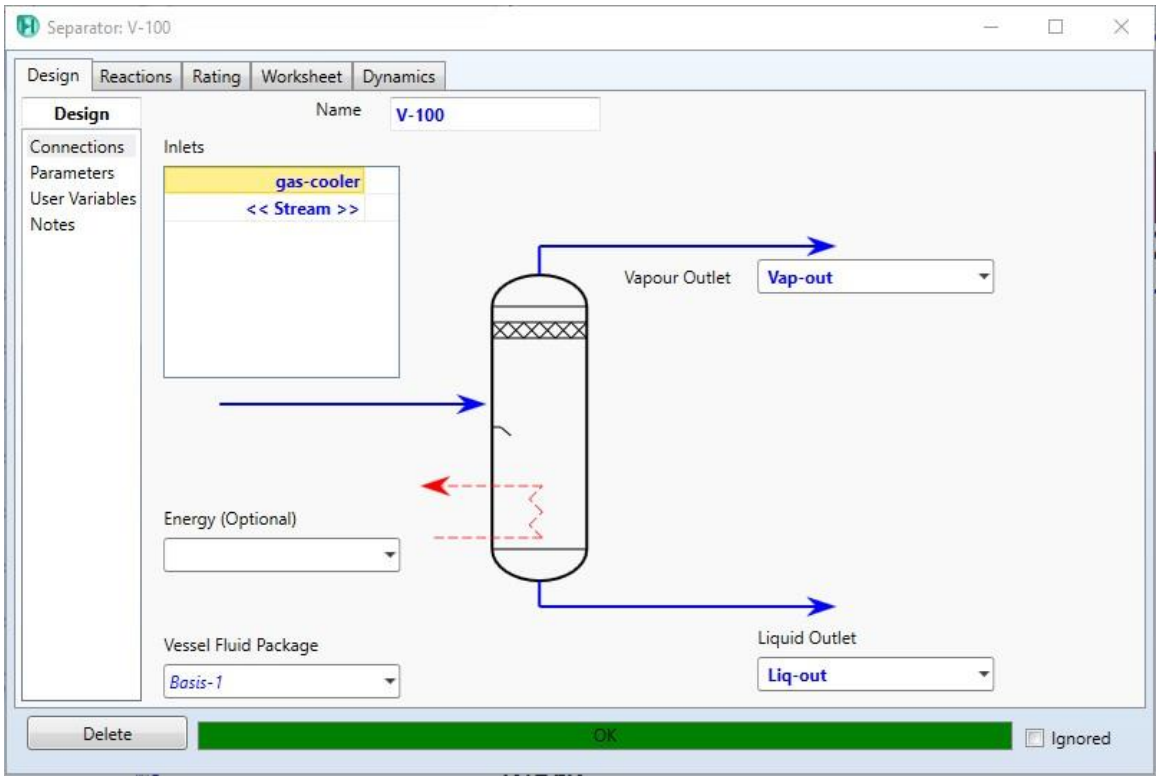


Name	gas-comp	gas-cooler	work2
Vapour	1.0000	0.9656	<empty>
Temperature [C]	68.55	1.667	<empty>
Pressure [kPa]	413.7	413.7	<empty>
Molar Flow [kgmole/h]	45.36	45.36	<empty>
Mass Flow [kg/h]	1937	1937	<empty>
Std Ideal Liq Vol Flow [m3/h]	4.126	4.126	<empty>
Molar Enthalpy [kJ/kgmole]	-1.024e+005	-1.082e+005	<empty>
Molar Entropy [kJ/kgmole-C]	182.2	163.1	<empty>
Heat Flow [kJ/h]	-4.647e+006	-4.909e+006	2.621e+005

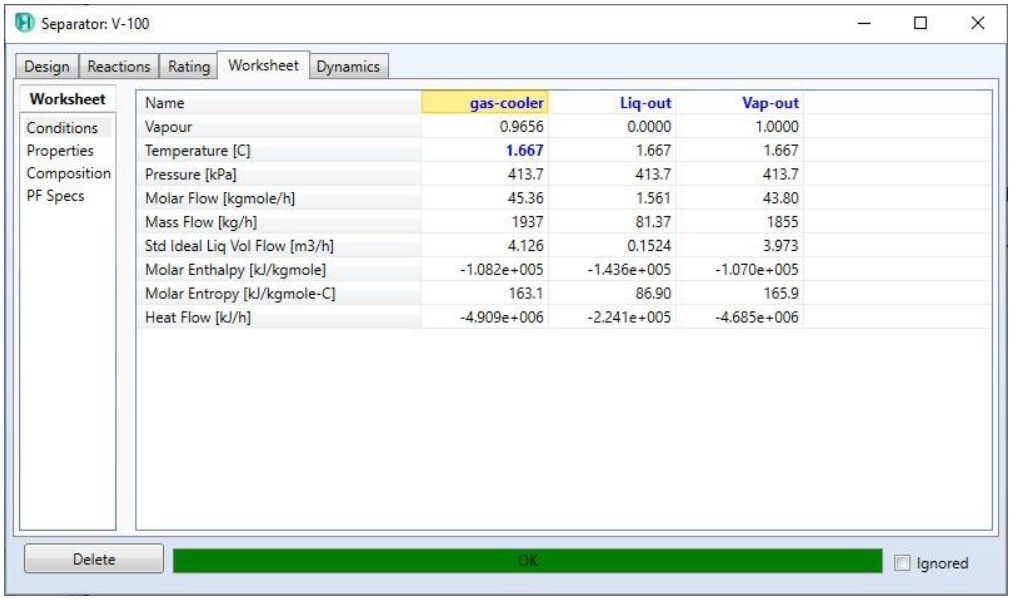
- Adding Flash Separator

1. Object palette.
2. Select flash separator.
3. Place the selected unit in the desired position.

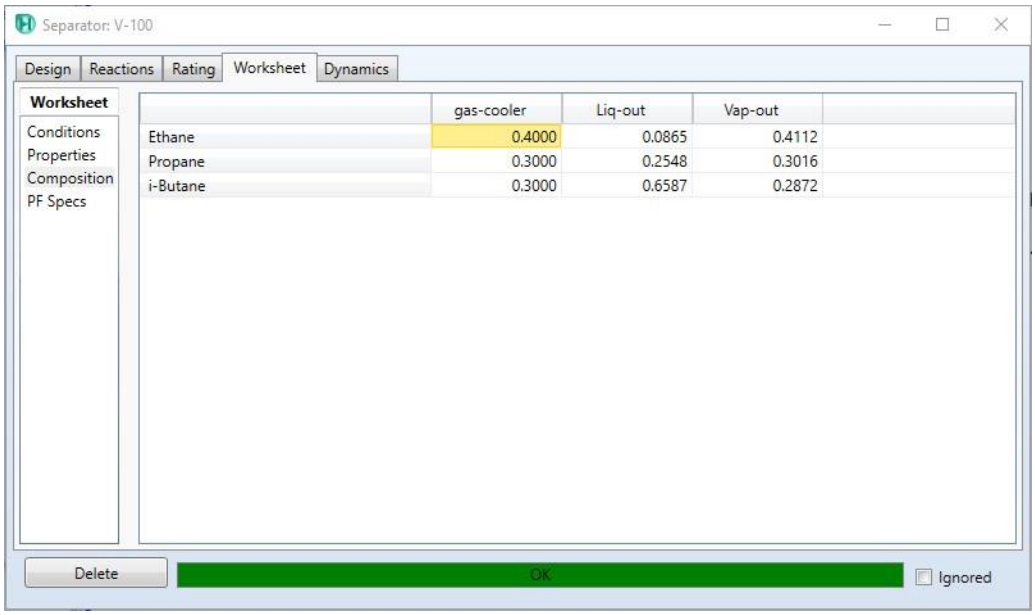
4. Double click on the flash separator
5. Select Design \ connections



6. In the Inlet field, select gas-cooler.
7. In the Vapour Outlet field, type (Vap-out). [a new material stream will be created and connected to the cooler]
8. In the Liquid outlet field, type (Liq-out). [a new material stream will be created and connected to the cooler]
9. Select Worksheet.
10. Read the flow rate values for the outlet streams.

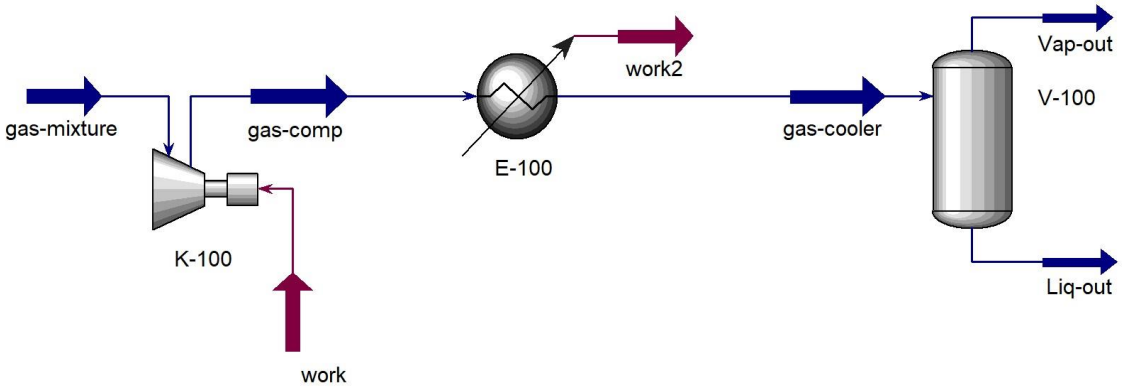


11. Select compositions
12. Read the compositions of the outlet streams



- Save the case:

1. File menu
2. Select save as
3. Give the name (flash separator)

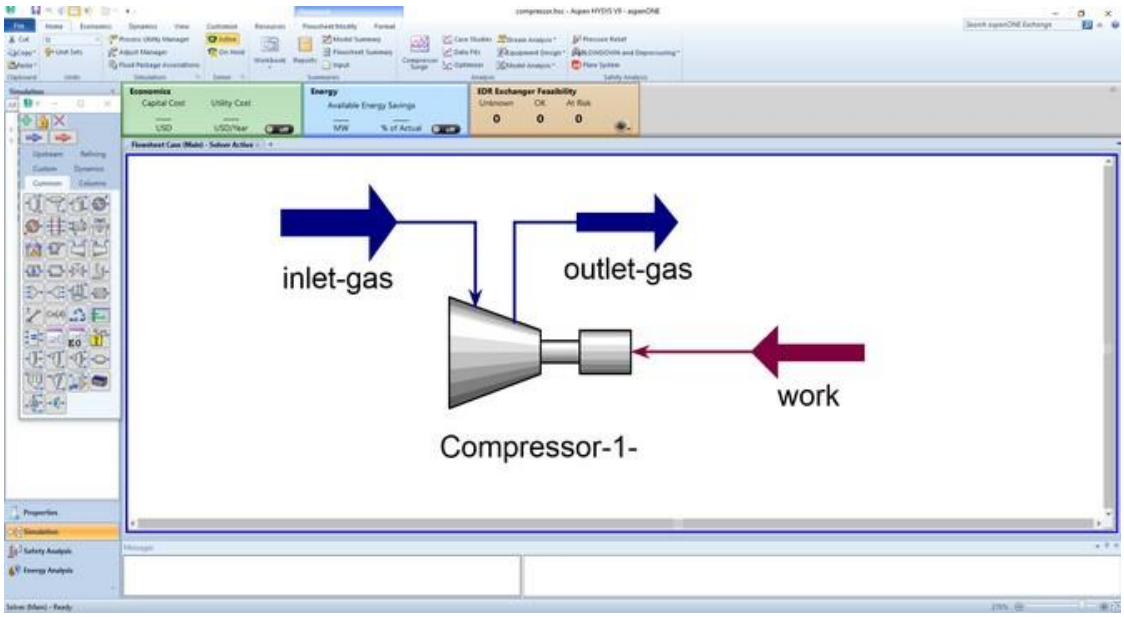


References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Modeling of Compressing Process using HYSYS V9

It is possible to model the process of compressing the gas mixtures using HYSYS. Compressors units in HYSYS are used to increase the pressure of the inlet streams giving the possibility to calculate the related properties such as the temperature and compression efficiency. In this subject, it is intended to learn how to work with the compressor unit to model the compressing process as well as set up the unit connections and other design parameters. In the end, it would be possible to operate the compressor according to the given information.



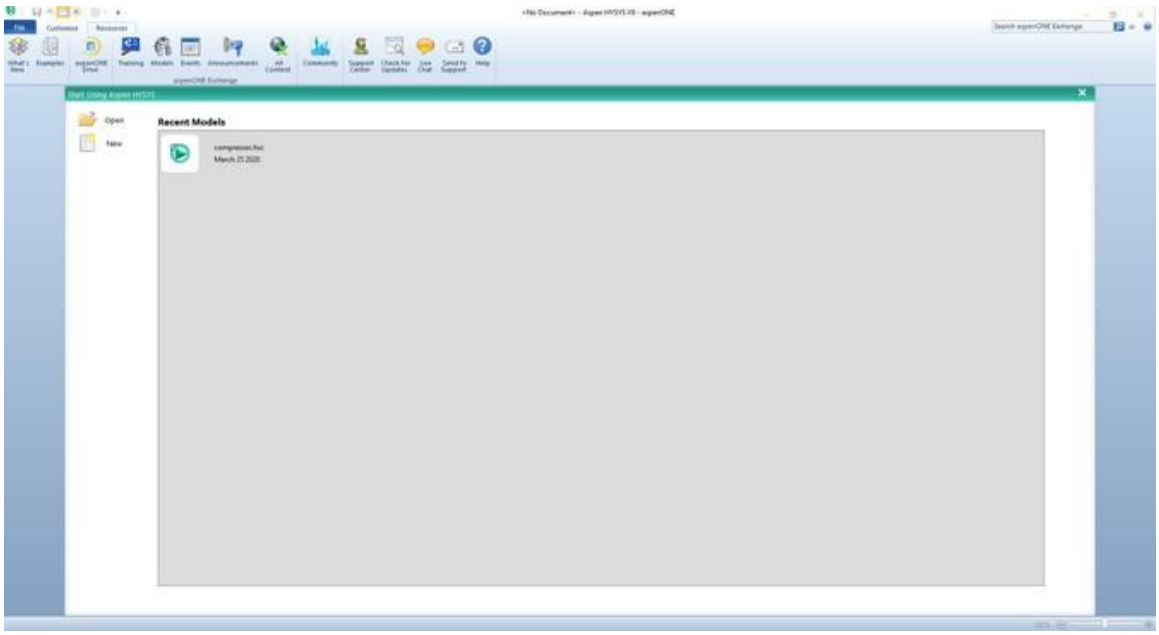
The figure above shows a simple model containing the compressor with inlet, outlet and energy streams using Aspen HYSYS V.9.

Example:

A mixture of (Methane, Ethane, Propane, and C-Hypo) at 120o C and 2 bar is fed into a compressor with 30% efficiency. the pressure of the outlet stream is 7 bar while the flow rate of the mixture is 100 kgmole/h. determine the outlet temperature using the Peng-Robinson equation of state.

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new window.

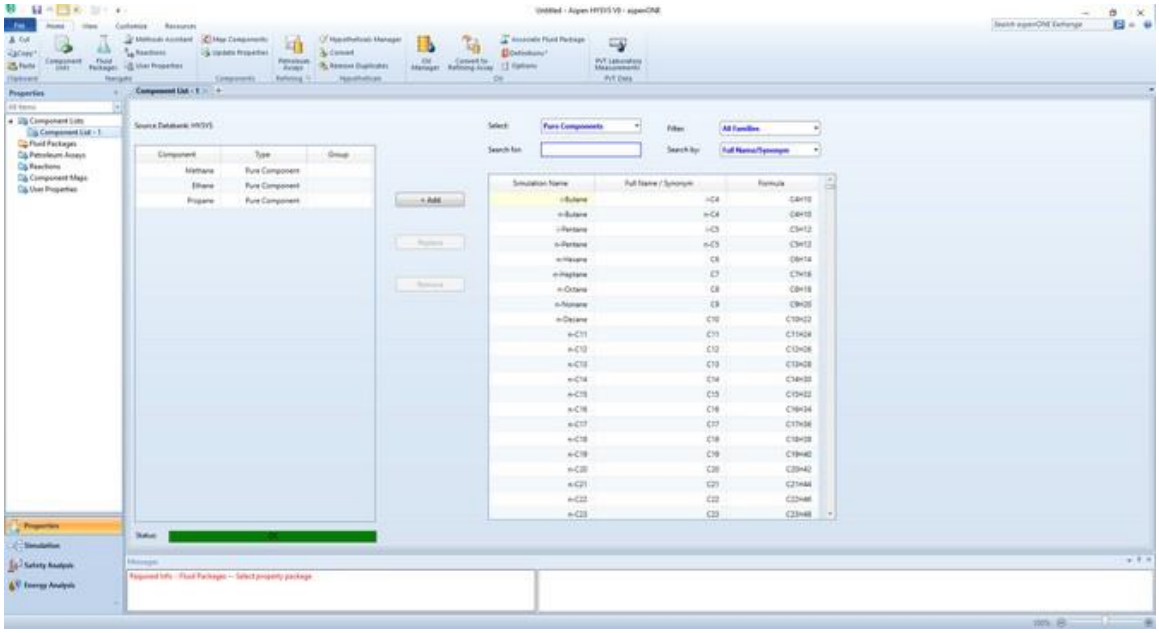
- Create a new case:

1. File menu
2. New \ case

- There are two main necessary information have to be given in the properties tab before starting the simulation:
    1. Property package : Peng – Robinson
    2. Components: C1, C2, C3 , C-hypo

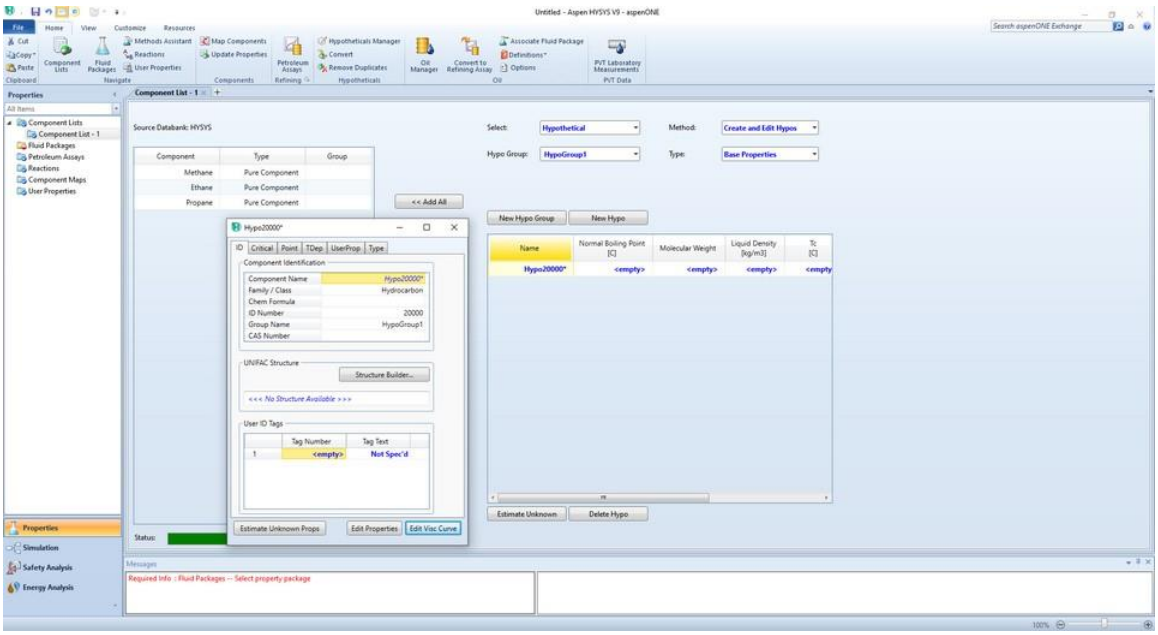
1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the serach field C1
5. Select C1 \ add
6. Repeat the steps (4,5) for C2 and C3

The component C-Hypo does not exist in the list of Pure components but, it is possible to create a new hypothetical component.

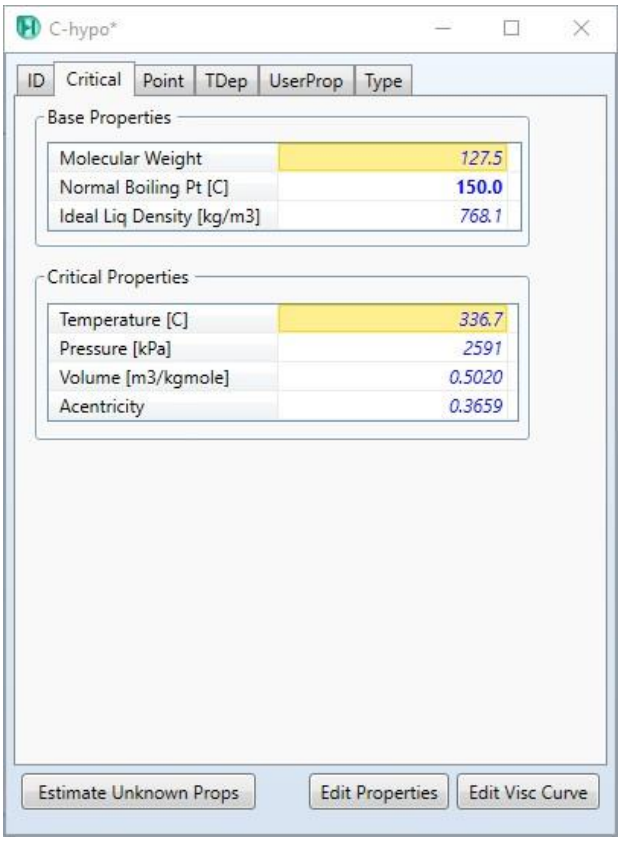


- Create new hypothetical component:

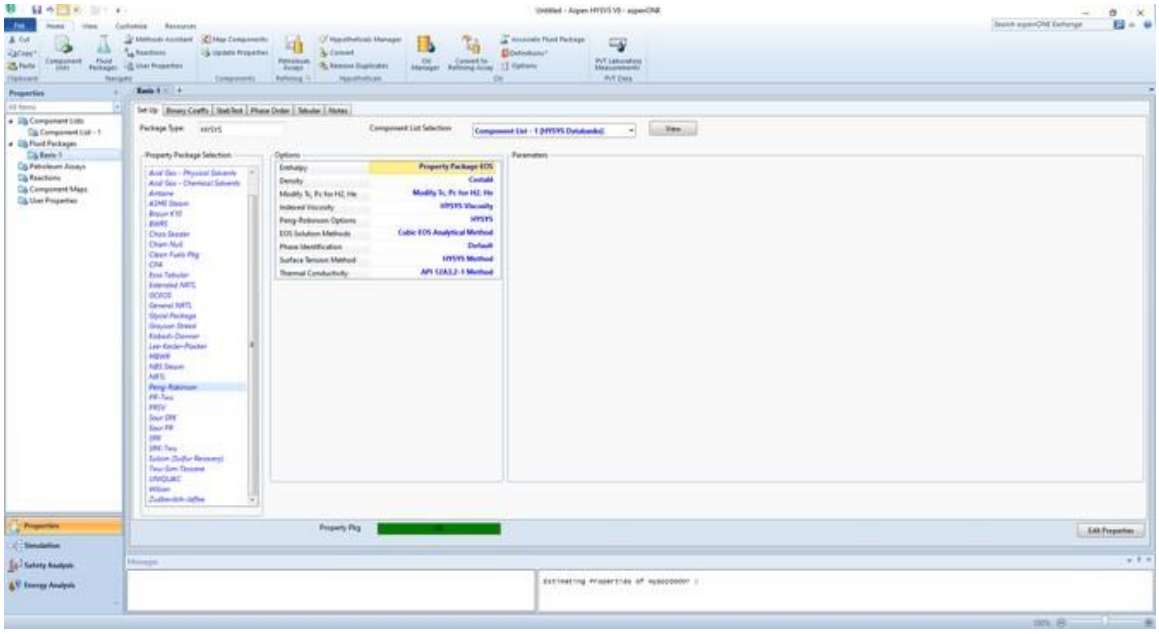
1. Select Hypothetical
2. In the mehtod field, select (create and edit hypos)
3. Click New Hypo
4. Double- Click on the added new component



5. Change thre component name to : C-Hypo
6. Select critical
7. Change the Normal Boiling point to : (150^{o} C). [the value of the normal Boinling point is given according to the application or example]
8. Click (estimate unknown props)
9. Change the name of the hypo group to : Hypo-compressor-group
10. Select the created component (C-hypo) to your component list
11. Click add



- Add fluid package:
  1. Select Fluid package
  2. Click Add
  3. Select (Peng – Robinson)



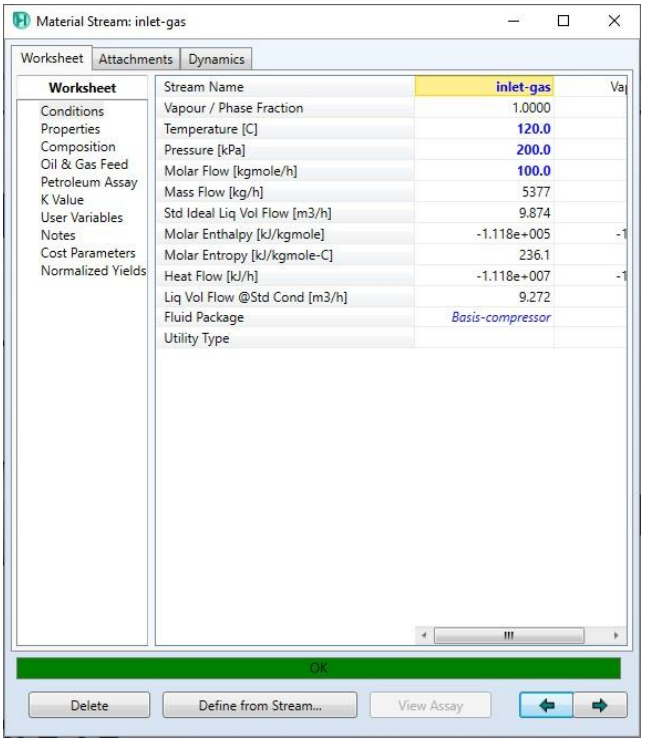
- Create new material stream:
  1. Select simulation.
  2. Object palette.
  3. Select the material stream icon.

