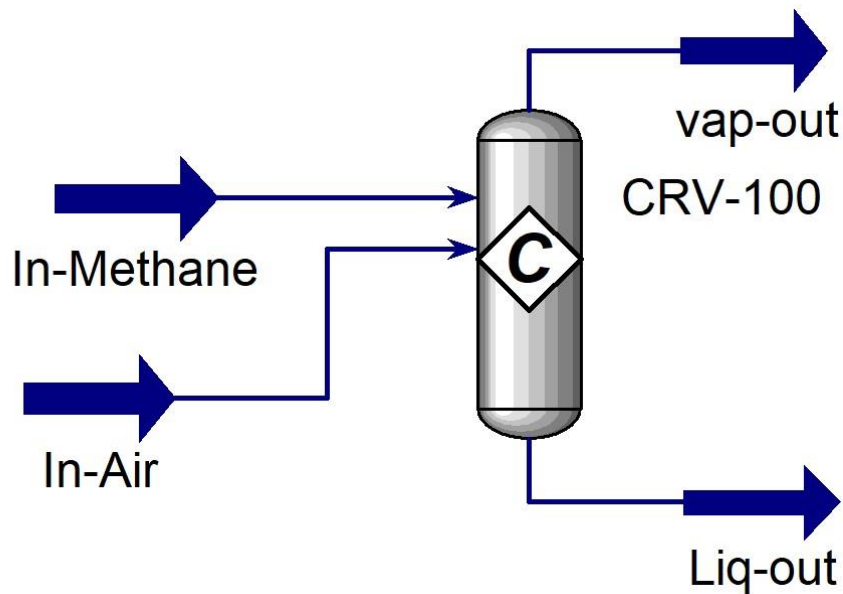


## Conversion Reaction Using HYSYS V9

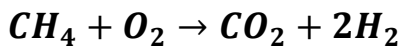
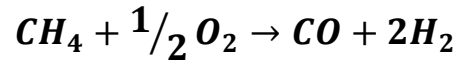
The reaction of methane with air producing hydrogen and carbon oxides is called the partial oxidation. Such kind of processes can be modeled using the conversion reaction in Aspen HYSYS V9. It is possible to perform more than one reaction in one group according to the given rank in order to operate them 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:**

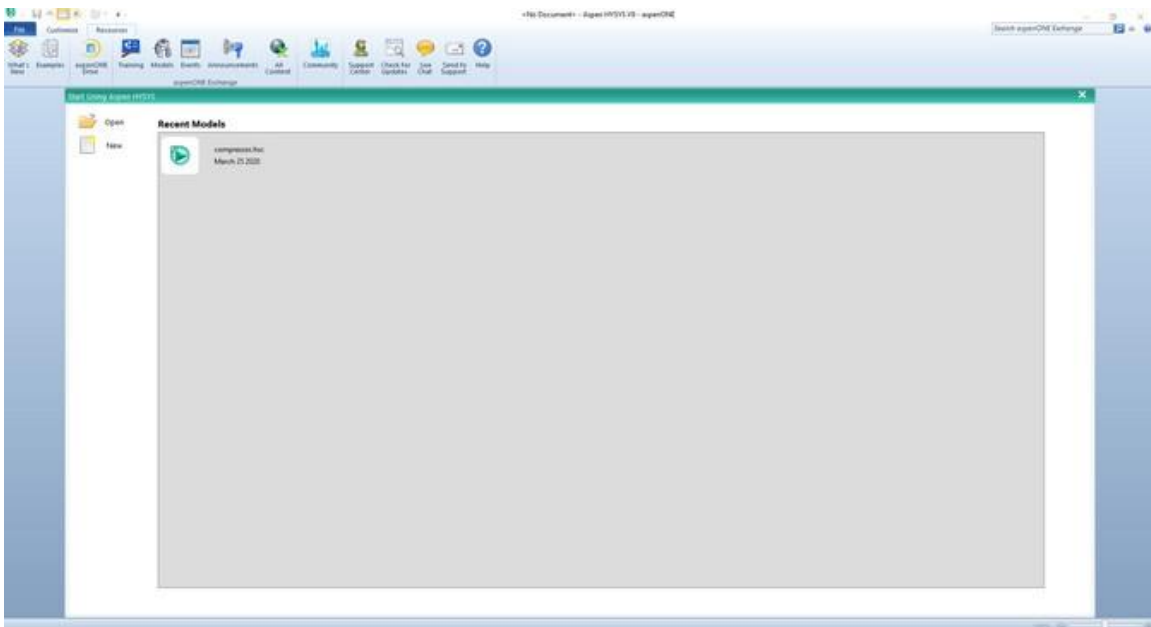
Hydrogen production from hydrocarbon is an enabling technology. The fuel is converted to hydrogen by the partial oxidation. The reaction of Methane with air producing the carbon oxides and the hydrogen is an example of the partial oxidation.



Model the partial oxidation of methane to produce hydrogen [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.

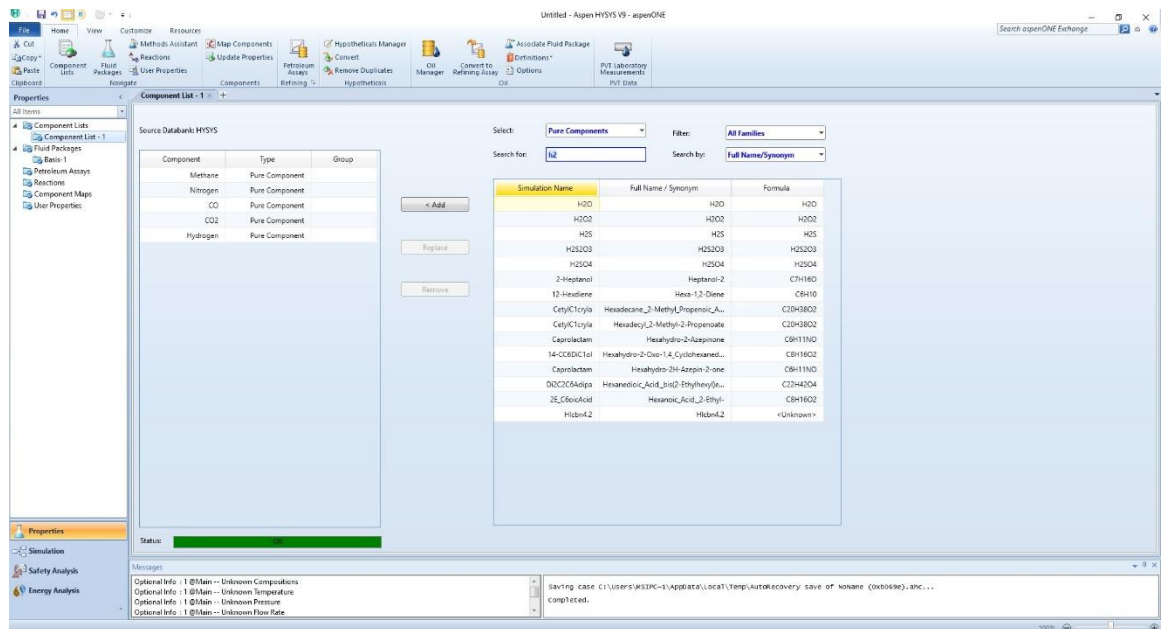
- Create a new case:

1. File menu
2. New \ case

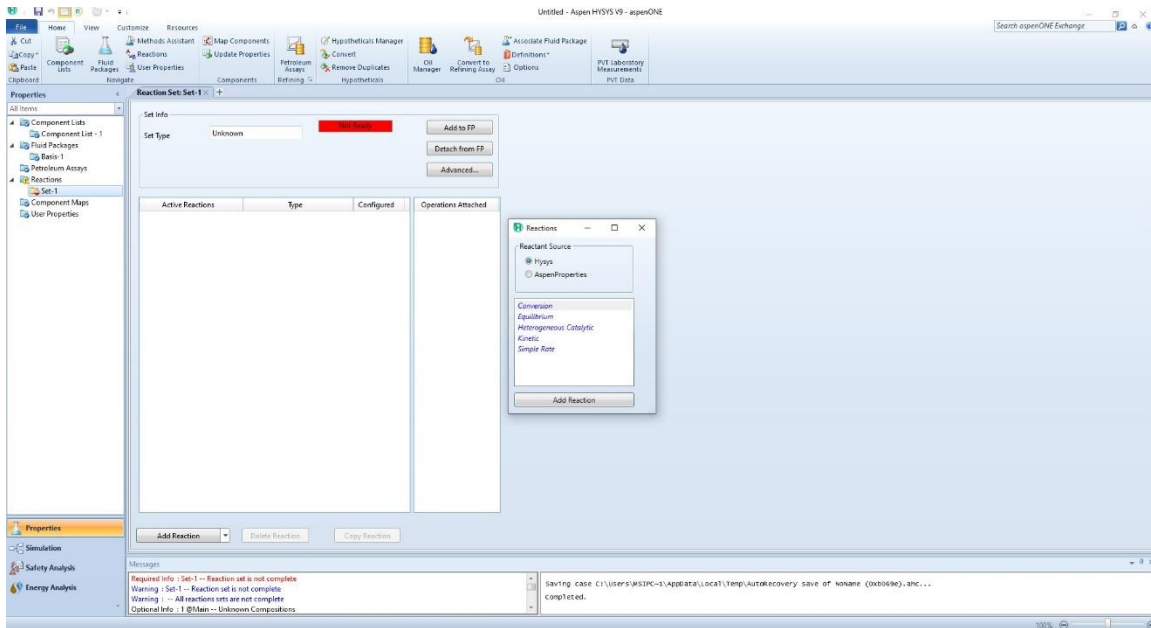
- There are two main necessary information have to be given in the properties tab before starting the simulation:

1. Property package : Peng-Robinson
2. Components: CH<sub>4</sub>, O<sub>2</sub>, N<sub>2</sub> , CO, CO<sub>2</sub>, H<sub>2</sub>

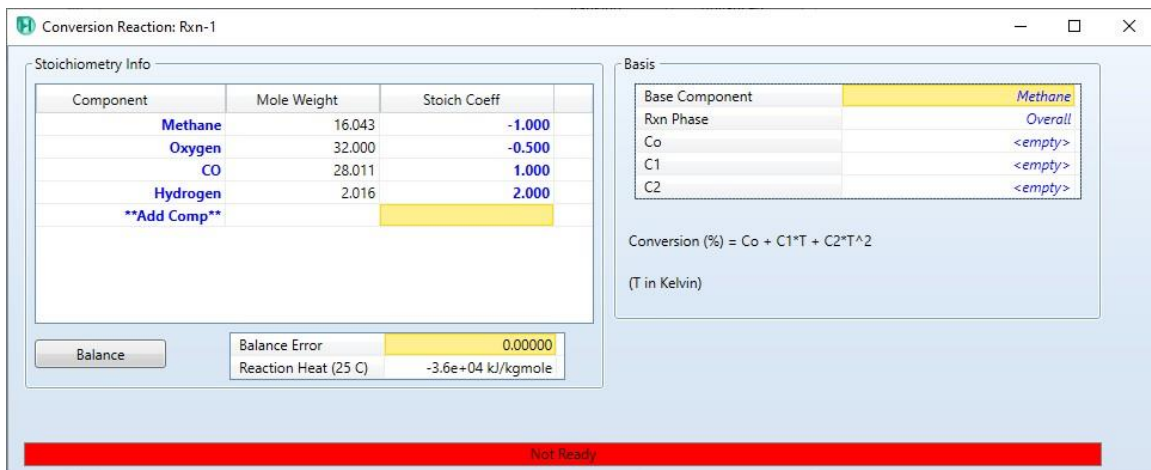
1. Properties
2. Component lists \ Add
3. Select: Pure components
4. Type in the search field CH<sub>4</sub>
5. Select CH<sub>4</sub> \ add
6. Repeat the steps (4,5) for N<sub>2</sub> , CO, CO<sub>2</sub>, O<sub>2</sub> and H<sub>2</sub>