Alternatively, you can add new material stream by pressing F11.

4. Double click on the added material stream
5. Give the below information:

Name	Inlet-gas
Conditions	
Temperature	120^{O} c
PRESSURE	2 bar
Molar flow	100 kgmole/h
Composition	
C1	0.1
C2	0.3
C3	0.4
C-hypo	0.2

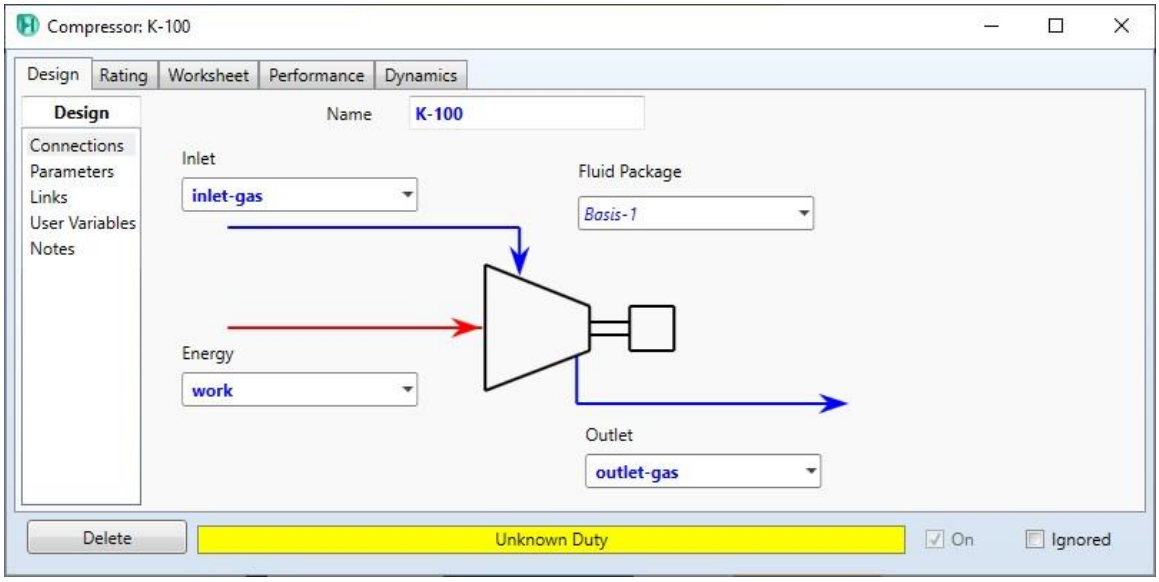
The above information should be given according to the application or example.



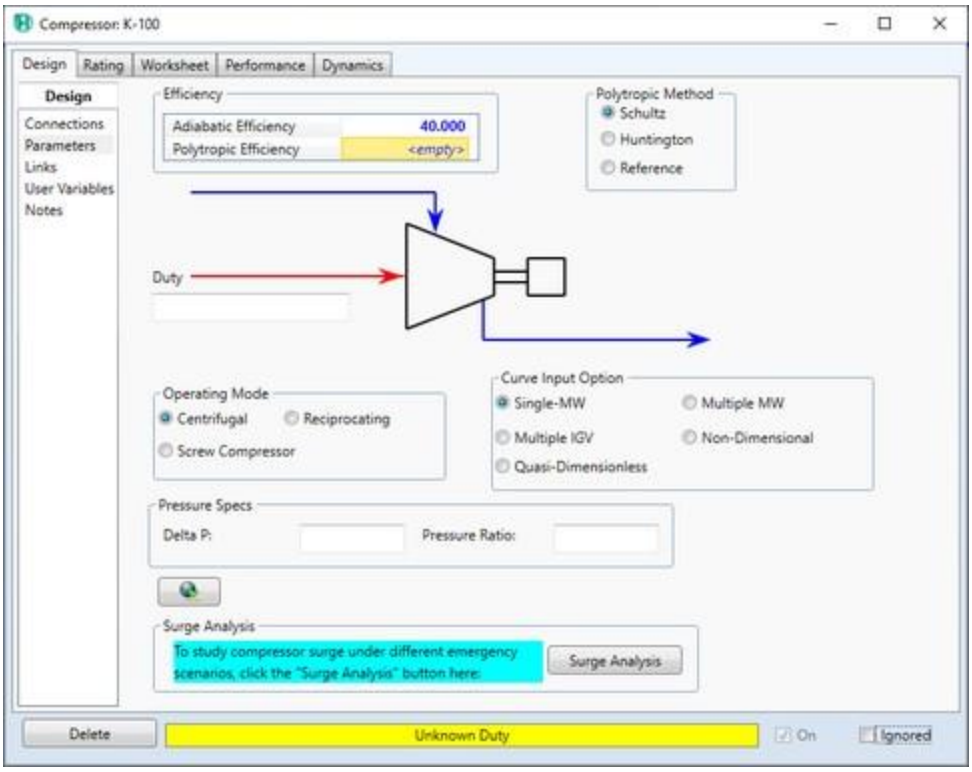
- Adding Compressor:
    1. Object palette.
    2. Select compressor
    3. Place the selected unit in the desired position.

You can add a new unit by pressing F12 and select the desired unit.

4. Double click on the compressor
5. Select Design \ connections
6. In the inlet field, select inlet-gas
7. In the outlet field, type (outlet-gas). [a new material stream will be created and connected to the compressor]
8. In the Energy field, type work. [a new energy stream will be created and connected to the compressor].

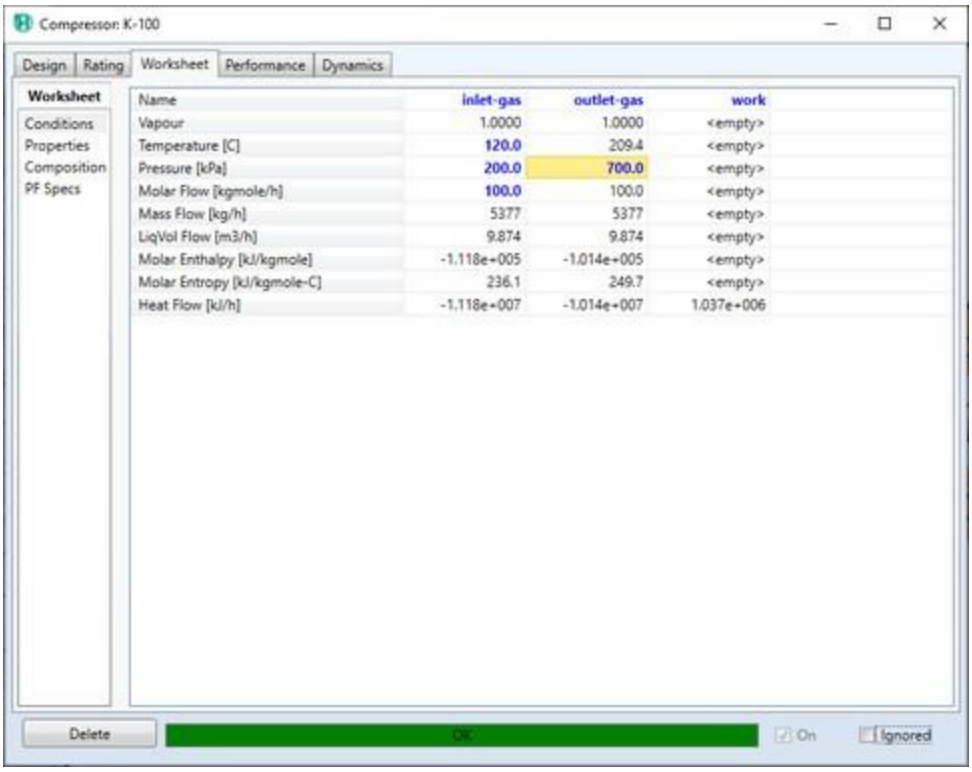


9. Select parameters \ Adiabatic Efficiency
10. Change the efficiency to 40 %.
11. Select worksheet



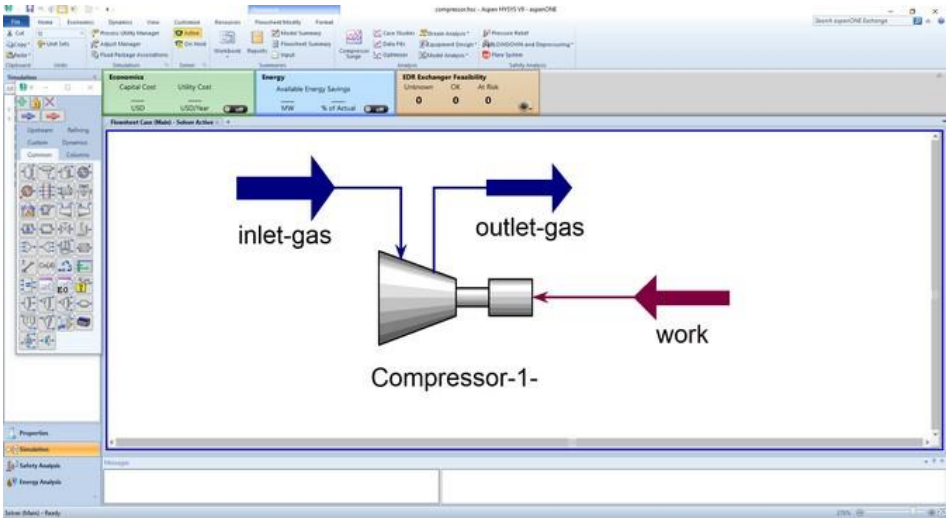
1. Change the outlet-gas pressure to 7 bar.
2. Read the temperature of the outlet-gas.

The temperature of the outlet stream is 209.4o C.



- Save the case:

1. File menu
2. Select save as
3. Give the name (compressor)

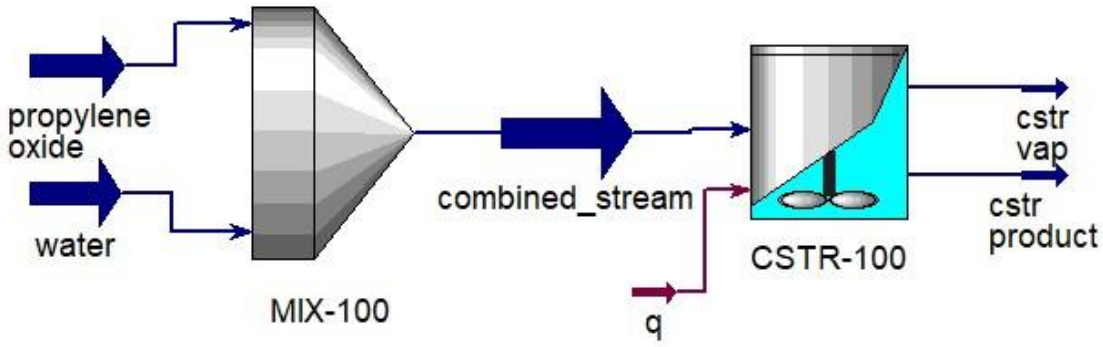


References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Modeling of CSTR Using HYSYS V9

The figure above shows a simple model containing the CSTR with inlet, and outlet streams using Aspen HYSYS V.9.



Example:

The propylene glycol is produced in CSTR by combining the propylene oxide with water. The propylene oxide and water streams are combined using a mixer while the the outlet stream is fed to the reactor operating at atmospheric pressure. Simulate the production of Propylene Glycol using CSTR:

$$H_2O + C_3H_6O \rightarrow C_3H_8O_2$$

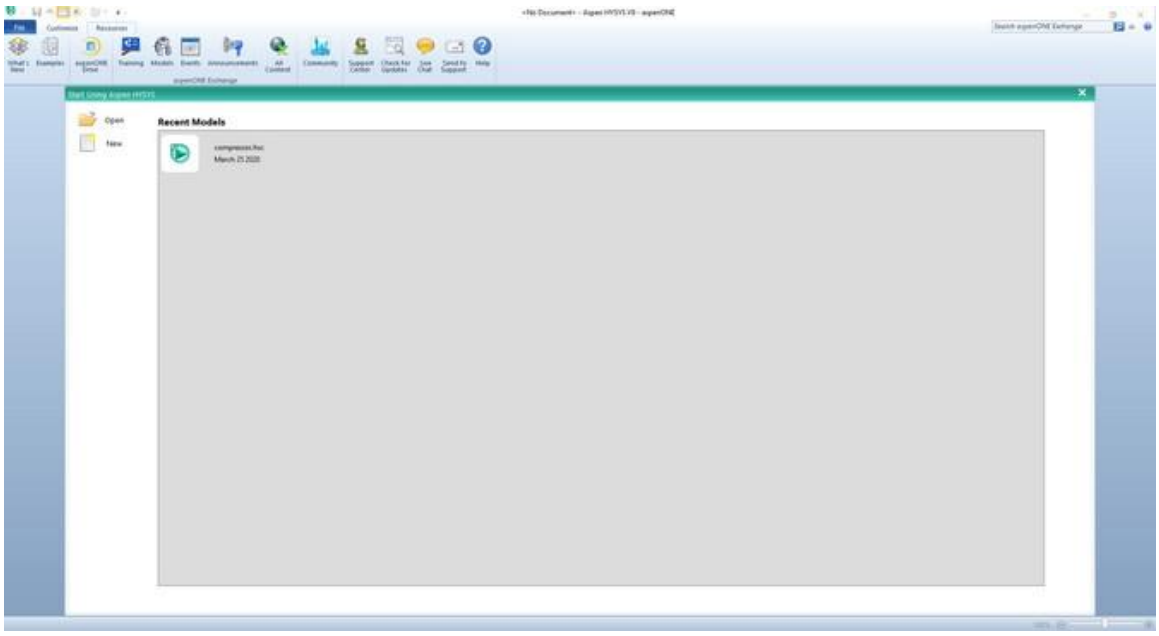
The forward reaction arrhenius parameters:

Frequency factor: 1.7 x 10^{13}, Activation Energy: 3.24 x 10^4

(fluid Package: UNIQUAC) [1]

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



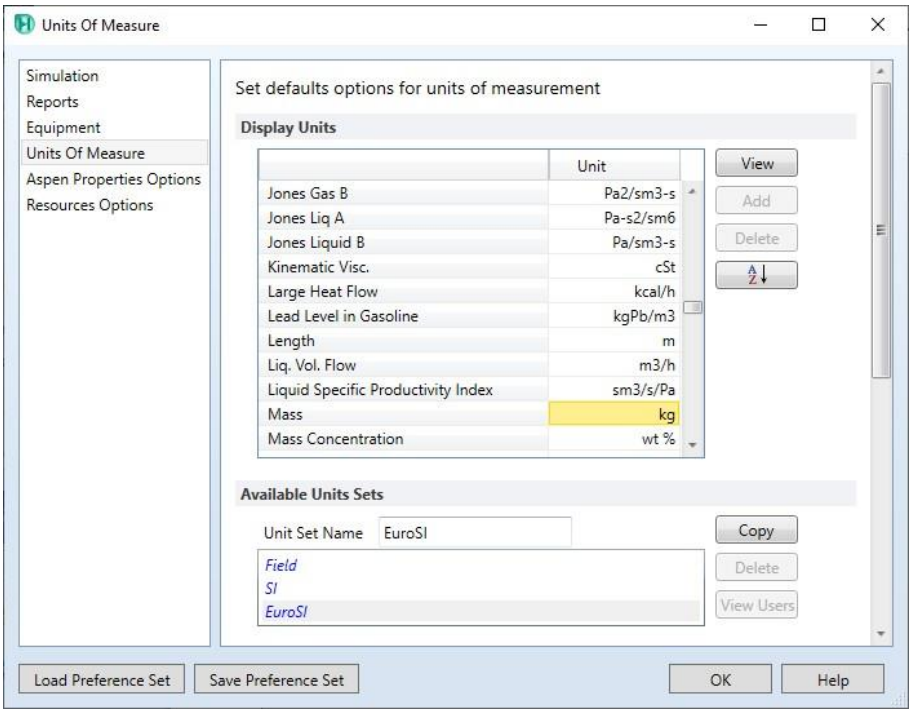
The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new window.

- Create a new case:

1. File menu
2. New \ case

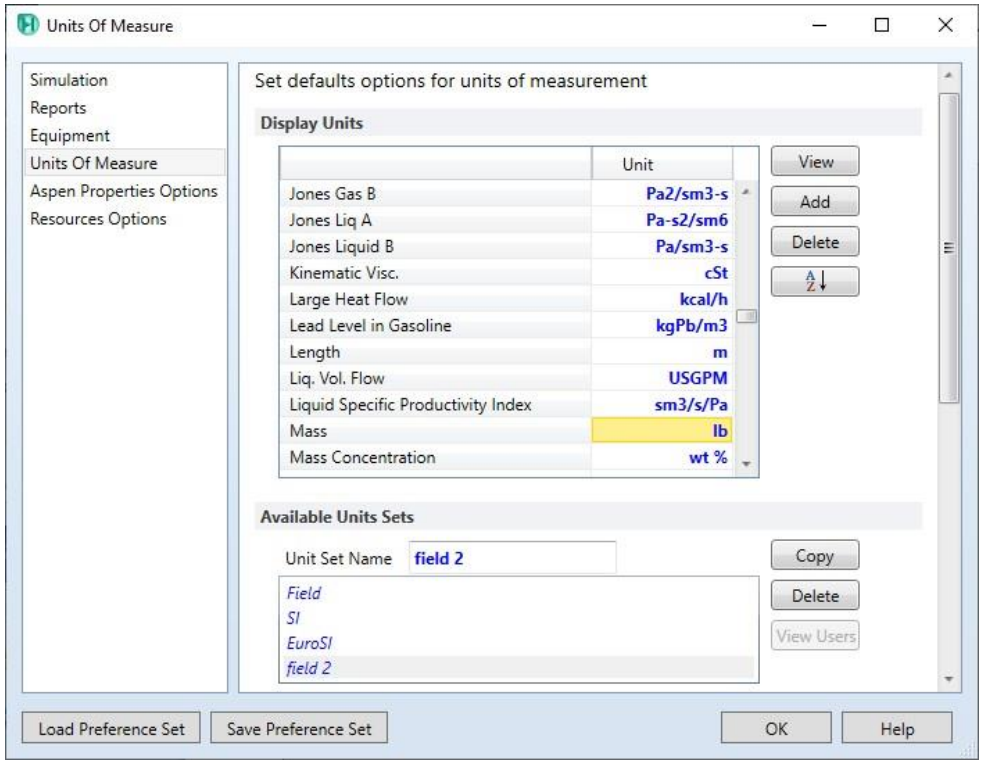
- There are two main necessary information have to be given in the properties tab before starting the simulation:
    1. Property package : UNIQUAC
    2. Components: Propylene_Glycol, H_2O, PropyleneOxide
- Preference Set:

1. File
2. Options
3. Click (unit of measure)



4. Avaialable unit set \ click (copy) : new unit set is given.
5. Chane the name of the added unit set to (field 2)
6. Display Units \ change the units as desired.
7. Change the unit of Liq. Vol. flow to (USGPM).
8. Change the unit of Mass to (lb).

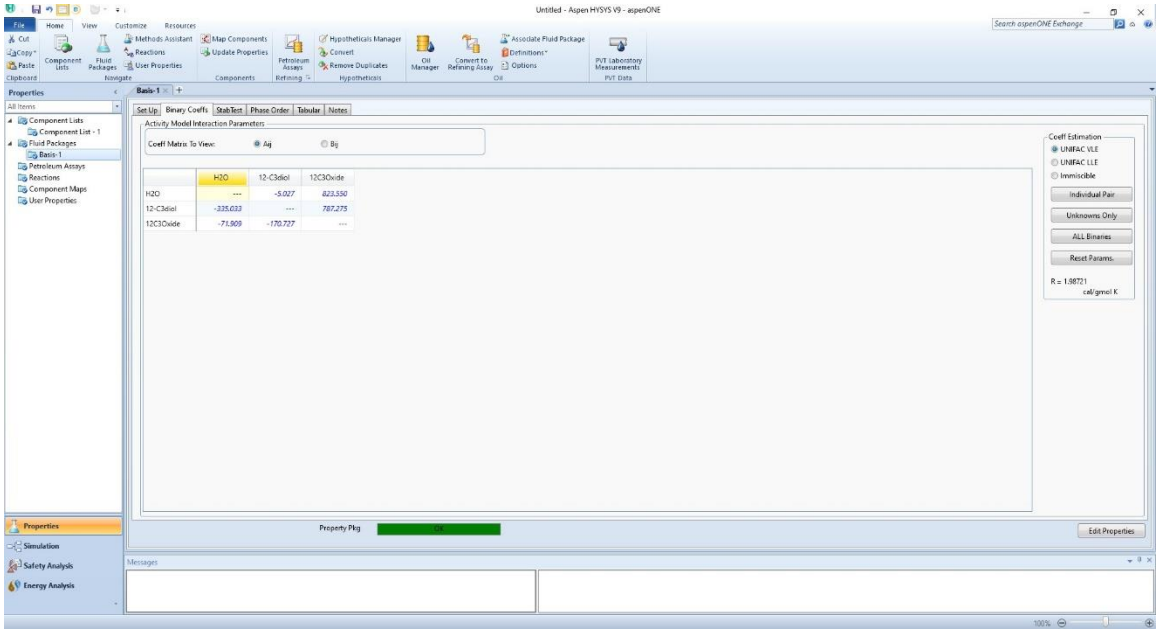
9. Click (save prefernce set) in order to save the set as a separate file. It is possible to use this prefernce set in another simulation case by clicking (load prefernce set).
10. Click ok



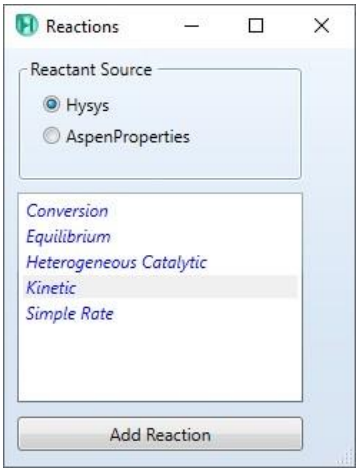
- Adding Component list:

1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the serach field Propylene_Glycol
5. Select Propylene_Glycol \ add
6. Repeat the steps (4,5) for PropyleneOxide and water

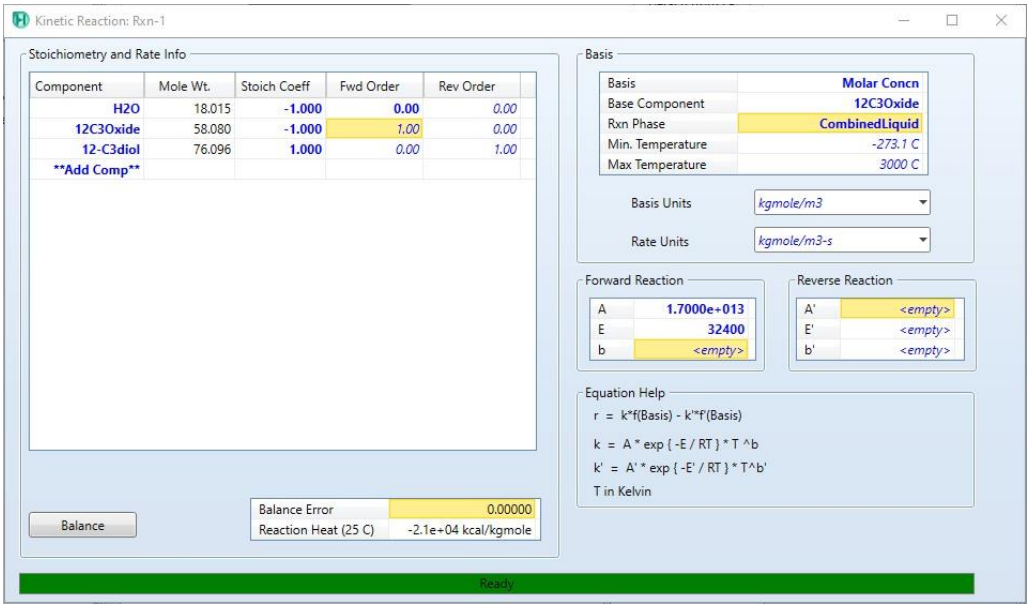
- Add fluid package:
  1. Properties
  2. Select Fluid package
  3. Click Add
  4. Select (UNIQUAC)
  5. Binary Coeffs
  6. Click (Unknown only)



- Adding reaction set:
  1. Properties
  2. Reactions
  3. Click (Add Reaction)
  4. Select kinetic
  5. Click (Add reaction)



6. Double click on (Rxn1)
7. Enter the related information of stoichiometry according to what are given in the equation.
8. Change (Fwd Order) of H_2O to 0.
9. Basis
10. Change the (basis component) to (Propylene Oxide)
11. Change the (Rxn phase) to (Combined_liquid)
12. Forward reaction
13. Set (A) to the value of the Frequency factor: 1.7 x 10^{13} as given above. [1.7e+13]
14. Set (E) to the value of the Activation Energy: 3.24 x 10^{4} as given above. [3.24e+4]



- Attach the reaction set to a fluid package:
  1. Click (Add to FP)
  2. Select the desired fluid package
  3. Click (Add Set to fluid package)

- Create new material streams:
  1. Select simulation.
  2. Object palette.
  3. Select the material stream icon.