- 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:

Conversion Reaction: Rxn-1

Stoichiometry Info

Component	Mole Weight	Stoich Coeff
Methane	16.043	-1.000
Oxygen	32.000	-0.500
CO	28.011	1.000
Hydrogen	2.016	2.000
**Add Comp**		

Balance

Balance Error: 0.00000  
Reaction Heat (25 C): -3.6e+04 kJ/kgmole

Basis

Base Component	
Rxn Phase	Overall
Co	40.00
C1	<empty>
C2	<empty>

Conversion (%) =  $Co + C1 \cdot T + C2 \cdot T^2$   
(T in Kelvin)

Ready

7. Enter the below information regarding the second reaction:

Conversion Reaction: Rxn-2

Stoichiometry Info

Component	Mole Weight	Stoich Coeff
Methane	16.043	-1.000
Oxygen	32.000	-1.000
CO2	44.010	1.000
Hydrogen	2.016	2.000
**Add Comp**		

Balance

Balance Error: 0.00000  
Reaction Heat (25 C): -3.2e+05 kJ/kgmole

Basis

Base Component	
Rxn Phase	Overall
Co	60.00
C1	<empty>
C2	<empty>

Conversion (%) =  $Co + C1 \cdot T + C2 \cdot T^2$   
(T in Kelvin)

Ready

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

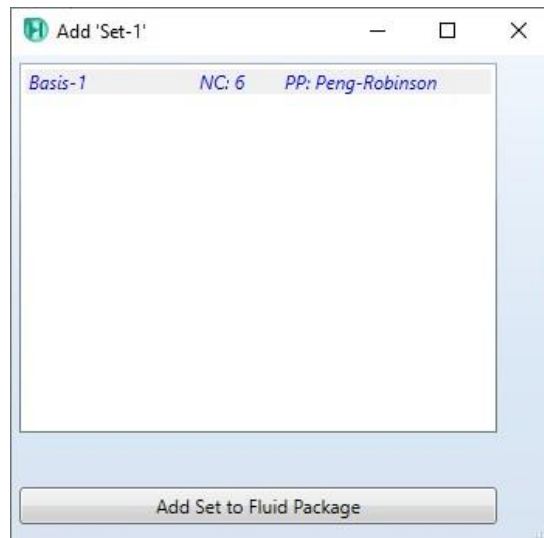
Reaction Ranks: Set-1

Reaction	Rank	User Spec
Rxn-1	0	<input checked="" type="checkbox"/>
Rxn-2	1	<input checked="" type="checkbox"/>

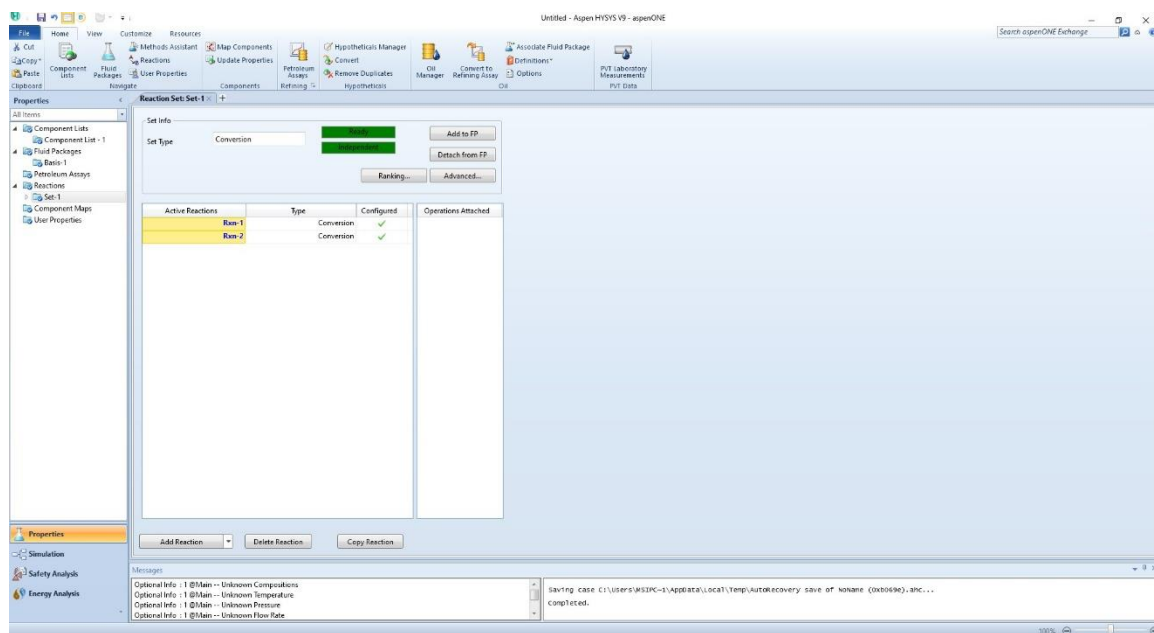
Reset

Close

- 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° C
Pressure	3 bar
Molar flow	100 kgmole/h
Composition	
C1	1

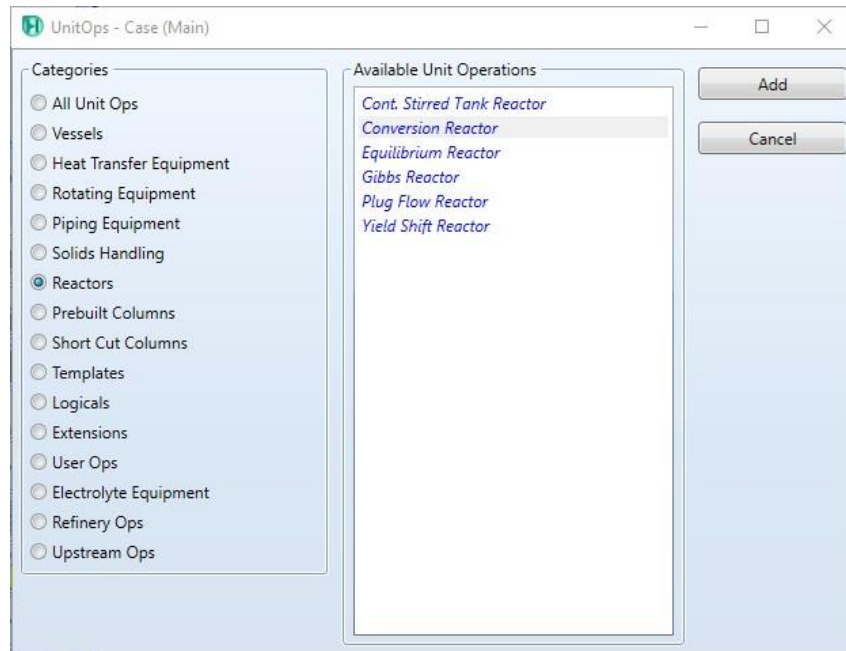
1. Add second material stream:

Name	In-Air
Conditions	
Temperature	20° C
Pressure	3 bar
Molar flow	250 kgmole/h
Composition	
N <sub>2</sub>	0.79
O <sub>2</sub>	0.21