Alternatively, you can add new material stream by pressing F11.

4. Double click on the added material stream
5. Give the below information:

Name	Propylene Oxide
Conditions	
Temperature	75^{O} F
PRESSURE	1.1 atm
Molar flow	150 lbmole/h
Composition	
Propylene Oxide	1

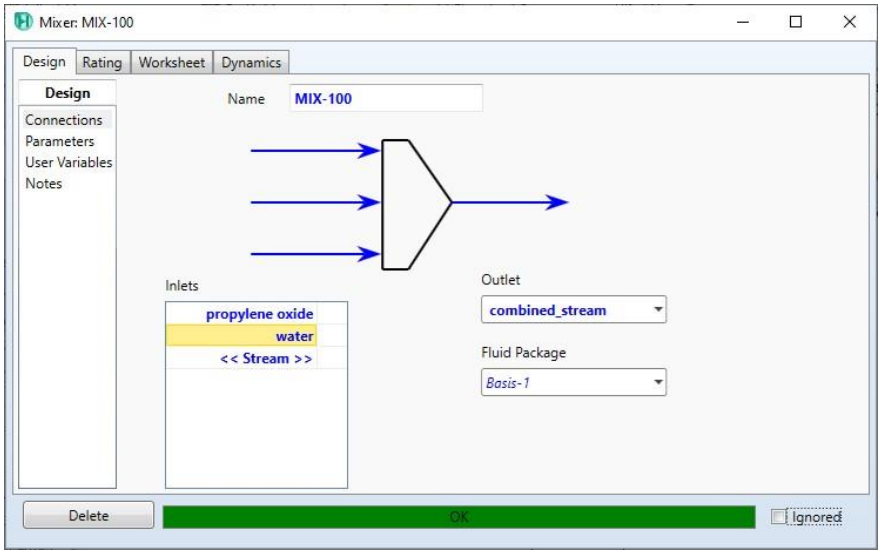
6. Repeat step 5 to add another stream and give the following information:

Name	Water
Conditions	
Temperature	75^{O} F
PRESSURE	1.1 atm
Molar flow	1.1e+4 lb/hr
Composition	
Water	1

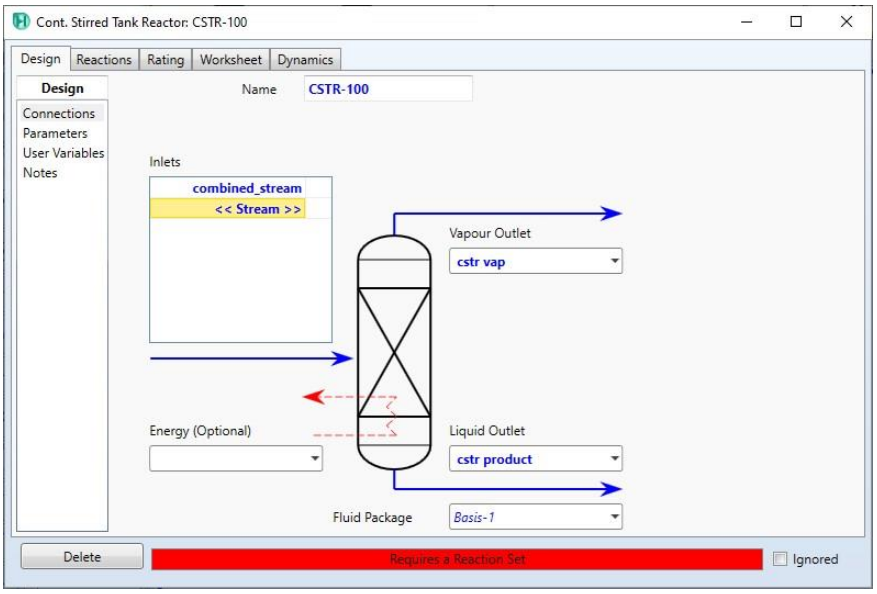
- Adding Mixer:
    1. Object palette.
    2. Select mixer
    3. Place the selected unit in the desired position.

You can add a new unit by pressing F12 and select the desired unit.

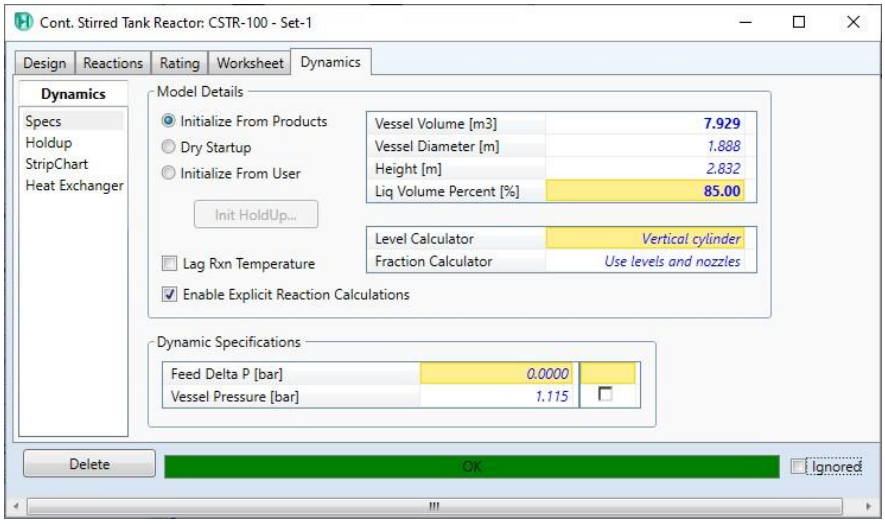
4. Double click on the mixer
5. In inlets field, select (propylene oxide) and (water)
6. In outlet field, type (combined stream). [a new material stream will be created and connected to the compressor]



- Adding CSTR:
    1. Object palette.
    2. Select CSTR (Continuously Stirred Tank Reactor)
    3. Place the selected unit in the desired position.
    4. Double click on the mixer
    5. In inlets field, select (combined stream)
    6. In Vapour outlet field, type (cstr vap). [a new material stream will be created and connected to the compressor]
    7. In Liquid outlet field, type (cstr product). [a new material stream will be created and connected to the compressor]



8. Reactions
9. In Reaction Set field , select Set-1
10. Dynamics
11. Model details
12. Set the vessel Volume to :280 ft3
13. Set the Liq Volume Percent [%] to 85%



14. Deign \connection
15. In Energy field, type (Q). [a new energy stream will be created and connected to the compressor]

16. Worksheet
17. Set the temperature in cstr product to 75^{o}F.

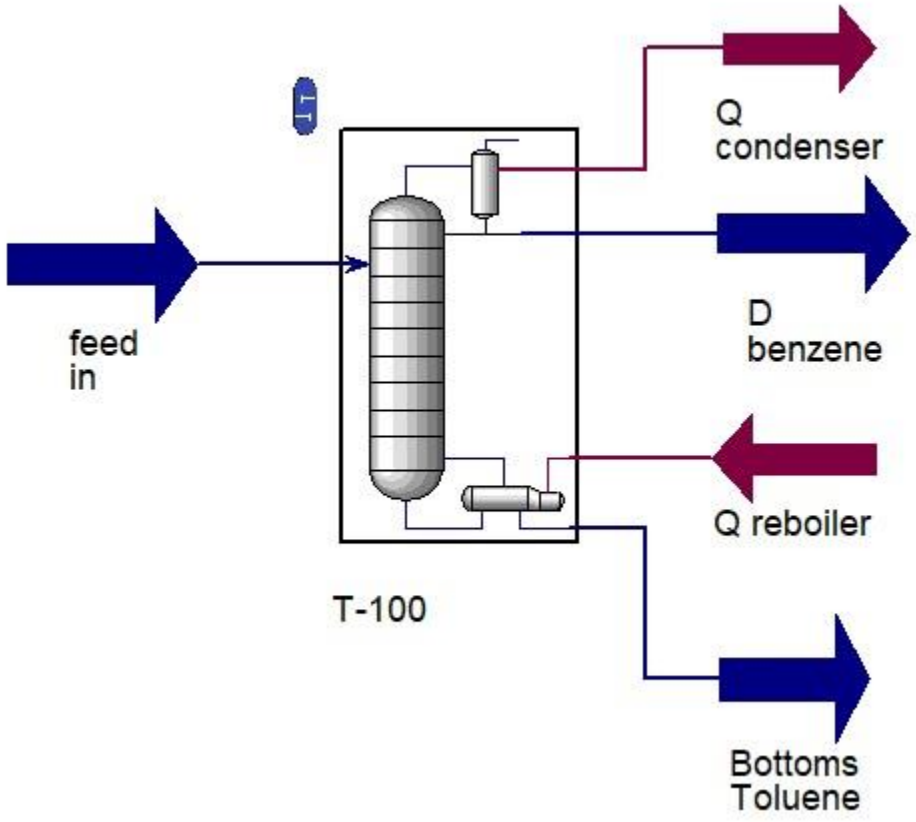
- Save the case:

1. File menu
2. Select save as
3. Give the name (compressor)

References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Modeling of Distillation Column Using HYSYS V9 -2-



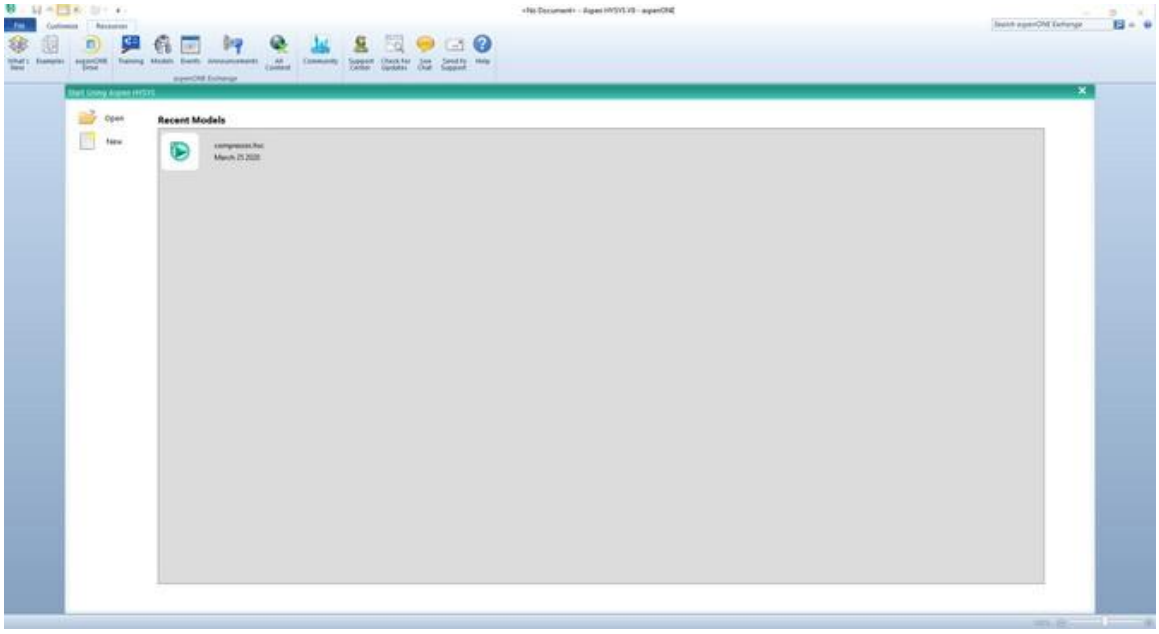
The figure above shows a simple model containing the Distillation Column with inlet, and outlet streams using Aspen HYSYS V.9.

Example:

A material stream consists of 40% Benzyn and 60% Toluene with temperatureof 35^{o}C, pressure of 1.1 atm, and flowrate of 140 kgmole/h is fed into a distillation column so that these components are separated into two material streams. Give the required steps to simulate this separation process using (distillation column sub0flowsheet).

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



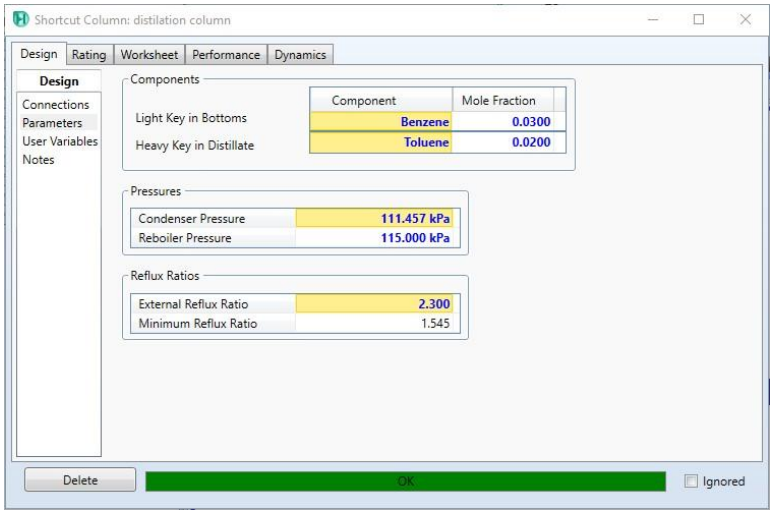
The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new window.

- Open the case (distillation):

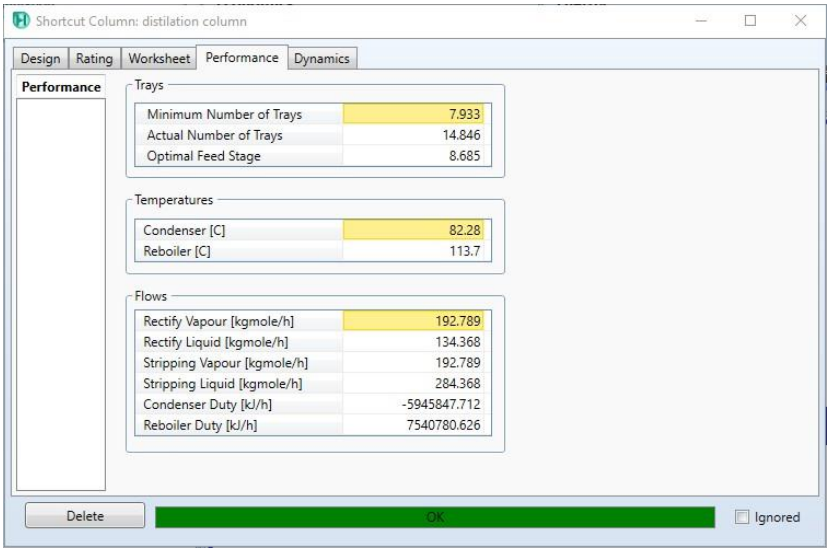
1. File menu
2. open \ dostillation

- checking the external reflux ratio and actual number of trays:

1. Simulation \ (short cut distillation)
2. double click
3. design \ parameters : read the (external reflux ratio)



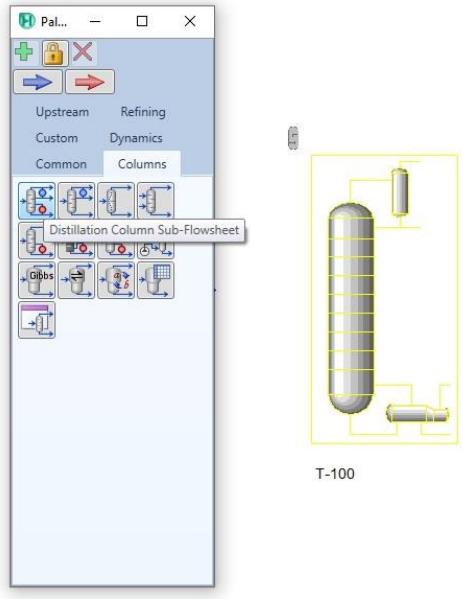
4. Performance \ trays : read (actual number of trays)



- Delete the (short cut distillation) and streams (Distillate benzene, Q condenser, Q reboiler, Vottoms toluen)

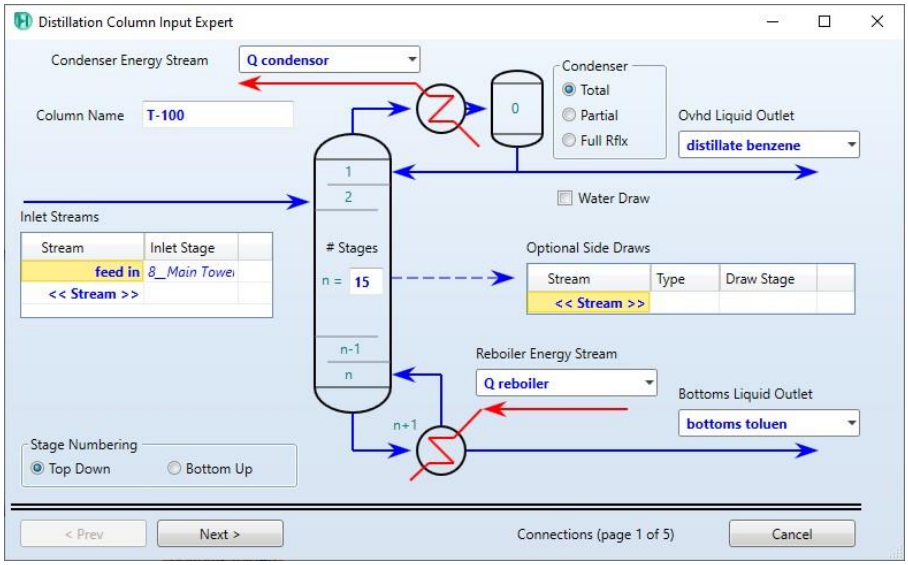
- Adding (distillation column sub-flowsheet)

1. Simulation
2. Object palette \ columns
3. Select (distillation column sub-flowsheet)
4. Place the selected unit in the deisred location inside the flowsheet

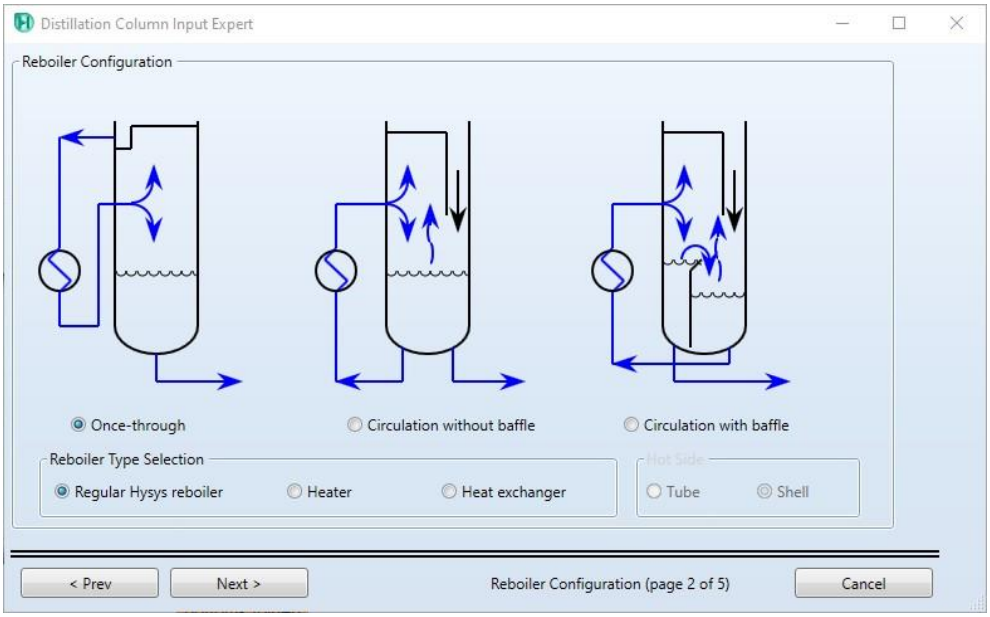


5. Double click
6. Set (Stages \ n=15)
7. In inlet streams, select (feed in)
8. In Condenser energy stream field, type (Q condenser). [a new energy stream will be created and connected to the distillation column]
9. In Reboiler energy stream field, type (Q Reboiler). [a new energy stream will be created and connected to the ditillation column]
10. Select condensor \ total
11. In Ovhd Liquid Outlet field, type (Distillate Benzene). [a new material stream will be created and connected to the distillation column]

12. In Bottoms Liquid Outlet field, type (Bottoms toluene). [a new material stream will be created and connected to the distillation column]
13. Click (Next)



14. In reboiler configuration select (once through)
15. Click (Next)

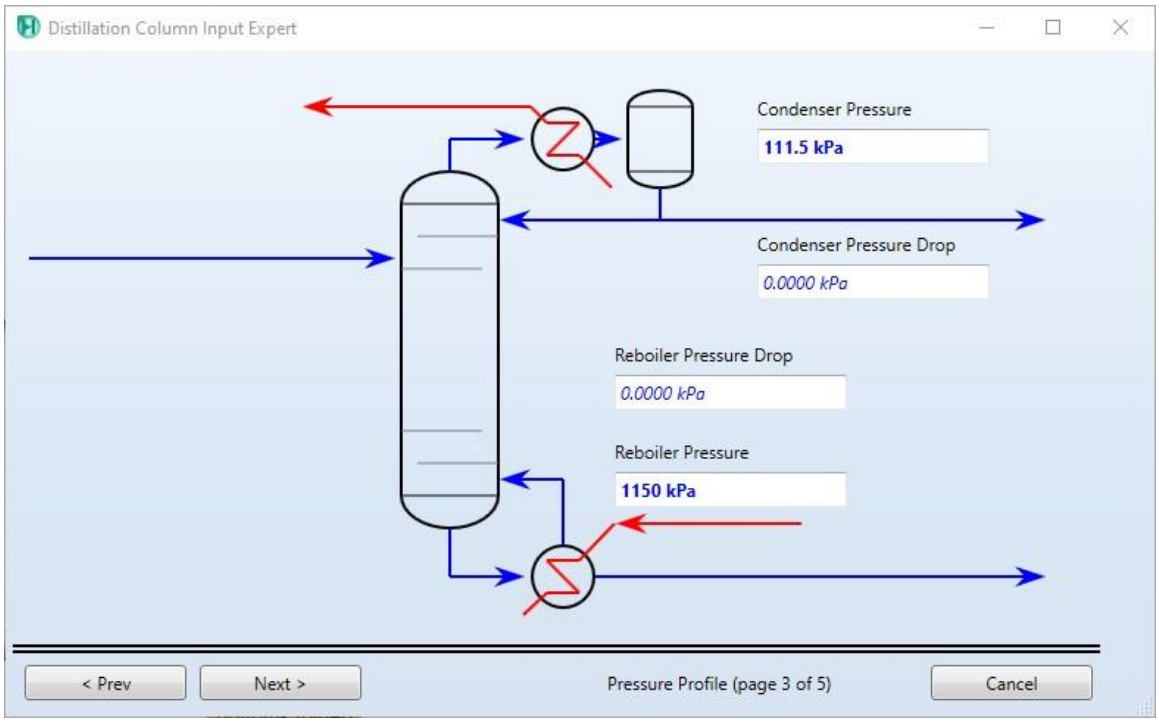


16.Set the condenser pressure to 1.1 atm

17.Set the reboiler pressure to 115 KPa

18.Set the pressure drop in both condenser and reboiler to 0 KPa

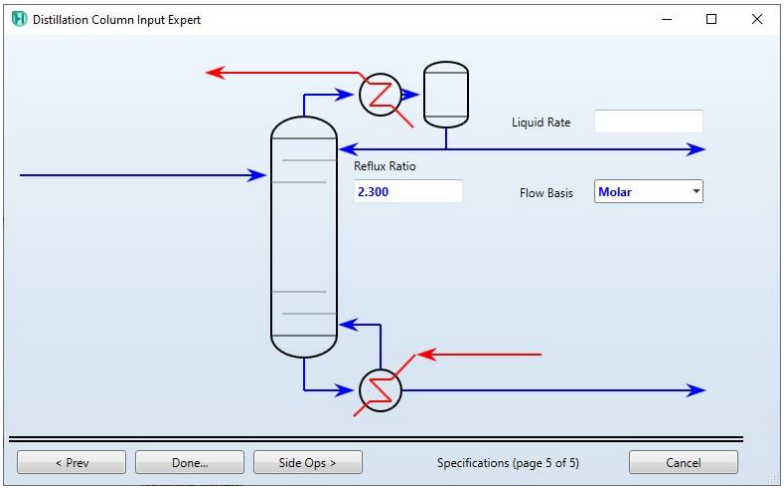
19.Click (Next)



20.In optional estimates page click (Next)

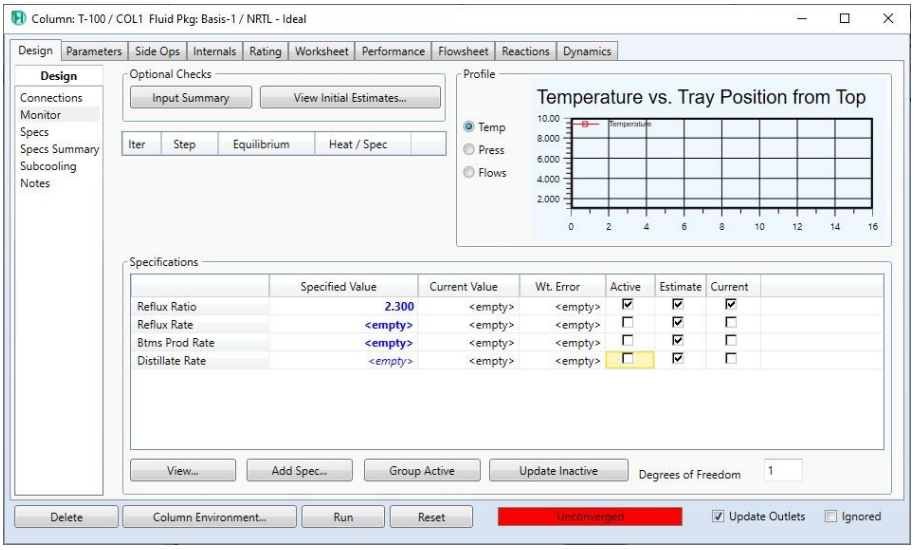
21.In specification page \ set the reflux ratio to 2.3

22.Click (Done)

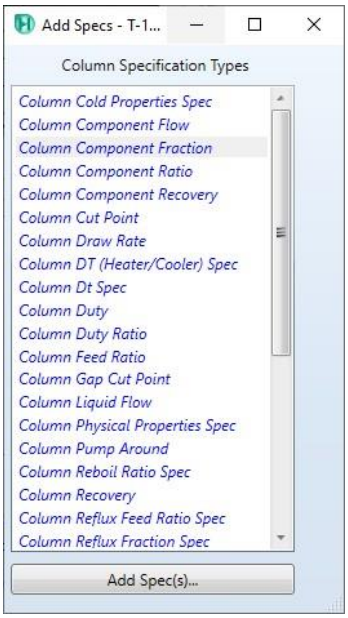


- Specifications

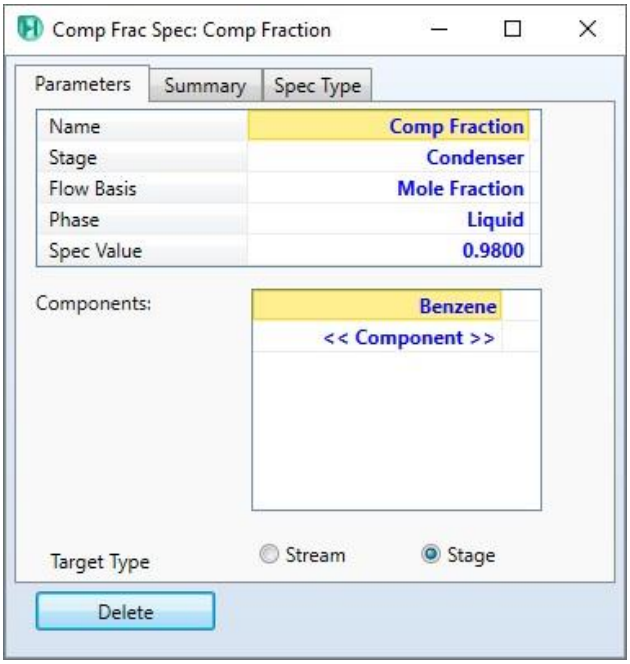
1. Design
2. Monitor \ specifications
3. Uncheck the active state of (Distillate rate)



4. Click (Add Spec…)
5. Select (Column component fraction)
6. Click (Add spec(s)…)



7. Select the added specification
8. Double click
9. In stage field : select (condenser)
10. In flow Basis : select (Mole fraction)
11. In Phase : select (Liquid)
12. Set the Spec Value to 0.98
13. In components select (Benzene)



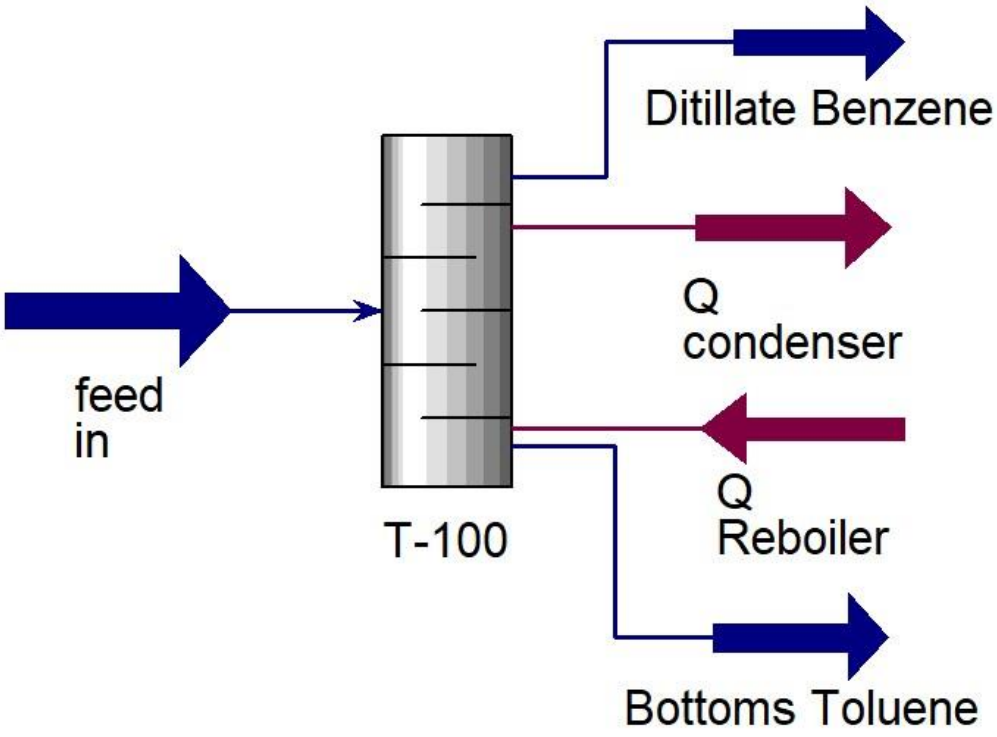
- Run

1. Click Run
2. Internals
3. Click (Auto sections)
4. Performance

References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Modeling of Distillation Column Using HYSYS V9



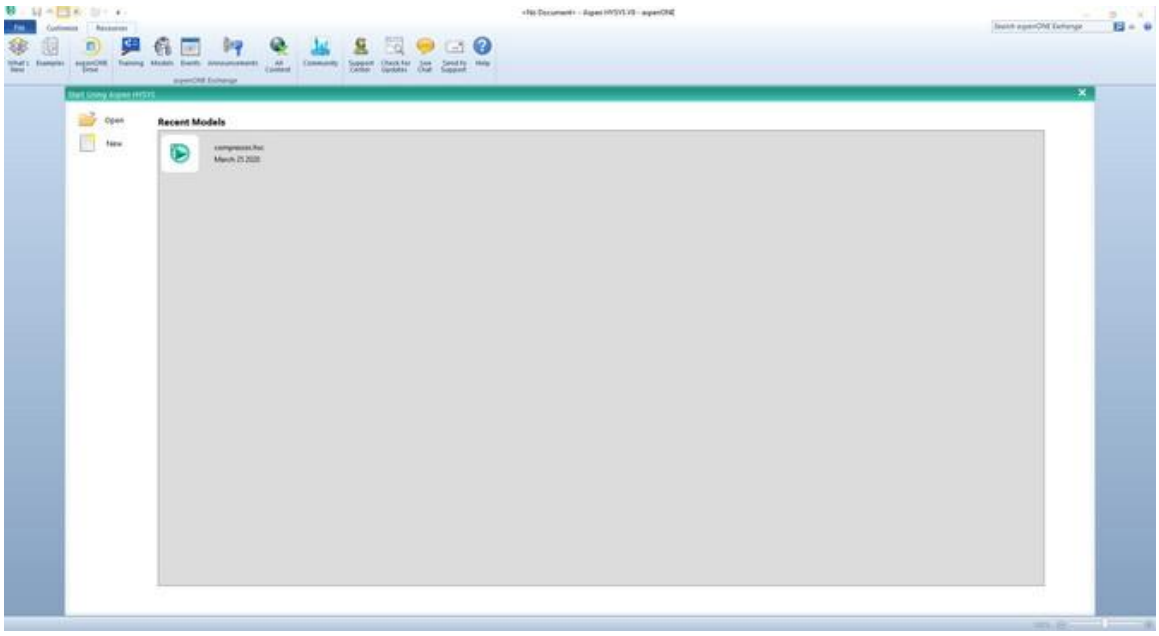
The figure above shows a simple model containing the Distillation Column with inlet, and outlet streams using Aspen HYSYS V.9.

Example:

A material stream consists of 40% Benzyn and 60% Toluene with temperatureof 35°C, pressure of 1.1 atm, and flowrate of 140 kgmole/h is fed into a distillation column so that these components are separated into two material streams. Give the required steps to simulate this separation process.

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new window.

- Create a new case:

1. File menu
2. New \ case

- There are two main necessary information have to be given in the properties tab before starting the simulation:

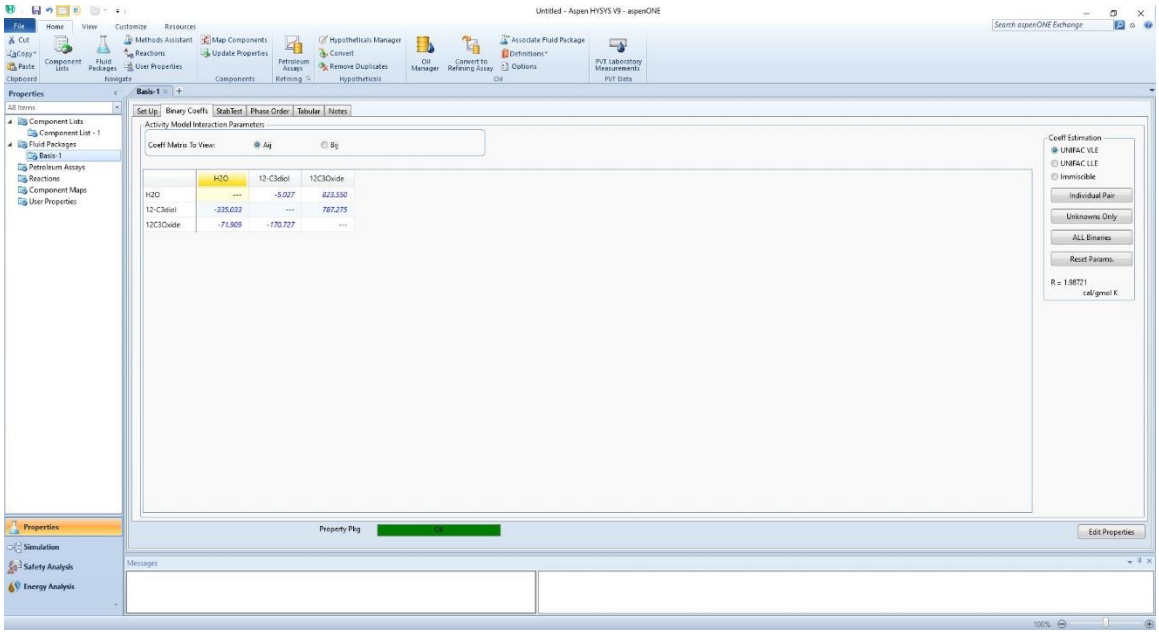
1. Property package : NRTL
2. Components: Benzyn, Toluene

- Adding Component list:

1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the serach field Benzyn
5. Select Benzyn \ add
6. Repeat the steps (4,5) for Toluen

- Add fluid package:

1. Properties
2. Select Fluid package
3. Click Add
4. Select (NRTL)
5. Binary Coeffs
6. Click (Unknown only)

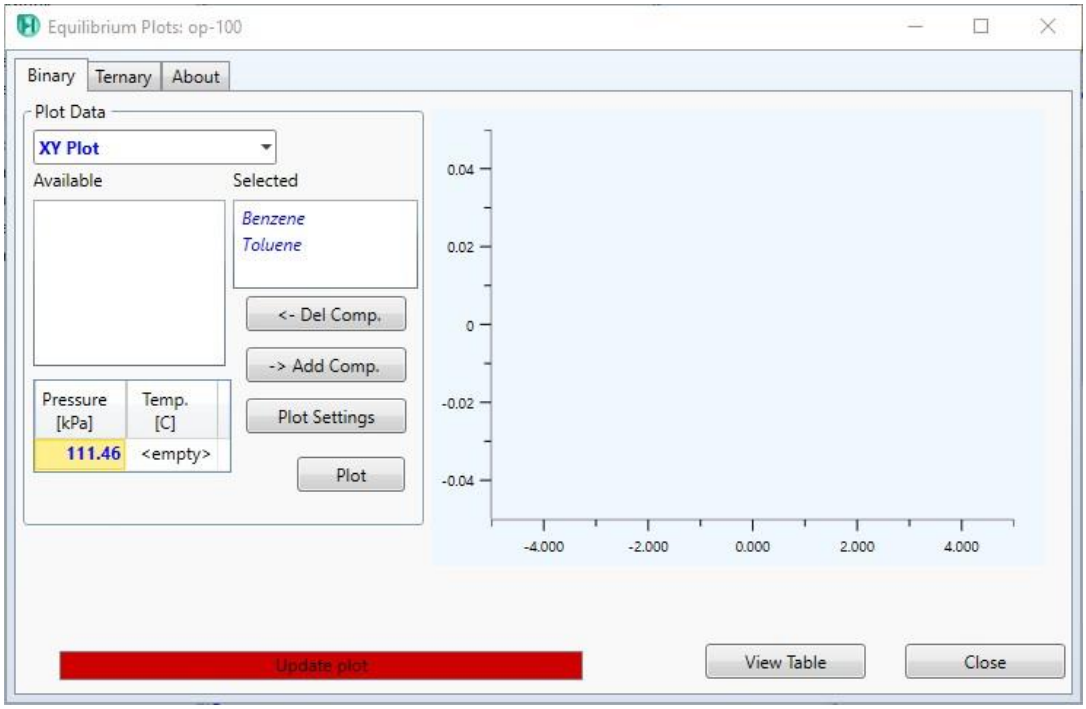


- Test the isotropic point:

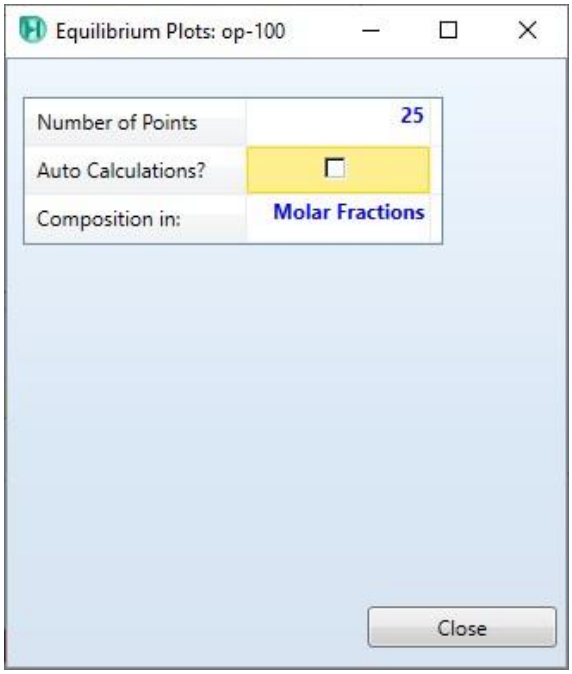
1. Select simulation.
2. Object palette \ custom
3. Select Equilibrium Unit Operation.
4. Place the selected unit in the desired position.

op-100

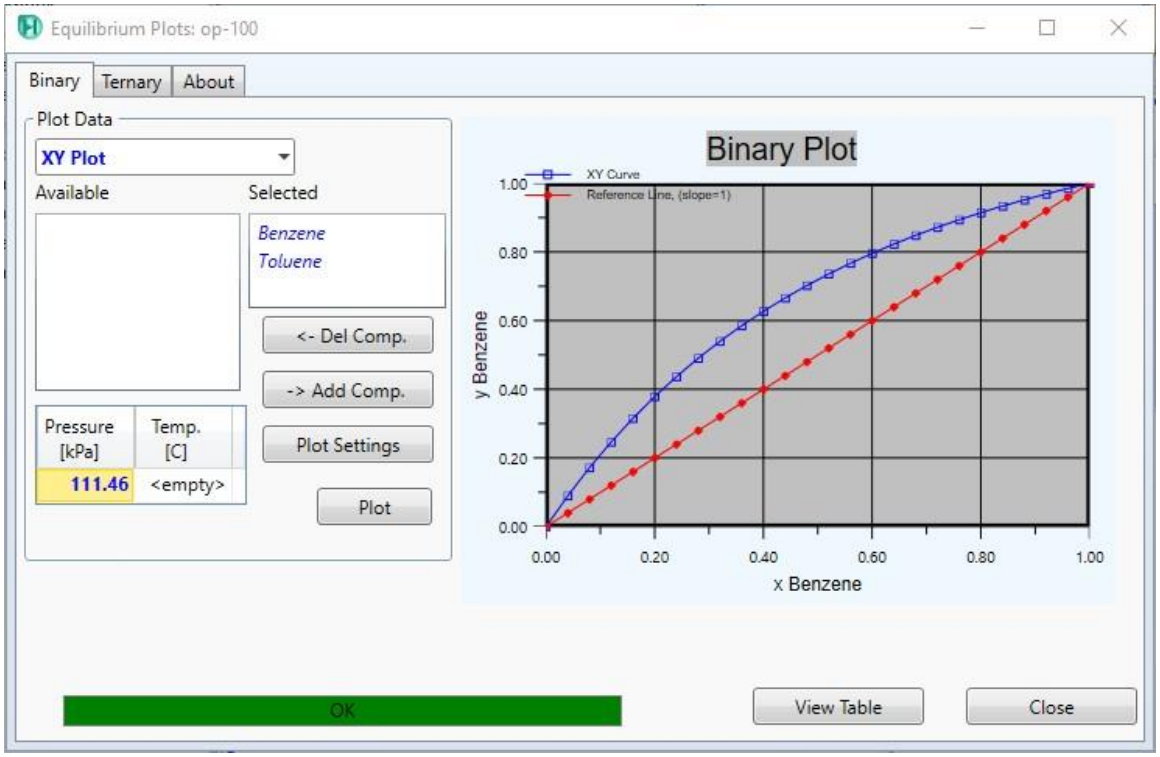
5. Double click on the added unit
6. Binary
7. Available
8. Select Benzene
9. Click (Add Comp.)
10. Select Toluene
11. Click (Add Comp.)
12. Set the pressure to 1.1 atm
13. Data plot
14. Select (XY plot)



15. Click plot settings
16. Set the number of points to 25
17. Click close



18. Click plot



- Create new material streams:

1. Select simulation.
2. Object palette.
3. Select the material stream icon.

Alternatively, you can add new material stream by pressing F11.