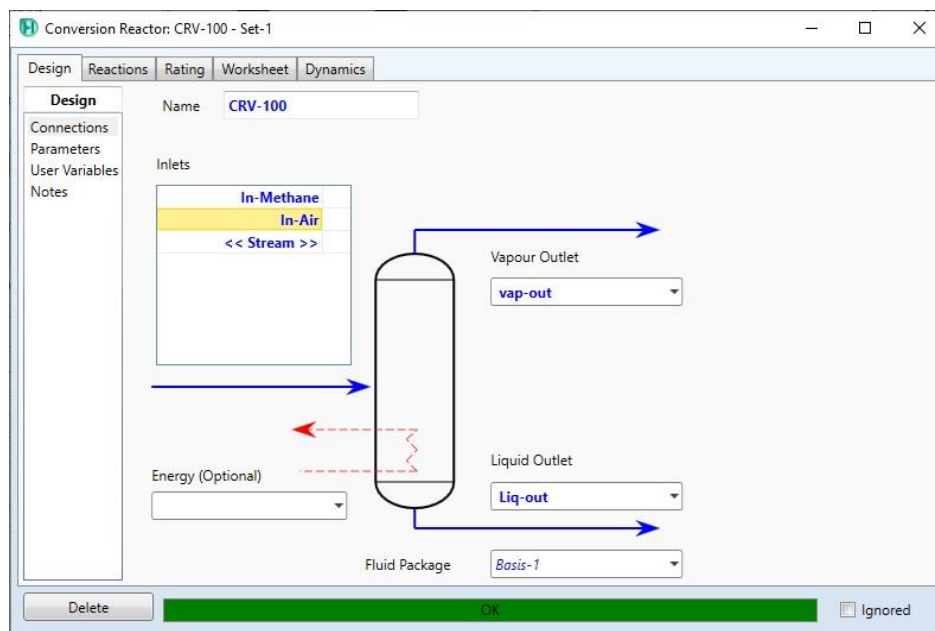
The above information should be given according to the application or example.

- 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)

Conversion Reactor: CRV-100 - Set-1

Design Reactions **Rating** Worksheet Dynamics

**Reactions**

Reaction Set: **Set-1** Reaction: **Rxn-1**

☒ Stoichiometry ☐ Basis ☐ Conversion % View Reaction...

Stoichiometry Info

Component	Mole Wgt.	Stoich Coeff
Methane	16.043	-1.000
Oxygen	32.000	-0.500
CO	28.011	1.000
Hydrogen	2.016	2.000
**Add Comp**		

Balance Error: 0.00000  
Reaction Heat (25 C): -3.6e+04 kJ/kgmole

Delete OK Ignored

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).