4. Double click on the added material stream
5. Give the below information:

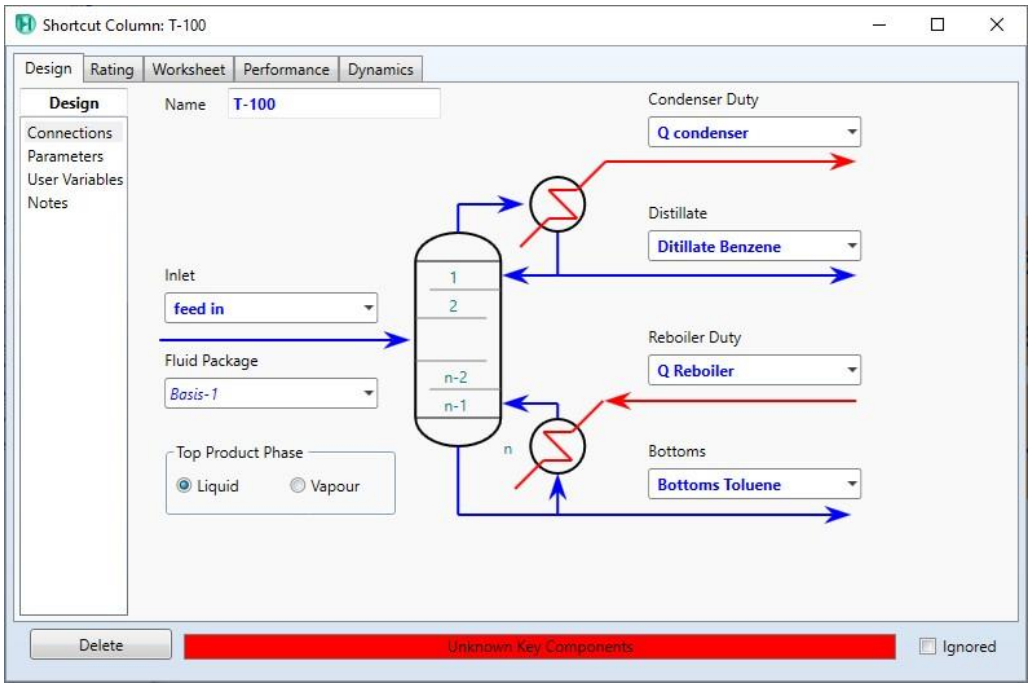
Name	Feed in
Conditions	
Temperature	35°C
PRESSURE	1.1 atm
Molar flow	140 lbmole/h
Composition	
Benzene	0.4
Toluene	0.6

- Adding distillation column:

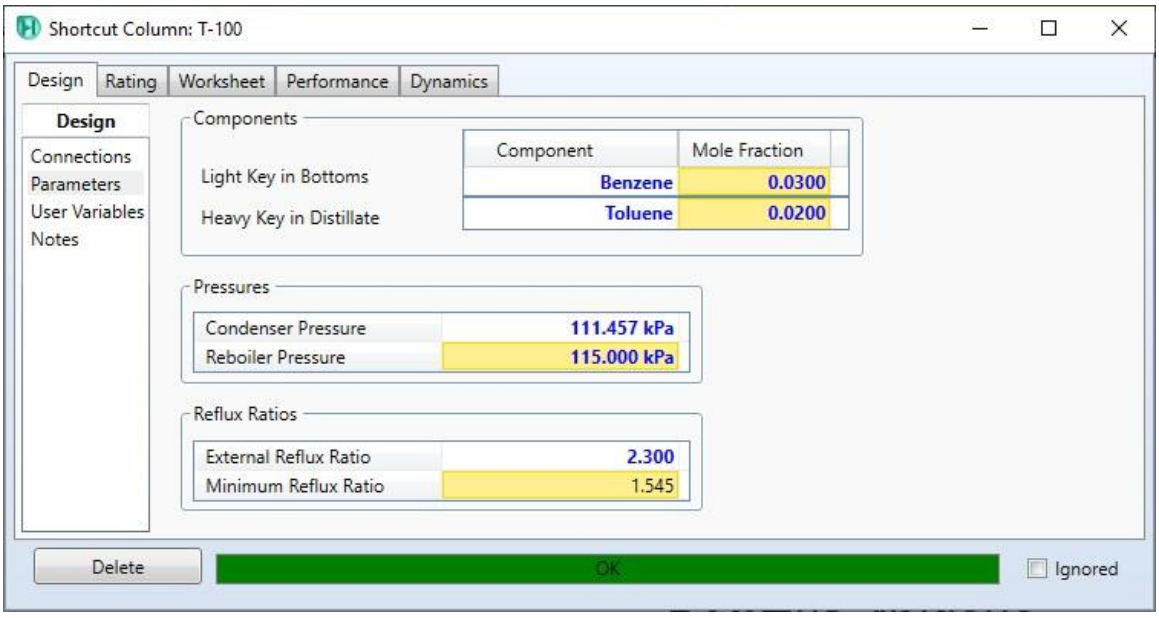
6. Object palette\ column
7. Select (short cut distillation)
8. Place the selected unit in the desired position.

You can add a new unit by pressing F12 and select the desired unit.

9. Double click on the distillation column
10. In inlet field, select (feed in)
11. In Condenser Duty field, type (Q condenser). [a new energy stream will be created and connected to the compressor]
12. In Dsitillate field, type (Distillate Benzene). [a new material stream will be created and connected to the compressor]
13. In Reboiler Duty field, type (Q Reboiler). [a new energy stream will be created and connected to the compressor]
14. In Dsitillate field, type (Bottoms Toluene). [a new material stream will be created and connected to the compressor]



15. Design \ parameters \ Components
16. Set the mole fraction in (Light key in Bottoms) to (0.03) for (Benzene).
17. Set the mole fraction in (Heavy key in Distillate) to (0.02) for (Toluene).
18. Set the condenser pressure to 1.1 atm
19. Set the condenser pressure to 115 KPa
20. Set the External Reflux ratio to 2.3



- Save the case:

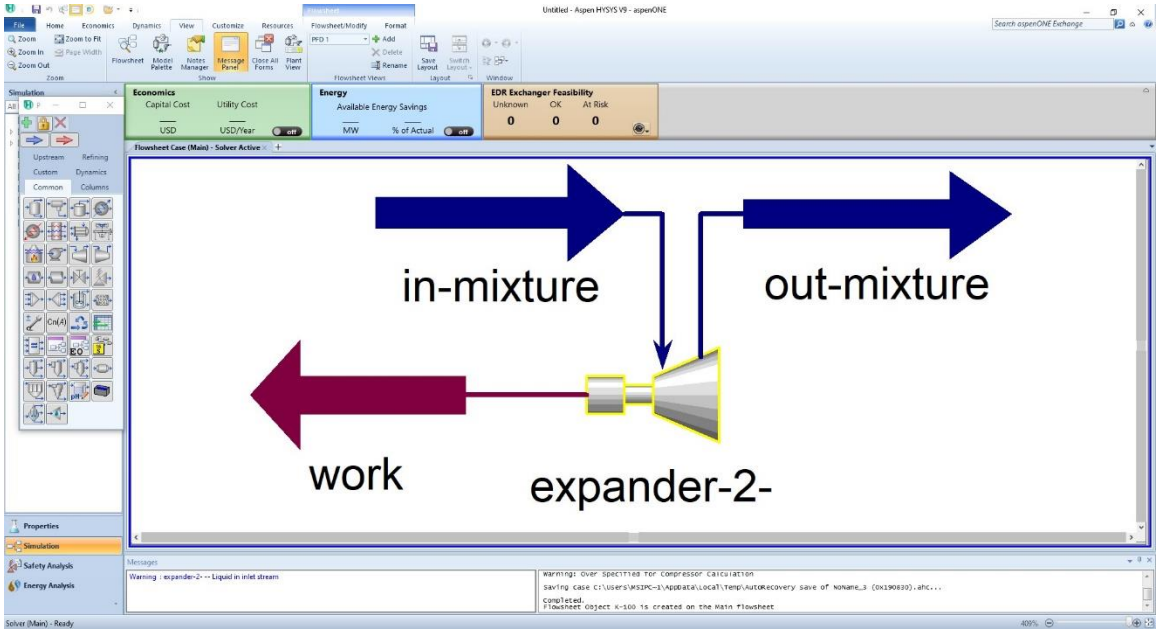
1. File menu
2. Select save as
3. Give the name (Distillation)

References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Modeling of Expander using HYSYS V9

High pressure gas stream can be processed by the expansion operation to produce an outlet mixture with low pressure and high velocity. The expansion process converts the internal energy of the gas to kinetic energy. Expanders units in HYSYS are used to decrease the pressure of the inlet streams giving the possibility to calculate the related properties such as the temperature and the operation efficiency. In this subject, it is intended to learn how to work with the expander unit to model the expansion process as well as set up the unit connections and other design parameters. In the end, it would be possible to operate the expander according to the given information.



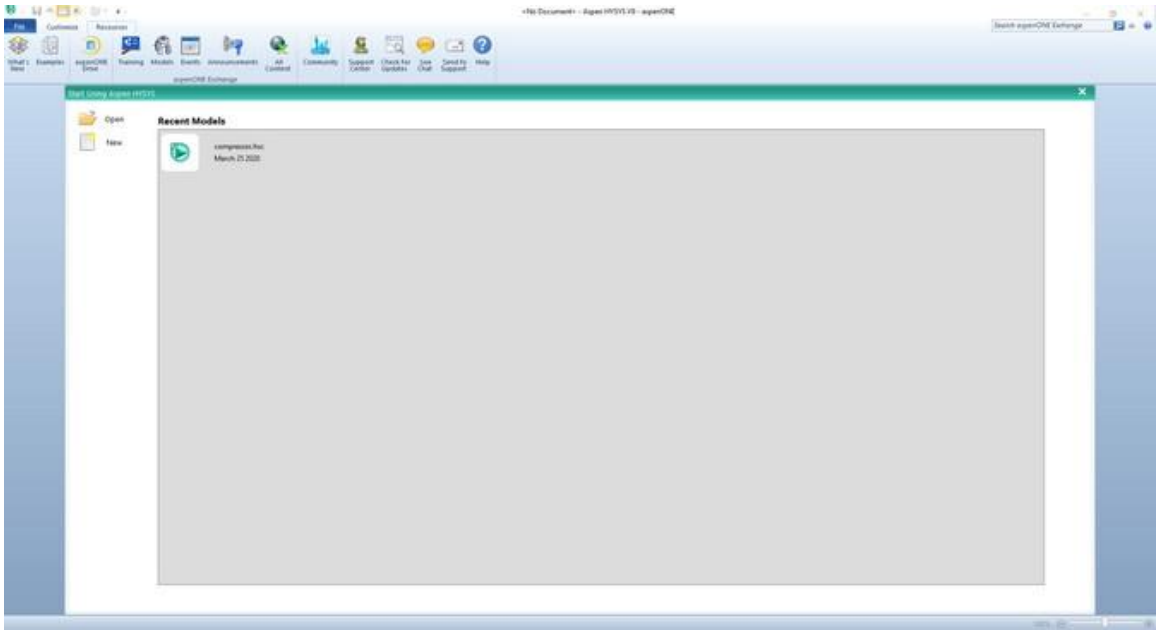
The figure above shows a simple model containing the expander with inlet, outlet and energy streams using Aspen HYSYS V.9.

Example:

A mixture of (Methane, Ethane, Propane, and and i-Butane) at 30^{o} C and 25 bar is fed into an expander with 20% efficiency. the pressure of the outlet stream is 10 bar while the flow rate of the mixture is 100 kgmole/h. determine the outlet temperature using the SRK equation of state.

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



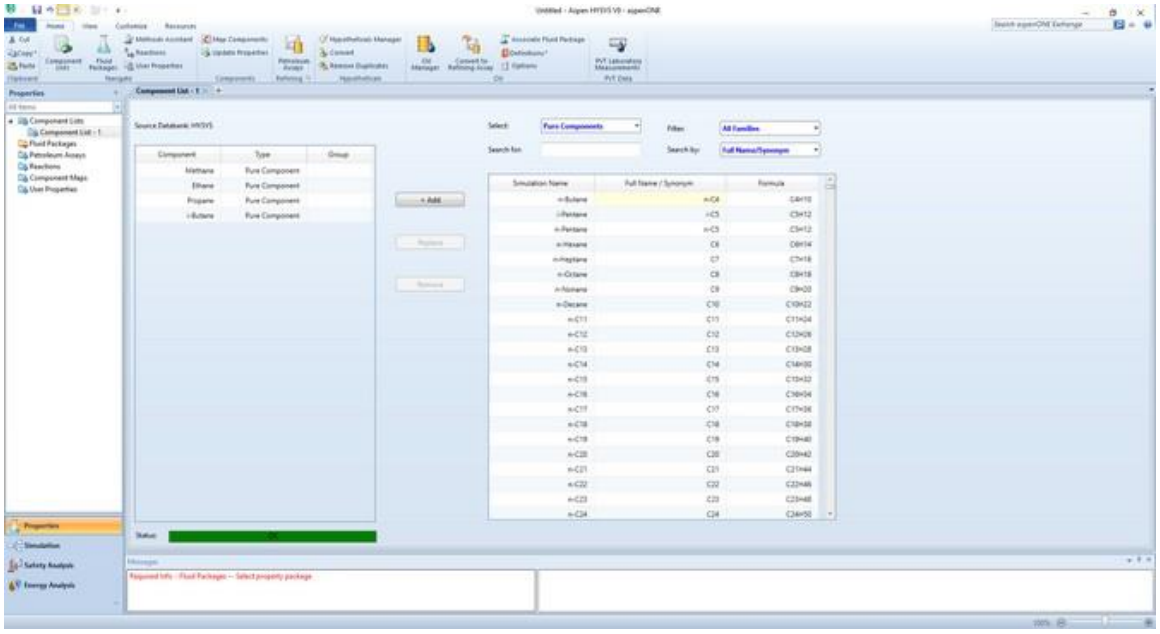
The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.

- Create a new case:

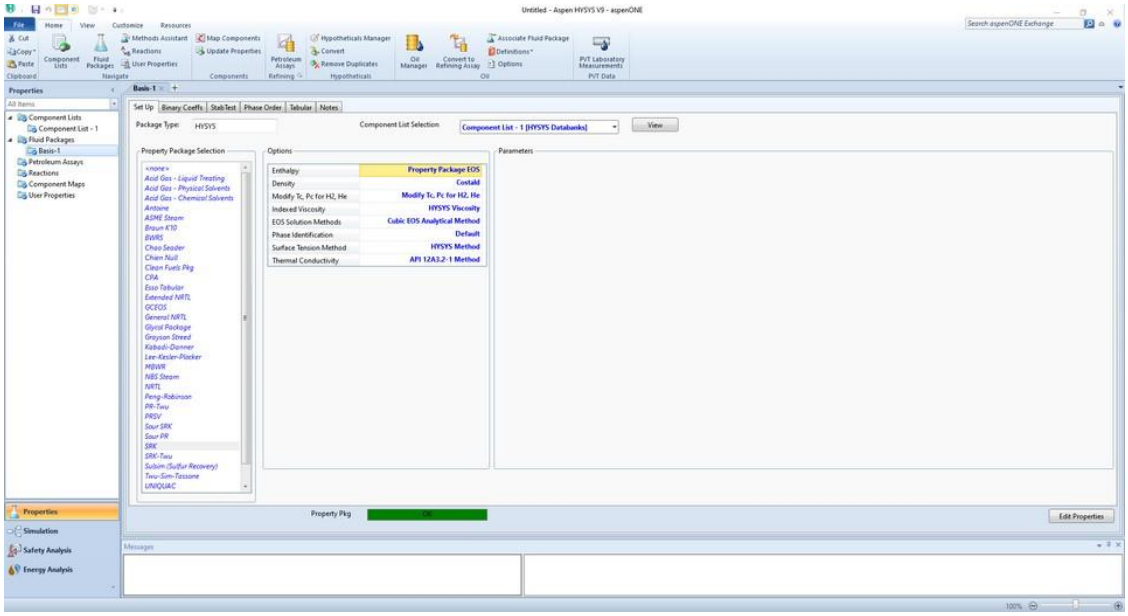
1. File menu
2. New \ case

- There are two main necessary information have to be given in the properties tab before starting the simulation:
    1. Property package : SRK
    2. Components: C1, C2, C3 , i-C4

1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the serach field C1
5. Select C1 \ add
6. Repeat the steps (4,5) for C2, C3 and i-C4



- Add fluid package:
  1. Select Fluid package
  2. Click Add
  3. Select (SRK)



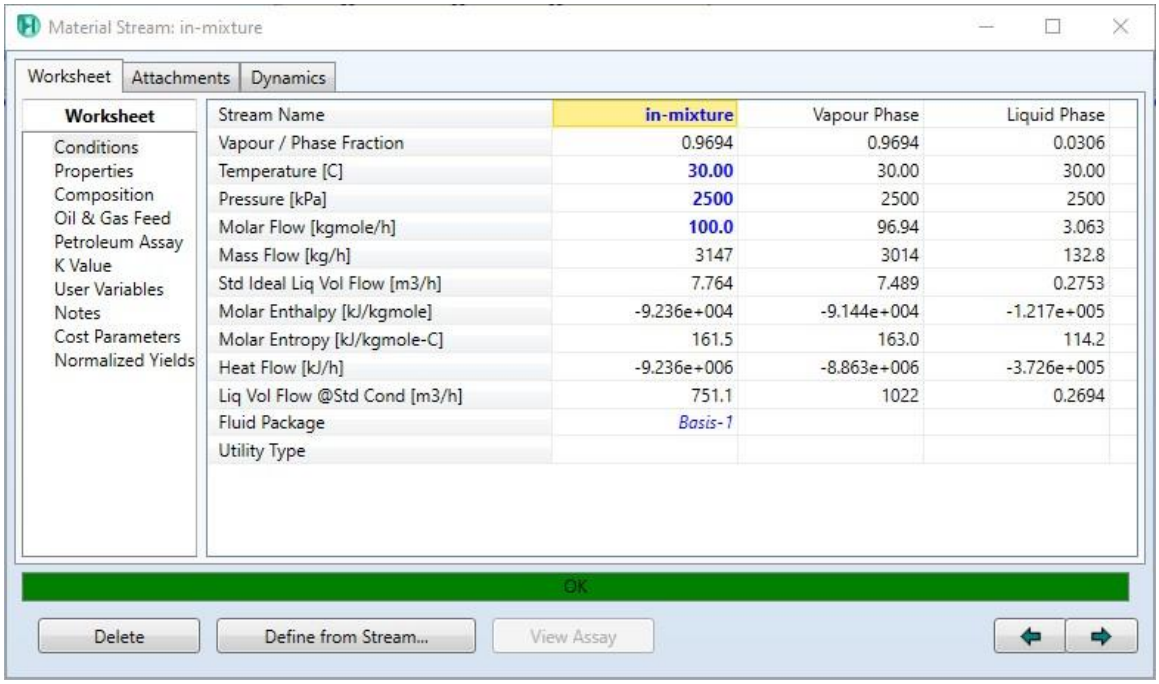
- Create new material stream:
  1. Select simulation.
  2. Object palette.
  3. Select the material stream icon.

Alternatively, you can add new material stream by pressing F11.

4. Double click on the added material stream
5. Give the below information:

Name	In-mixture
Conditions	
Temperature	30^{O} C
Pressure	25 bar
Molar flow	100 kgmole/h
Composition	
C1	0.3
C2	0.4
C3	0.2
i-C4	0.1

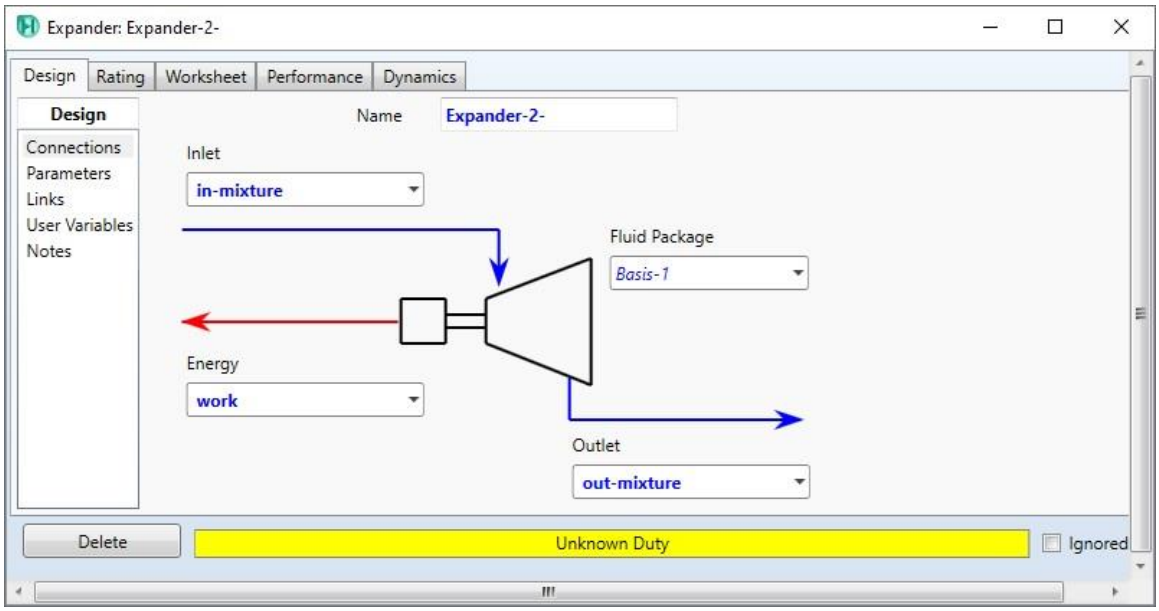
The above information should be given according to the application or example.



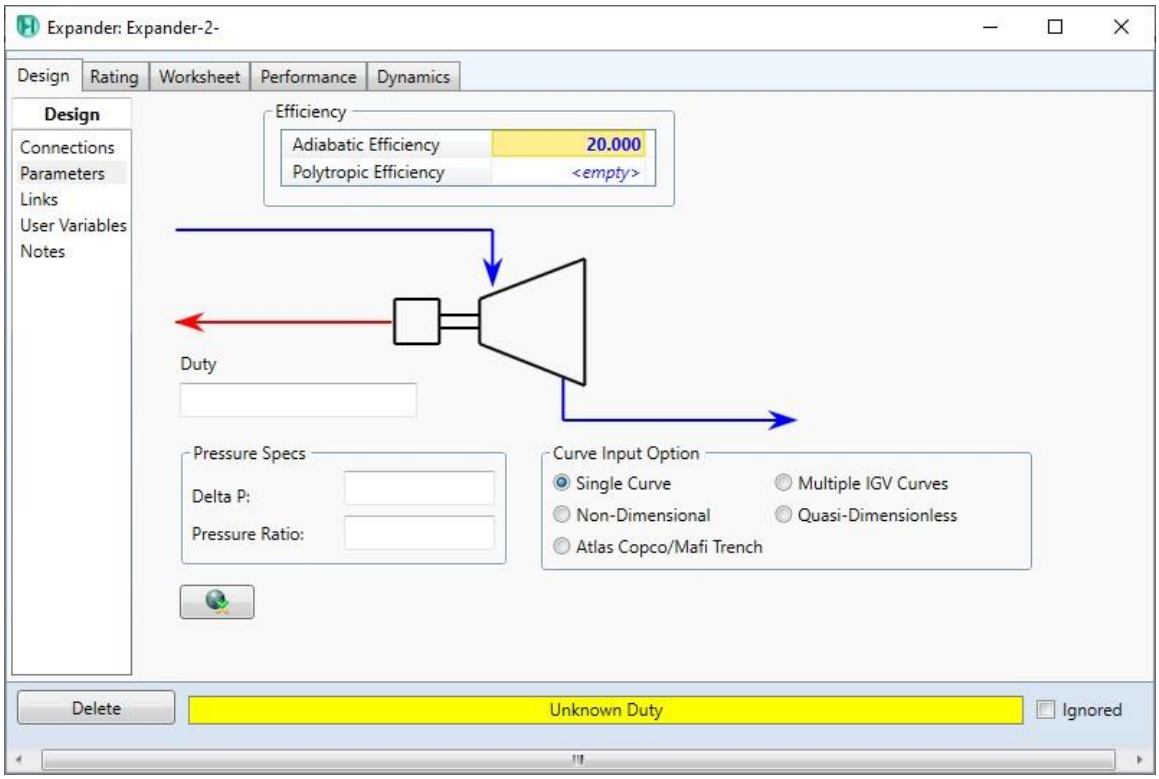
- Adding Expander:
    1. Object palette.
    2. Select expander
    3. Place the selected unit in the desired position.

You can add a new unit by pressing F12 and select the desired unit.

4. Double click on the expander
5. Select Design \ connections
6. In the inlet field, select in-mixture
7. In the outlet field, type (out-mixture). [a new material stream will be created and connected to the expander]
8. In the Energy field, type work. [a new energy stream will be created and connected to the expander].