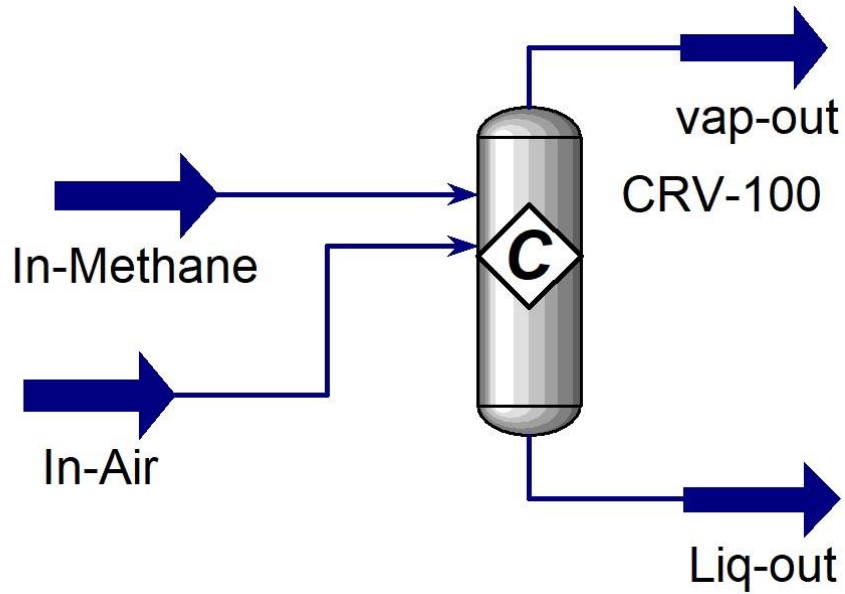
Conversion Reactor: CRV-100 - Set-1

Design Reactions Rating **Worksheet** Dynamics

**Worksheet**

Name	In-Methane	In-Air	Liq-out	vap-out
Vapour	1.0000	1.0000	0.0000	1.0000
Temperature [C]	20.00	20.00	817.1	817.1
Pressure [kPa]	300.0	300.0	300.0	300.0
Molar Flow [kgmole/h]	100.0	250.0	0.0000	442.5
Mass Flow [kg/h]	1604	7213	0.0000	8817
Std Ideal Liq Vol Flow [m3/h]	5.358	8.338	0.0000	15.65
Molar Enthalpy [kJ/kgmole]	-7.513e+004	-170.6	-1.708e+004	-1.708e+004
Molar Entropy [kJ/kgmole-C]	173.8	142.1	189.1	189.1
Heat Flow [kJ/h]	-7.513e+006	-4.266e+004	-0.0000	-7.556e+006

Delete OK Ignored



- 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**

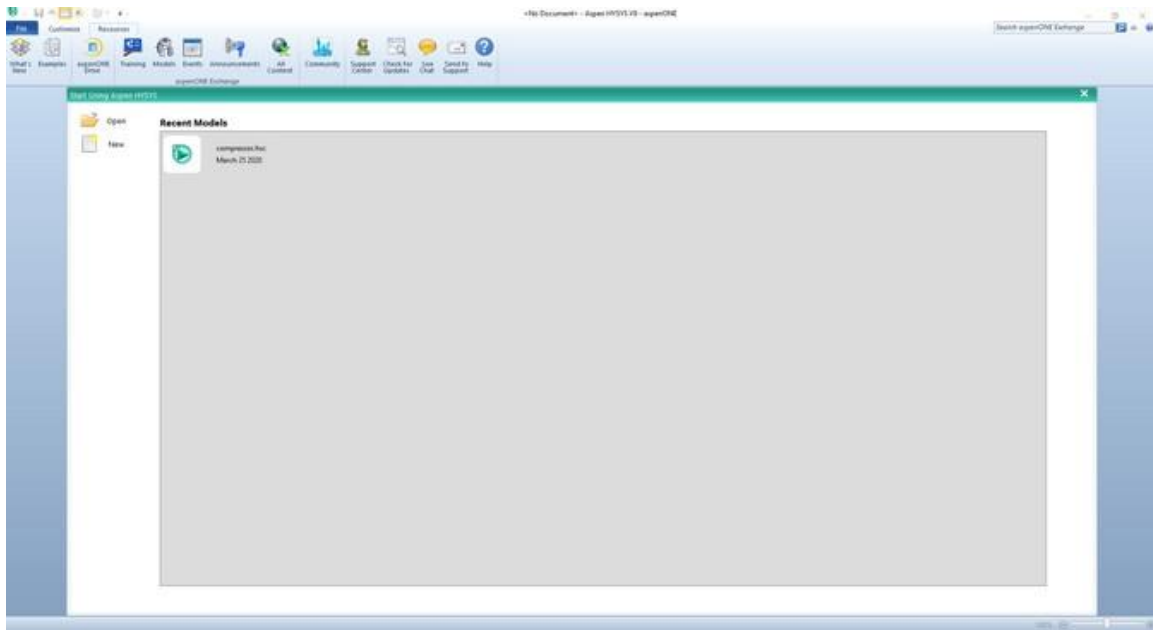
It is possible to find the molar volume of a mixture of material using an equation of state. Aspen HYSYS V9 give an access to several packages like Peng-Robinson (PR) equation of state which can fit with various operation processes. In this subject, it is intended to learn how to determine the specific 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].