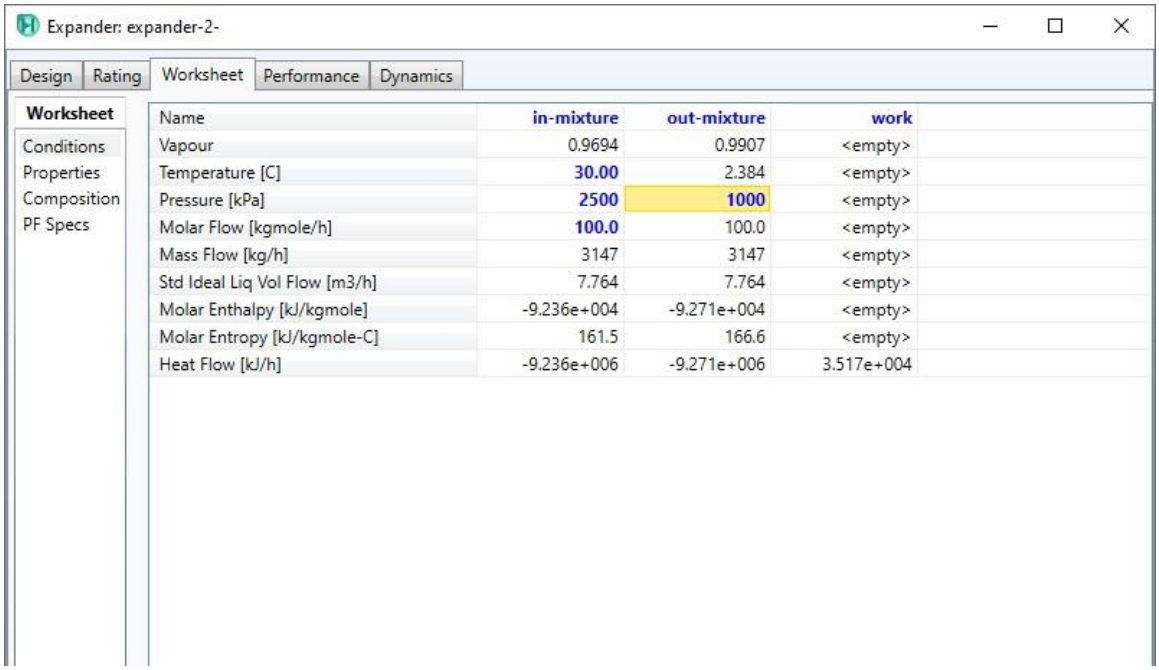


9. Select parameters \ Adiabatic Efficiency
10. Change the efficiency to 20 %.
11. Select worksheet



12. Change the outlet-gas pressure to 10 bar.
13. Read the temperature of the outlet-gas.

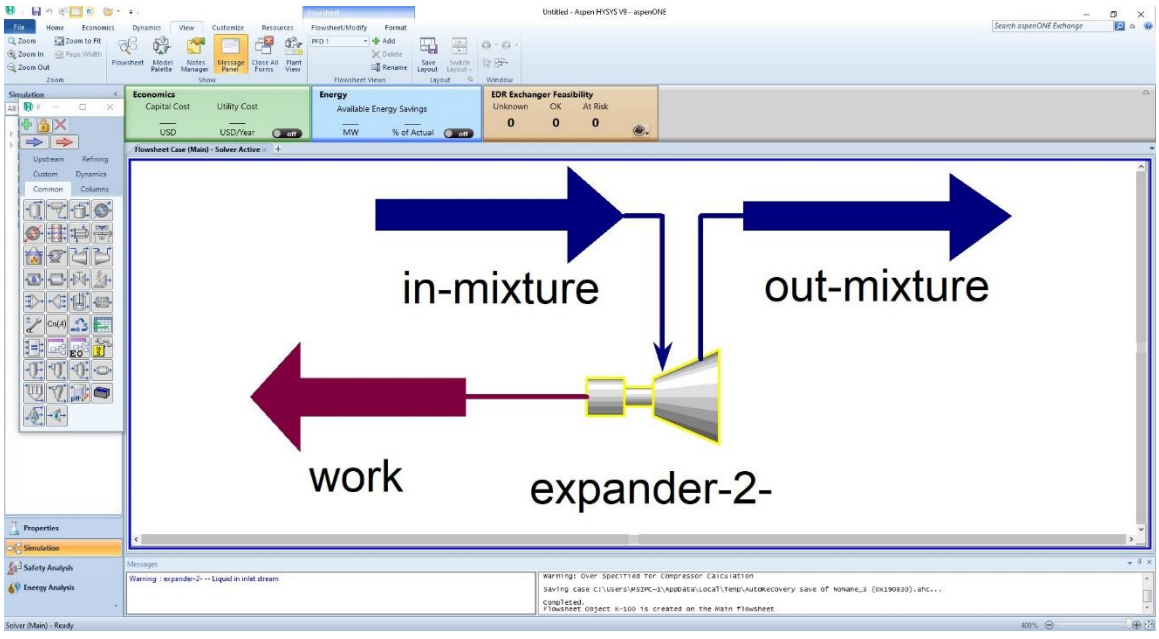
The temperature of the outlet stream is 2.384º C.



Name	in-mixture	out-mixture	work
Vapour	0.9694	0.9907	<empty>
Temperature [C]	30.00	2.384	<empty>
Pressure [kPa]	2500	1000	<empty>
Molar Flow [kgmole/h]	100.0	100.0	<empty>
Mass Flow [kg/h]	3147	3147	<empty>
Std Ideal Liq Vol Flow [m3/h]	7.764	7.764	<empty>
Molar Enthalpy [kJ/kgmole]	-9.236e+004	-9.271e+004	<empty>
Molar Entropy [kJ/kgmole-C]	161.5	166.6	<empty>
Heat Flow [kJ/h]	-9.236e+006	-9.271e+006	3.517e+004

- Save the case:

1. File menu
2. Select save as
3. Give the name (expander)

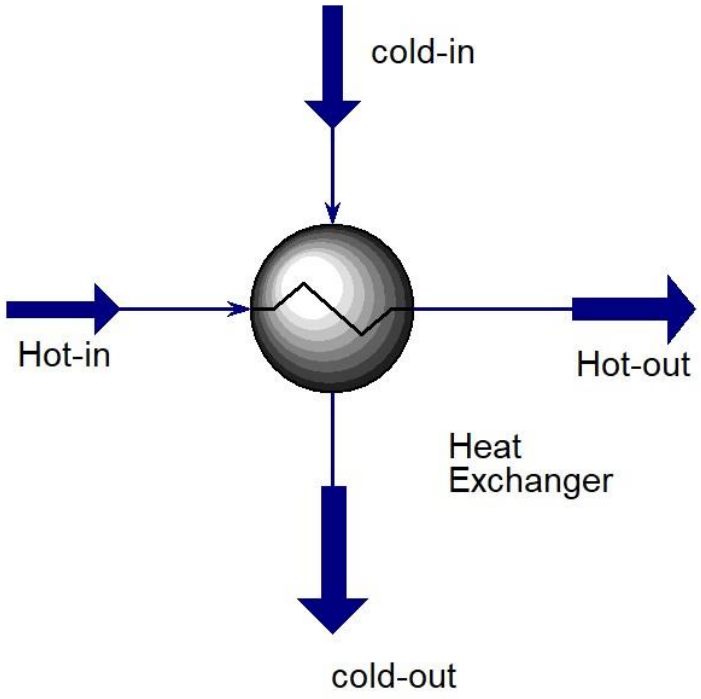


References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Modeling of heat Exchanger using HYSYS V9

HYSYS can be used to model the heat exchanger and determine the flowrate of the material stream passing through the unit at certain conditions. Shell and tube heat exchanger in Aspen HYSYS V9 can give material balance calculations. In this subject, it is intended to learn how to work with this unit to model such process and how to connect the right streams in their optimum directions as well as setting up the other related parameters.



The figure above shows a simple model containing the heat exchanger unit with the two sided inlet, outlet streams using Aspen HYSYS V.9.

Example:

Given that a shell and tube heat changer is used to heat a cold water at 20^{o} C and 110 psig via a hot water stream at 300^{o} C and 1100 psig. The temperatures of the outlet cold and hot streams are 135^{o} C and 220^{o} C. The flow rate of the hot stream is 100 kg/h. using Peng-Robinson as a fluid package, determine the mass low of the cold stream.

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.

- Create a new case:

1. File menu
2. New \ case

- There are two main necessary information have to be given in the properties tab before starting the simulation:
  1. Property package : Peng-Robinson
  2. Components: H_2O

- Create list of components

1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the serach field H_2O
5. Select H_2O \ add

- Add fluid package:
    1. Select Fluid package
    2. Click Add
    3. Select (Peng-Robinson)
- Create new material stream:
    1. Select simulation.
    2. Object palette.
    3. Select the material stream icon.

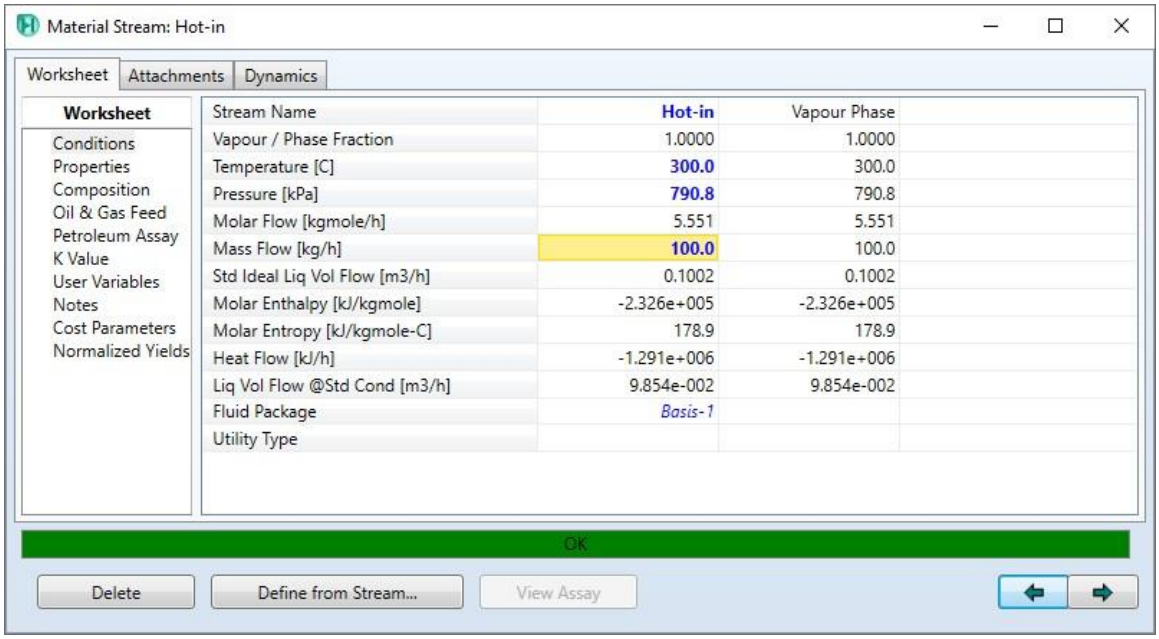
Alternatively, you can add new material stream by pressing F11.

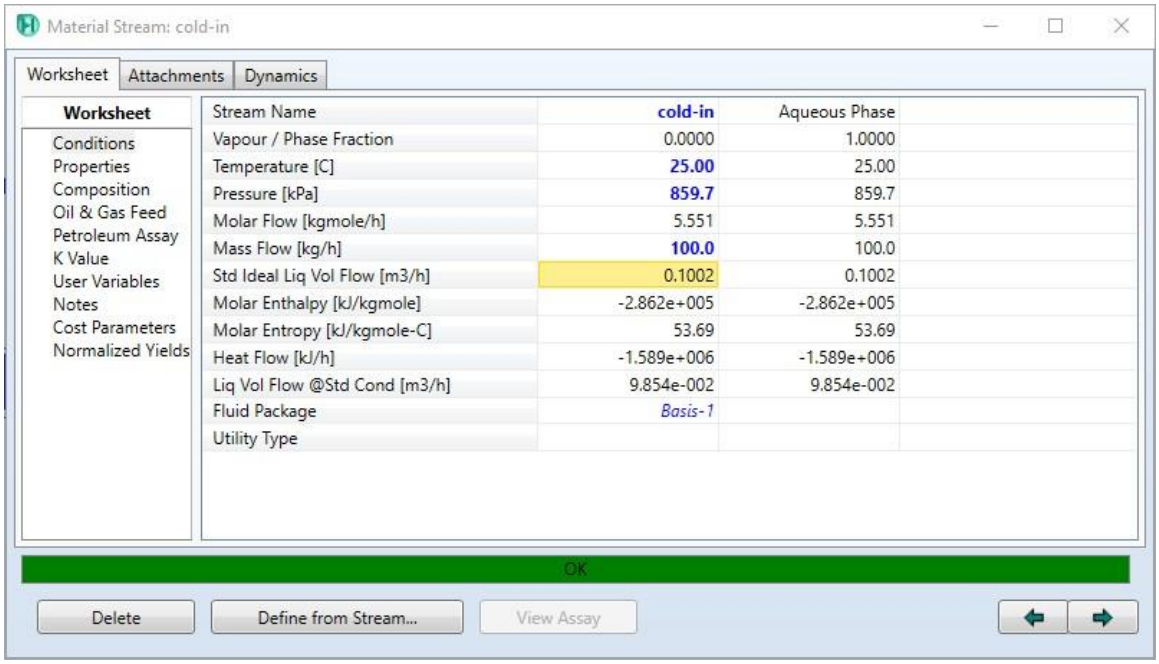
4. Double click on the added material stream
5. Give the below information:
6.

Name	Hot-in
Conditions	
Temperature	300^{O} C
Pressure	1100 psig
Mass flow	100 kg/h
Composition	
H_2O	1

7. Repeat the steps (2,3,4) for adding a material stream with the following information:

Name	Cold-in
Conditions	
Temperature	20^{O} C
Pressure	110 psig
Composition	
H_2O	1

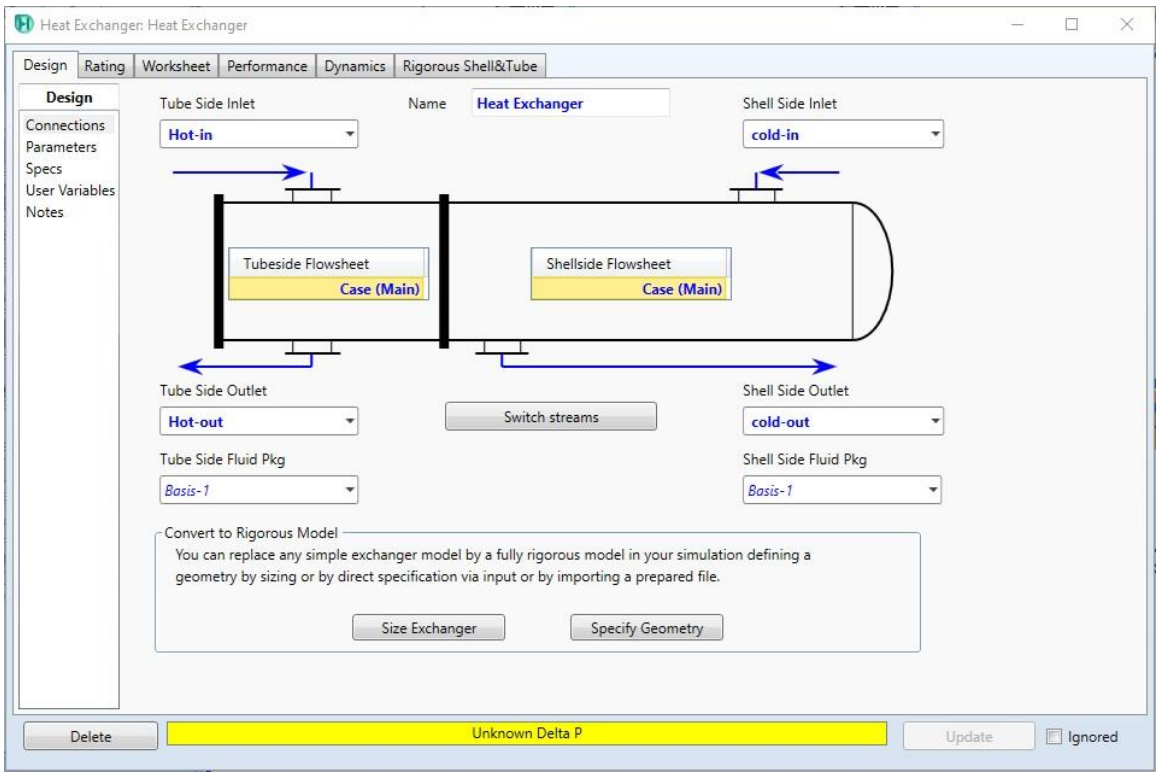




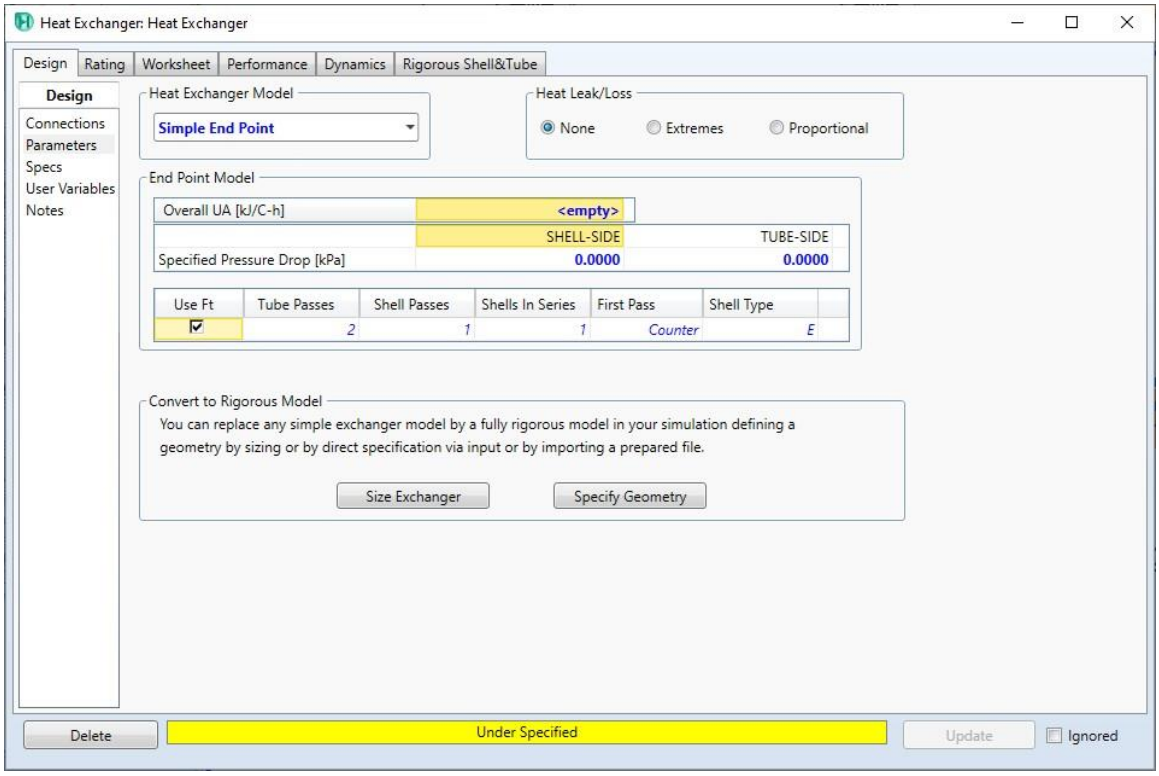
- Adding heat exchanger:
    1. Object palette.
    2. Select heat exchanger
    3. Place the selected unit in the desired position.

You can add a new unit by pressing F12 and select the desired unit.

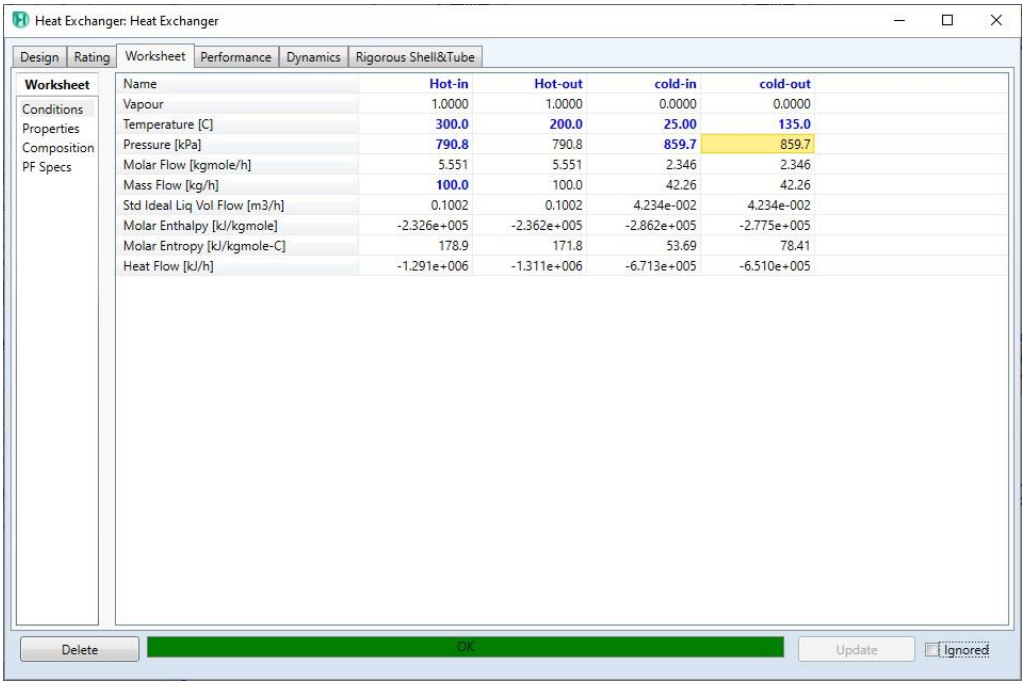
4. Double click on the heat exchanger
5. Select Design \ connections
6. In the Tube side Inlet field, select Hot-in
7. In the Tube side outlet field, type (Hot-out). [a new material stream will be created and connected to the heat exchanger]
8. In the Shell side Inlet field, select cold-in
9. In the Tube side outlet field, type (cold-out). [a new material stream will be created and connected to the heat exchanger]



10. Select parameters \ Specified Pressure Drop
11. Change the drop to (0) in shell side and tube side.

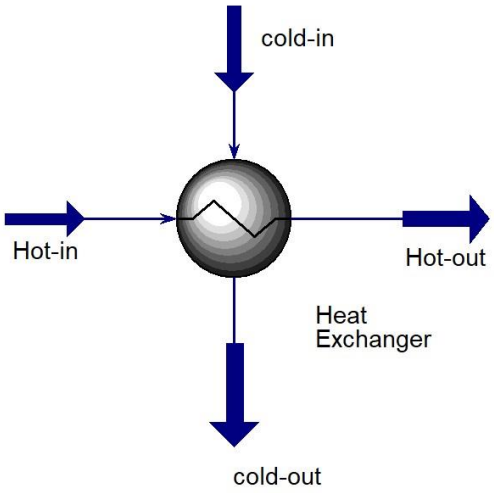


12. Select worksheet
13. Change the temperature in hot-out to 200º C
14. Change the temperature in cold-out to 135º C



15. Read the mass flow of the cold stream.

The mass flow of the cold stream is 42.26 Kg/h.



- Save the case:

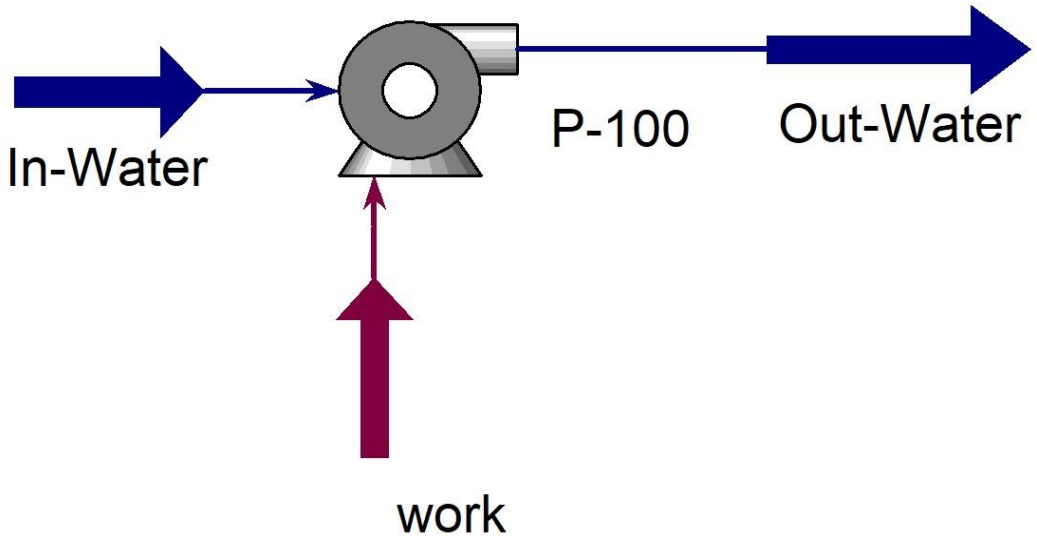
1. File menu
2. Select save as
3. Give the name (expander)

References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Modeling of Pump using HYSYS V9

It is possible to increase the pressure of the liquid stream using the pump unit. Pumping process for inlet material streams is modeled in Aspen HYSYS V9 including the calculation of the desired properties like temperature and efficiency. In this subject, it is intended to learn how to work with the Pump unit to model the pumping process as well as set up the unit connections and other design parameters. In the end, it would be possible to operate the pump according to the given condition.



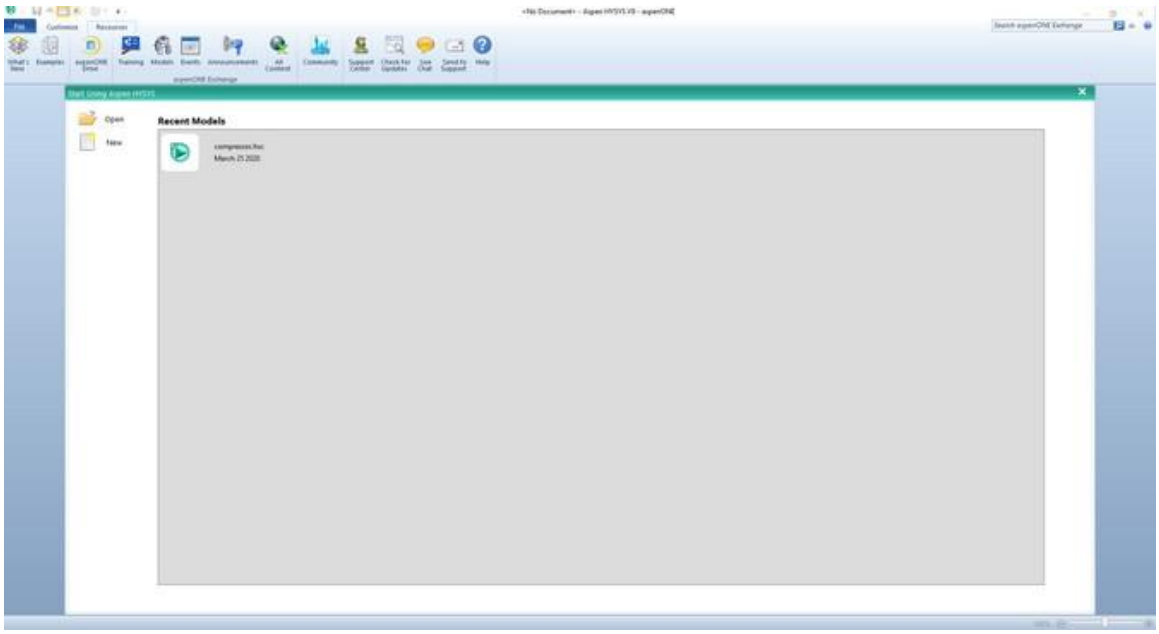
The figure above shows a simple model containing the Pump with inlet, outlet and energy streams using Aspen HYSYS V.9.

Example:

Material stream of Water at 130^{o}C and 4 bar is fed into a pump with 15% efficiency. The pressure of the outlet stream is 90 bar and the flow rate of the water is 100 kgmole/h. Deteremine the outlet temperature of the water using Peng-Robinson equation [1].

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



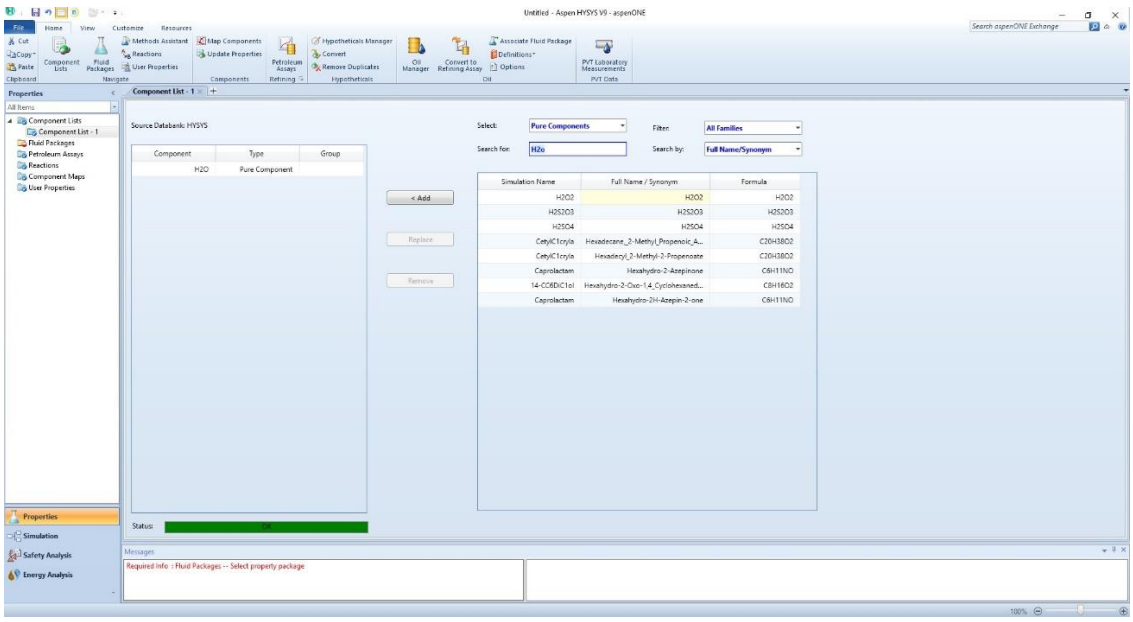
The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.

- Create a new case:

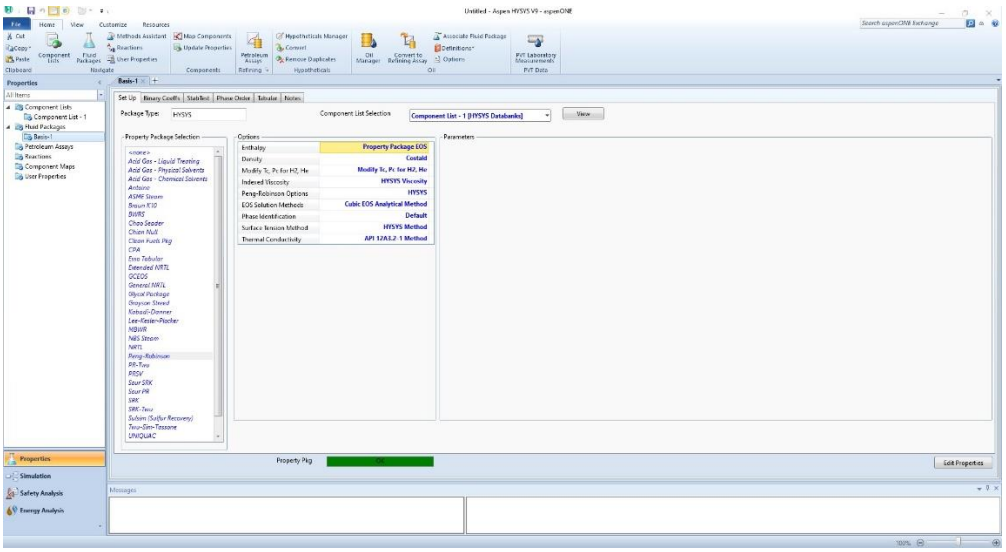
1. File menu
2. New \ case

- There are two main necessary information have to be given in the properties tab before starting the simulation:
    1. Property package : Peng-Robinson
    2. Components: H_2O

1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the search field H_2O



- Add fluid package:
    1. Select Fluid package
    2. Click Add
    3. Select (Peng-Robinson)



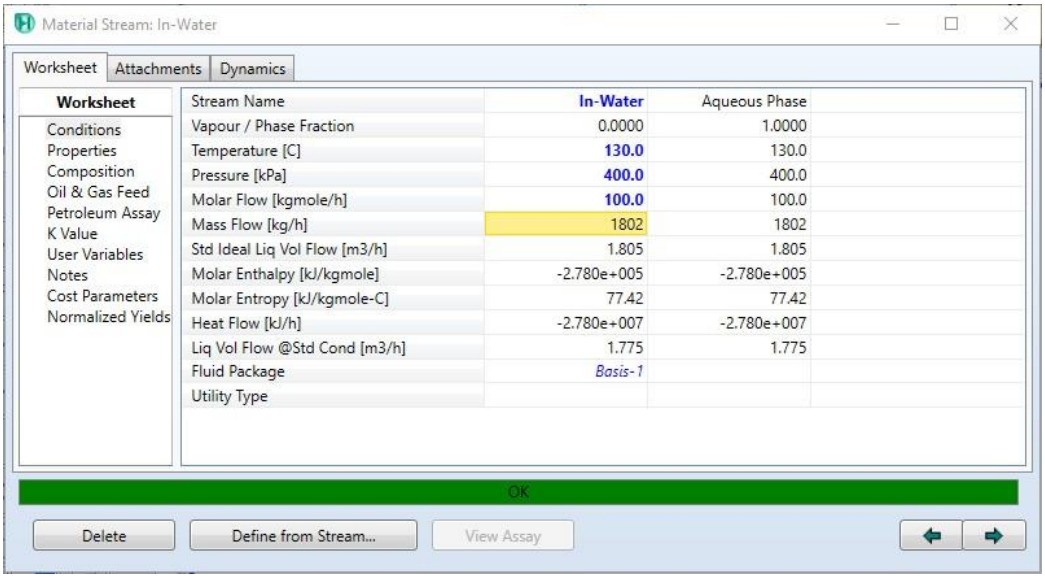
- Create new material stream:
  1. Select simulation.
  2. Object palette.
  3. Select the material stream icon.

Alternatively, you can add new material stream by pressing F11.

4. Double click on the added material stream
5. Give the below information:

Name	In-Water
Conditions	
Temperature	130^{O} C
Pressure	4 bar
Molar flow	100 kgmole/h
Composition	
H_2O	1

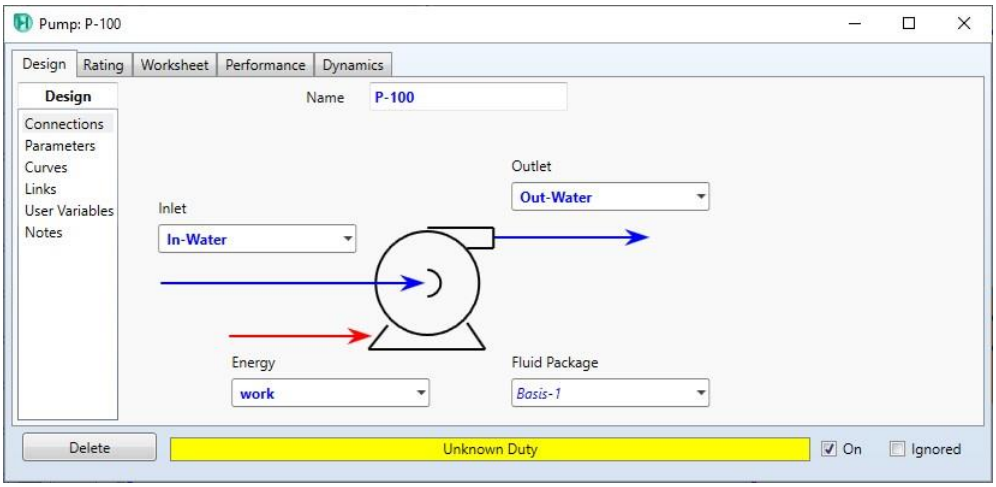
The above information should be given according to the application or example.



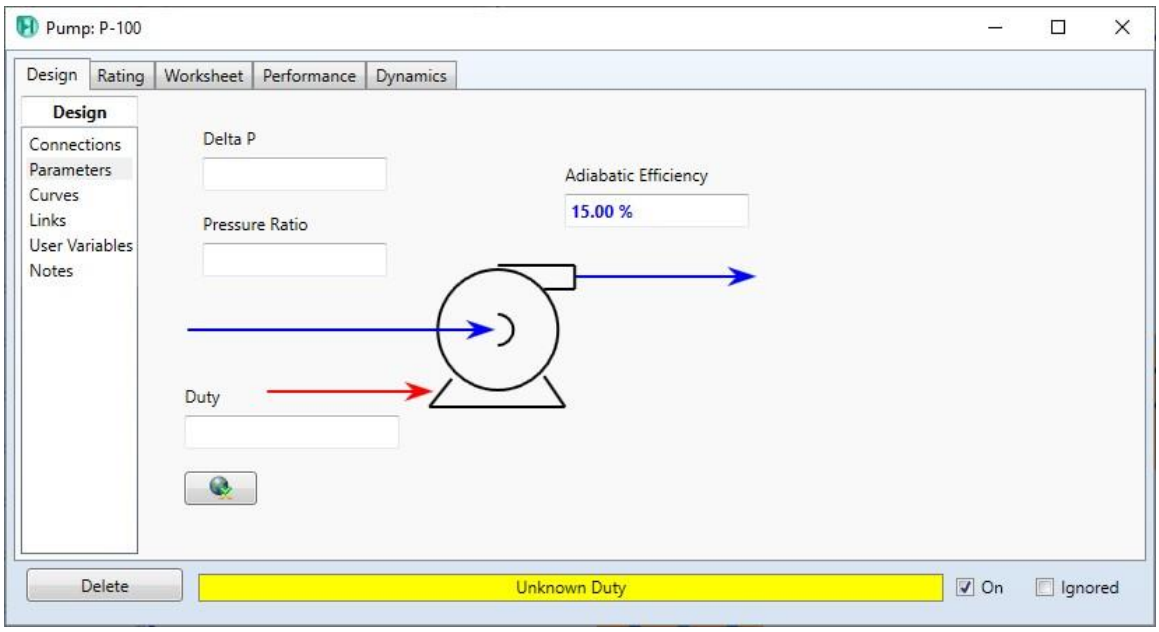
- Adding Pump:
    1. Object palette.
    2. Select pump
    3. Place the selected unit in the desired position.

You can add a new unit by pressing F12 and select the desired unit.

4. Double click on the Pump
5. Select Design \ connections
6. In the inlet field, select In-Water
7. In the outlet field, type (Out-water). [a new material stream will be created and connected to the pump]
8. In the Energy field, type work. [a new energy stream will be created and connected to the Pump].

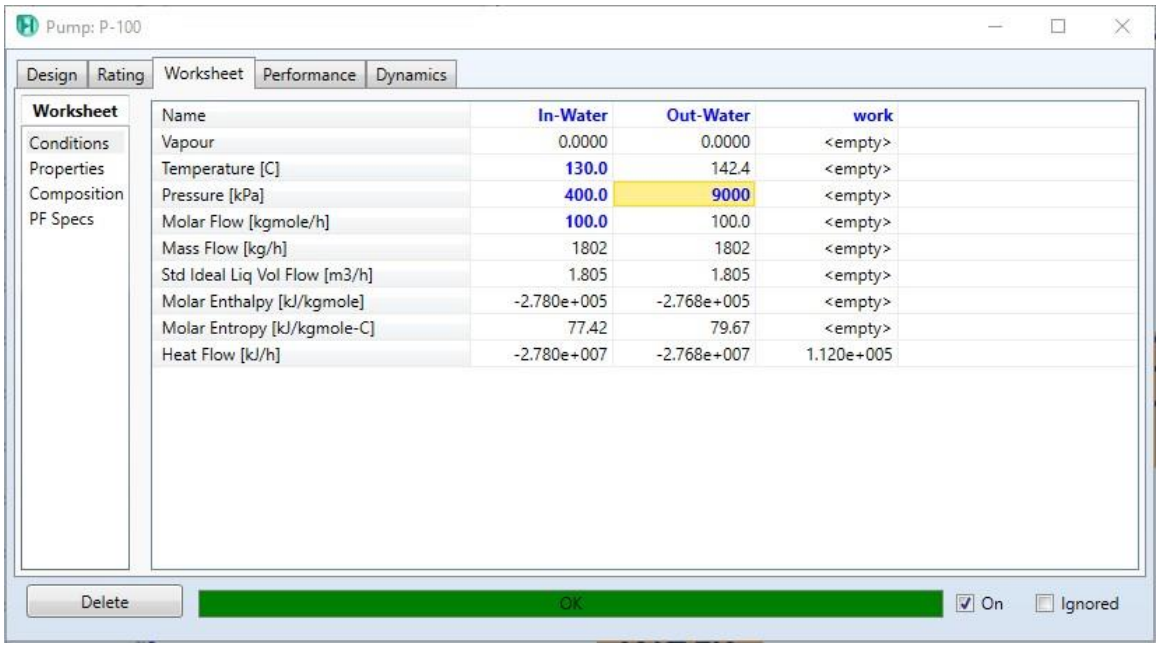


9. Select parameters \ Adiabatic Efficiency
10. Change the efficiency to 15 %.



11. Select worksheet
12. Change the outlet-stream pressure to 90 bar.
13. Read the temperature of the outlet-stream.

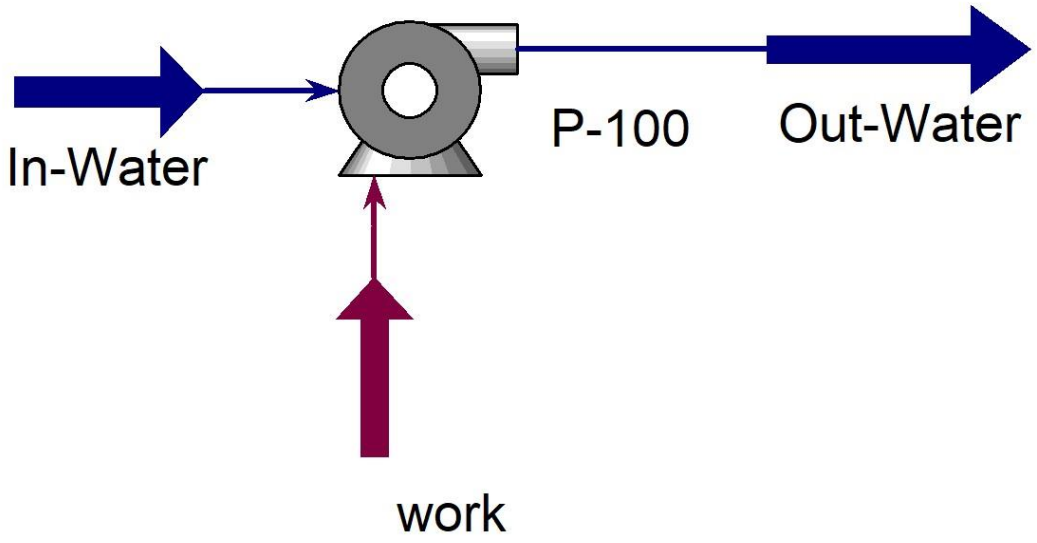
The temperature of the outlet stream is 142.4^{o} C.



Name	In-Water	Out-Water	work
Vapour	0.0000	0.0000	<empty>
Temperature [C]	130.0	142.4	<empty>
Pressure [kPa]	400.0	9000	<empty>
Molar Flow [kgmole/h]	100.0	100.0	<empty>
Mass Flow [kg/h]	1802	1802	<empty>
Std Ideal Liq Vol Flow [m3/h]	1.805	1.805	<empty>
Molar Enthalpy [kJ/kgmole]	-2.780e+005	-2.768e+005	<empty>
Molar Entropy [kJ/kgmole-C]	77.42	79.67	<empty>
Heat Flow [kJ/h]	-2.780e+007	-2.768e+007	1.120e+005

- Save the case:

1. File menu
2. Select save as
3. Give the name (pump)



References:

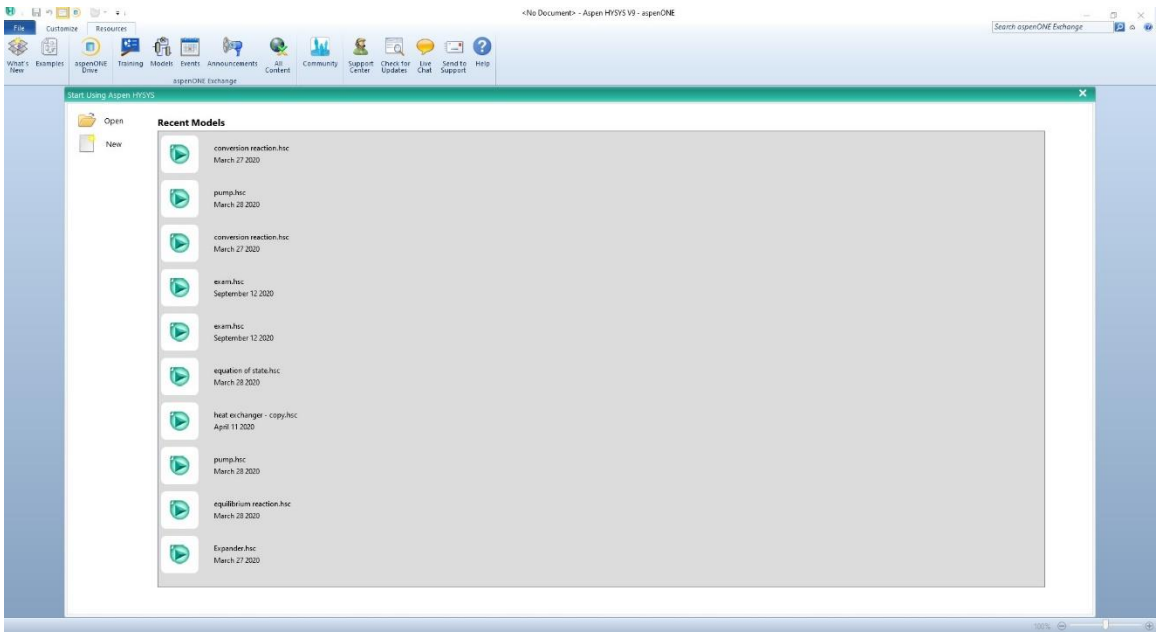
1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Starting HYSYS V9

HYSYS V9 is a professional simulation tool in chemical engineering applications. It presents a comprehensive environment including the design and modeling, facilitated interface, active interactivity and result visualizations. HYSYS is commonly given in universities and laboratories as a simulation and modeling software for chemical engineers with different levels. In this lecture, the main steps for starting HYSYS V9 are detailed thorough the software interface, component selection, Fluid package selection, working with material streams.

How to start HYSYS:

1. Start menu.
2. Type in the search field: Aspen HYSYS V9.
3. Select open.



The above window will pop up once you start HYSYS. Mainly, there are two options to start working:

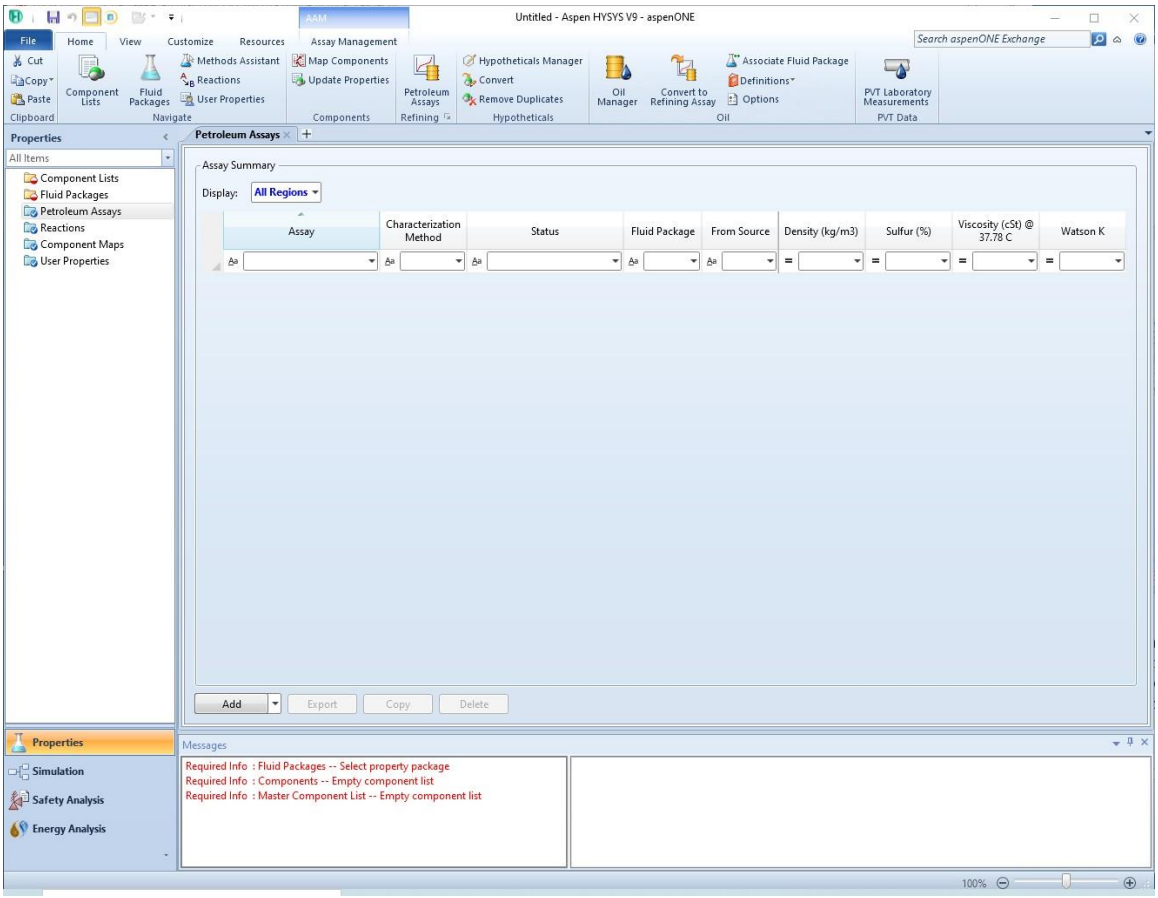
- **Open**: Enables the user to work with the models and projects which have been created previuosly. If (open) is chosen, it will be possible to browse you computer and select the desired project. However, it can be seen in the above figure that there are shortuts for recently opened files that have been edited by HYSYS V9. Alternatively, it is possible to open the HYSYS files by:
  1. (ctrl+o) buttons on keyboard
  2. file menu \ open
- **New**: Enables the user to create a new simulation project. As (new) is chosen, it will be ncessary to define the main propeties of the created project. Alternatively, it is possible to create new HYSYS files by:
  3. (ctrl+n) buttons on keyboard
  4. file menu \ new

Properties of the simulation case:

The figure below shows the initial view of HYSYS V9 desktop windowfor a new simulation case. The properties tab is exist on the the left down corner. It is possible to access and edit the realted information regarding the opened project from (properties). This includes the selection of components and choosing the fluid package. The first step before adding the project information is to save the file in a well known location in your computer as:

1. file \ save
2. browse your computer and give the file name in the desired location. [create a new folder (name: chemical fourth {your name})] and a file name of (stating hysys).
3. save

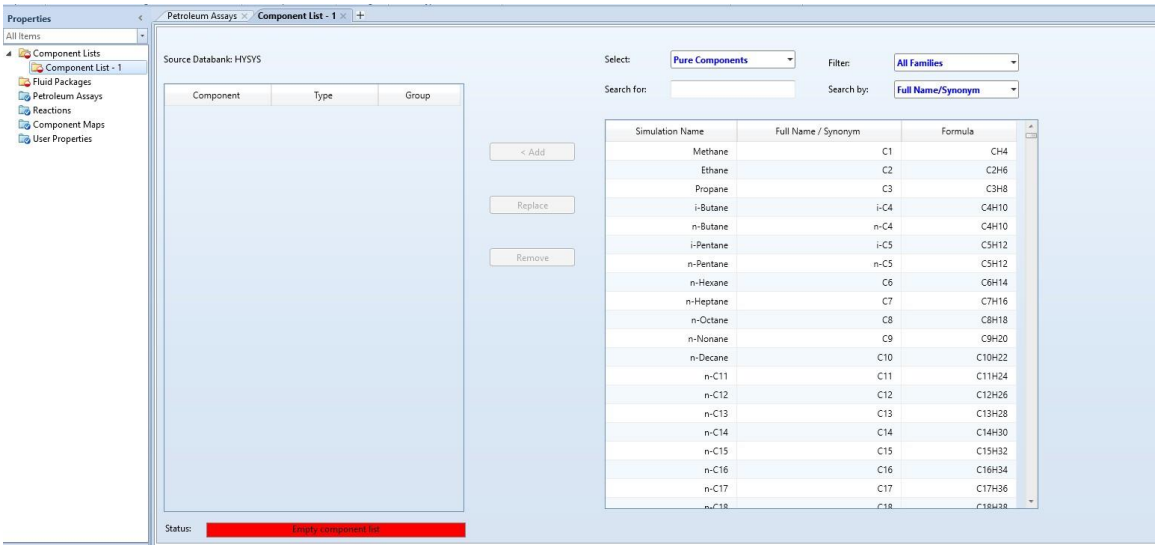
Moreover, the information of component lists and fluid package can be stored seprately in order to use them with other projects.



Adding component lists:

1. properties \ component lists window is opened.

2. Add (Add button is exist in the left down corner of the component lists window). A new window with the component library is opened as shown below.



3. Select the desired components. It is possible to search for a certain component in the field (search for) according to one of three entries in (search by) field: Full name/Synonym, Simulation name and formula.

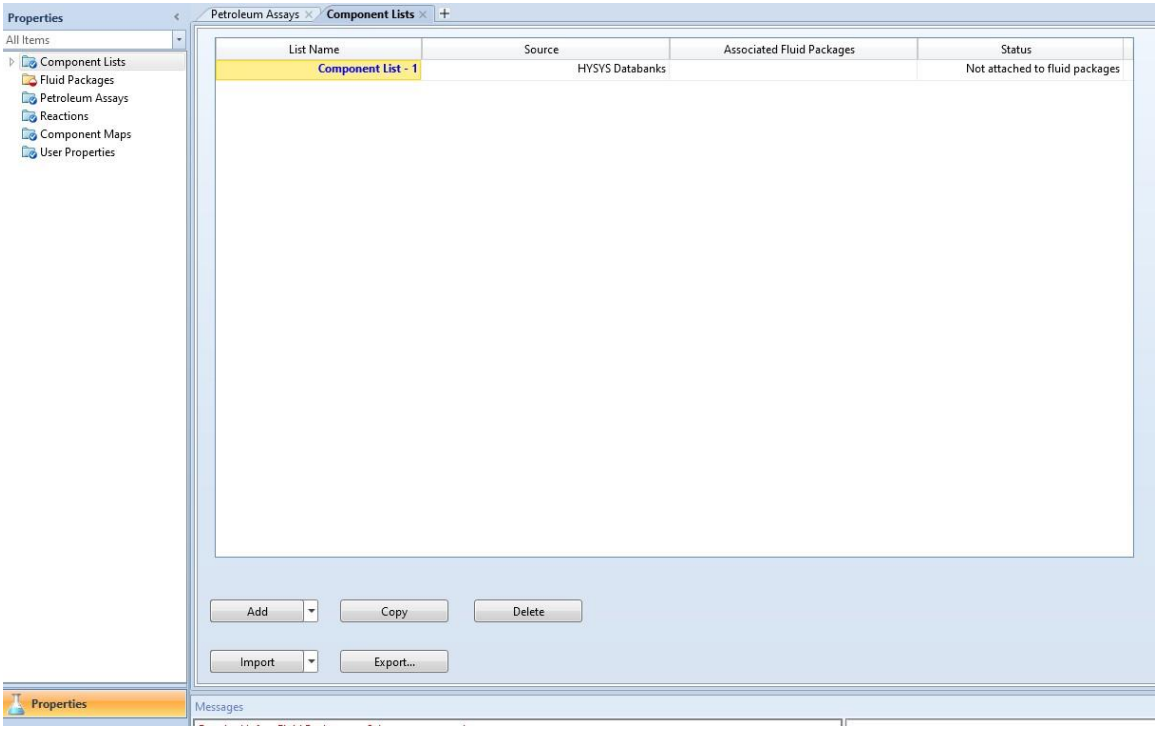
[Choose the (Full name/Synonym) and write (water) in search for field. Select water]

4. Add

A new component list is created (component List – 1) with single component (H_2O). It is possible to add or remove component from the component lists using add, remove and replace buttons. Moreover, the component list can be saved separately as:

1. Component Lists

2. Select the desired component list
3. Export
4. browse your computer and give the file name in the desired location



Once the component list is saved in a certain location. It will be allowed to use it in other project as:

1. Component Lists
2. browse your computer and select the desired file.
3. Import

Adding the fluid package:

The fluid package is chosen in order to calculate the desired properties of the chemical mixtures accompanied in the simulation.

References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

Case Study in HYSYS V9

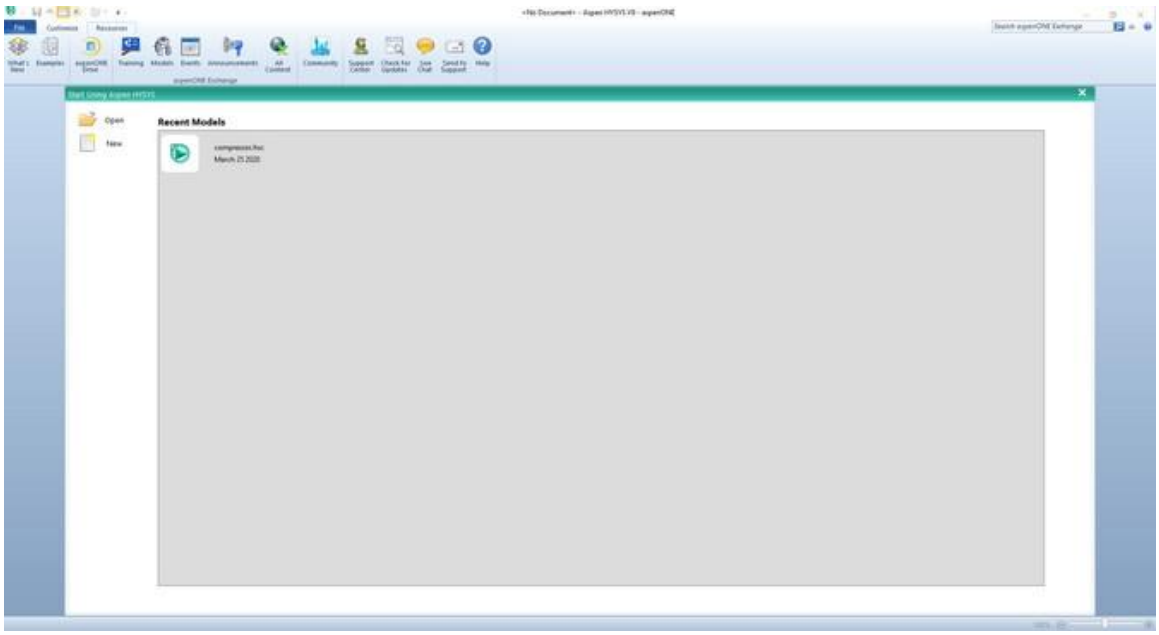
We can analyze the molar volume with a range of temperature values using the case study utility in Aspen HYSYS V9.

Example:

Show how the specific volume of a material stream of i-pentane when the temperature is changing from 250 k to 350 k [1].

Solution:

- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.

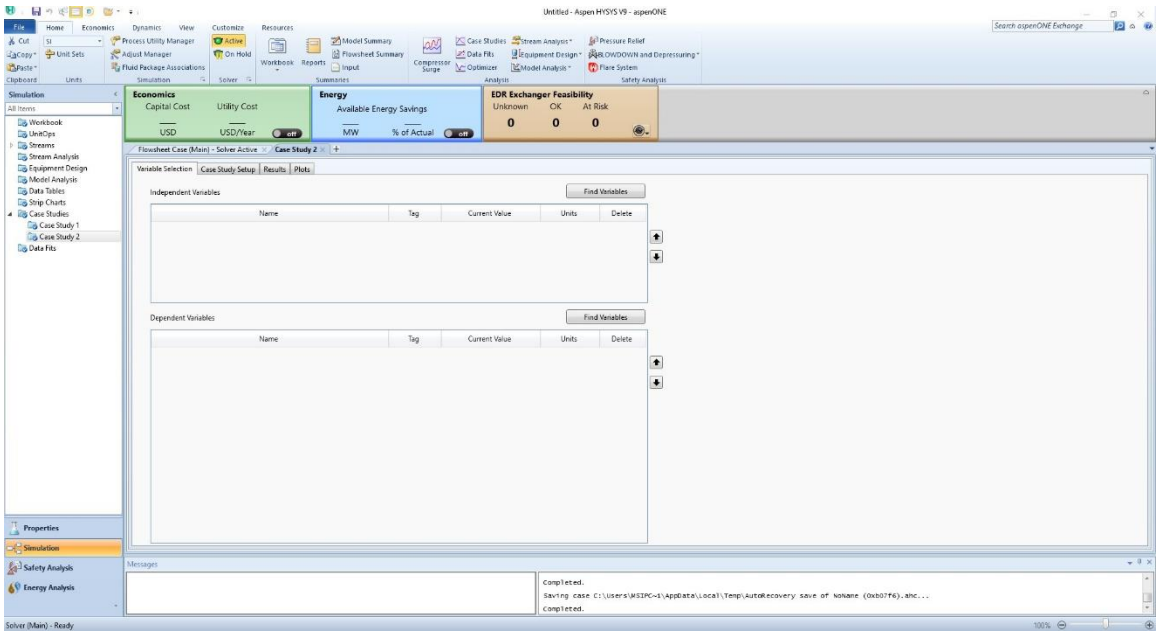


The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.

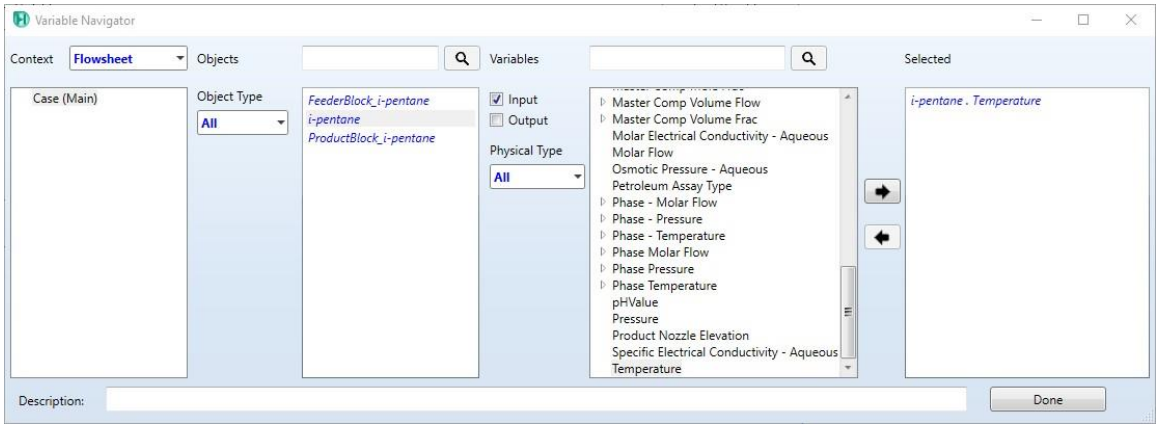
- Open the case of the previuos example:

1. File menu
2. Open \ equation of state

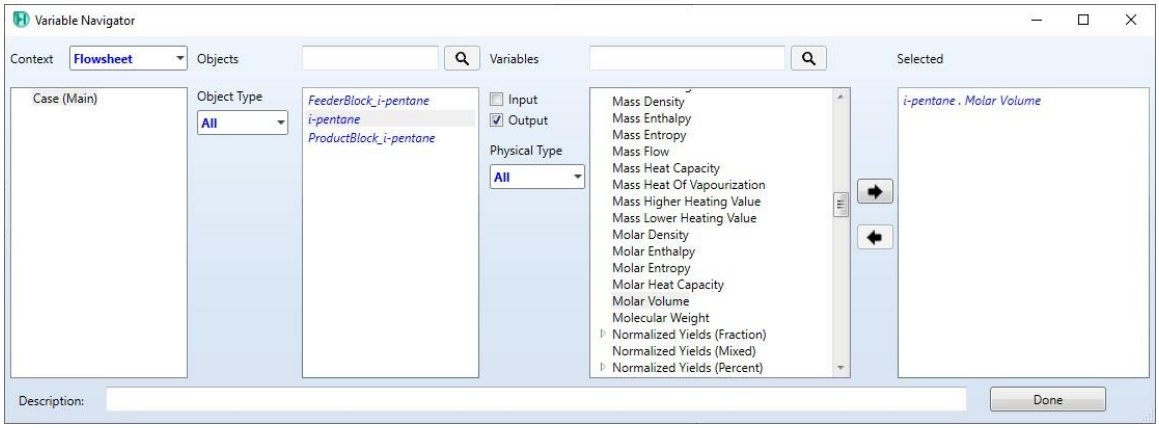
- Working with databook:
    1. From the Home toolbar, click on case studies
    2. Add

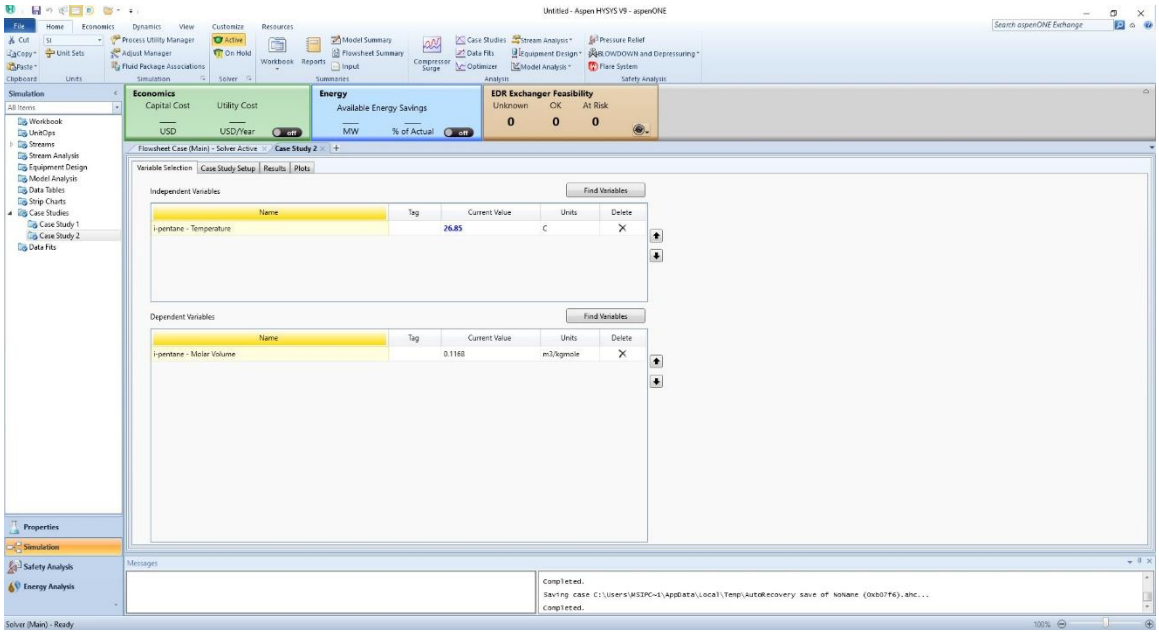


3. Variable selection
4. In Independent Variable click on Find variables
5. Highlight the desired material stream
6. Select the desired variable (temperature) \ Add
7. Done

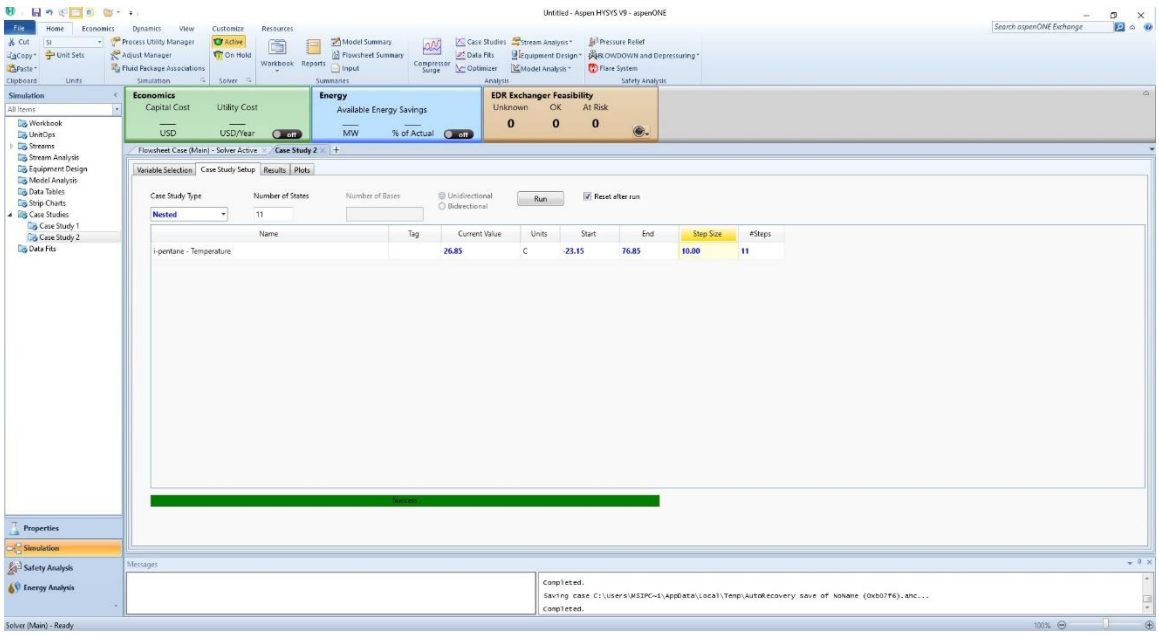


8. In Dependent Variable click on Find variables
9. Highlight the desired material stream
10. Select the desired variable (Molar Volume) \ Add
11. Done

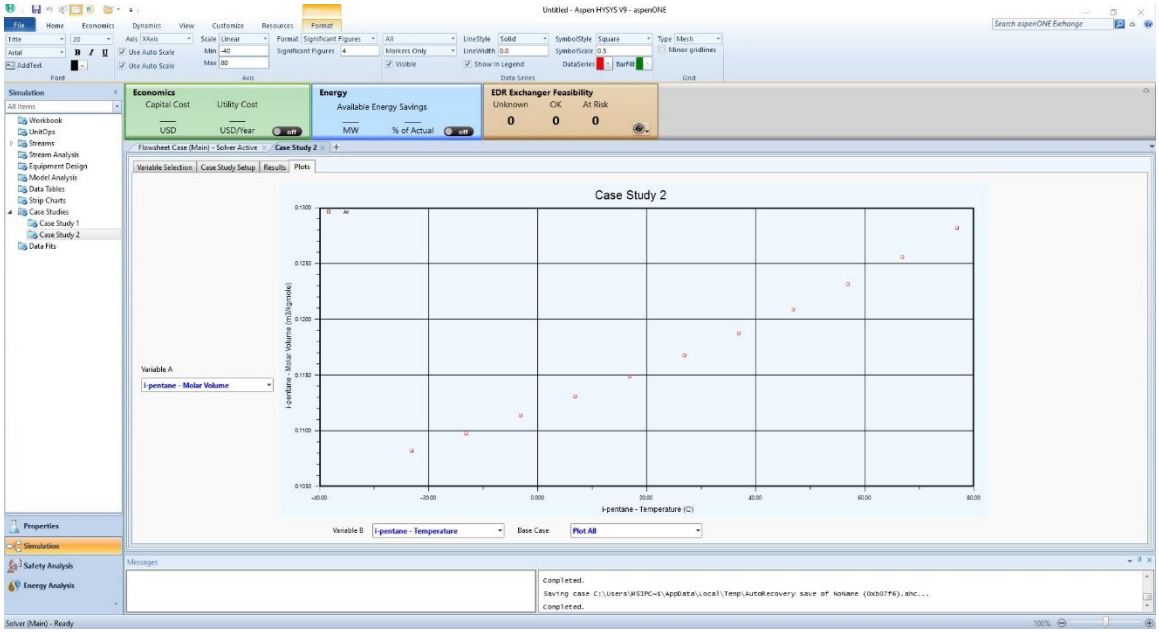




12. Select the Case Study Setup
13. Change the start value to 250 K
14. Change the end value to 350 K
15. Change the step size to 10 K
16. Click Run



17. Select results and read the volume values with temperature
18. Select plots



- Save the case:

1. File menu
2. Select save as
3. Give the name (case study)

References:

1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).