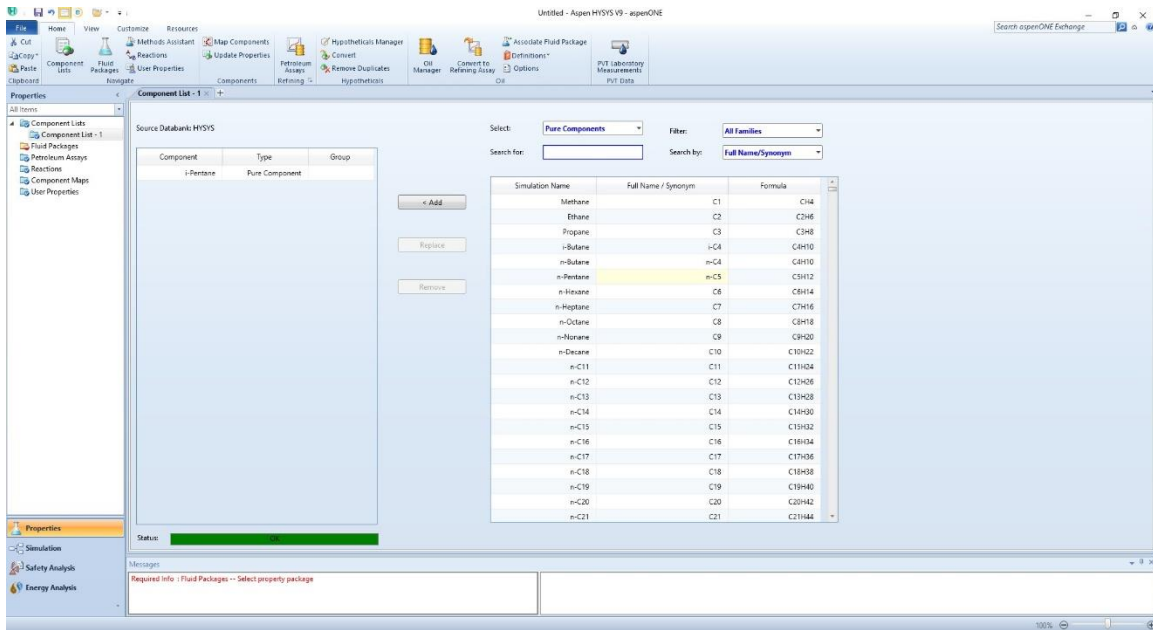
### **Solution:**

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

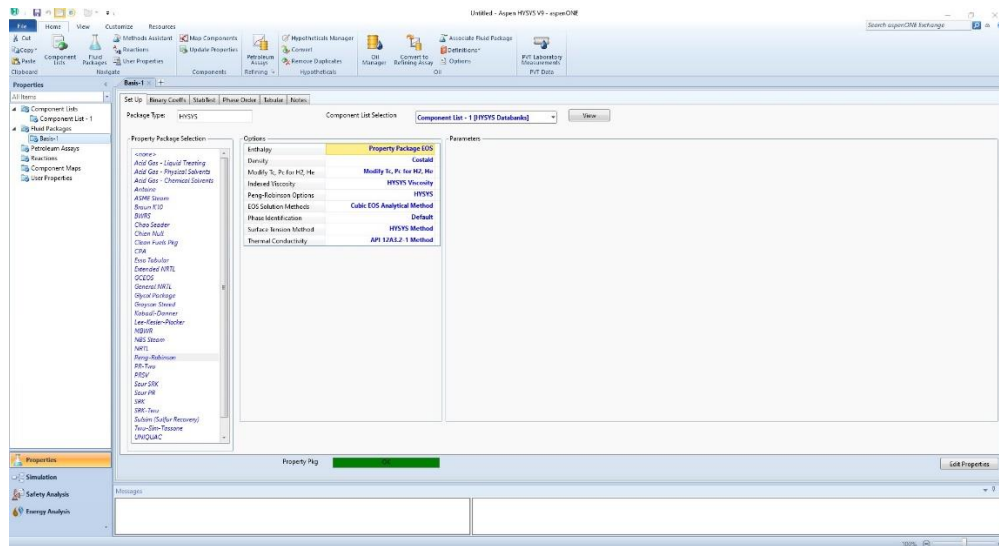


The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.

- 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 search field i-pentane



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



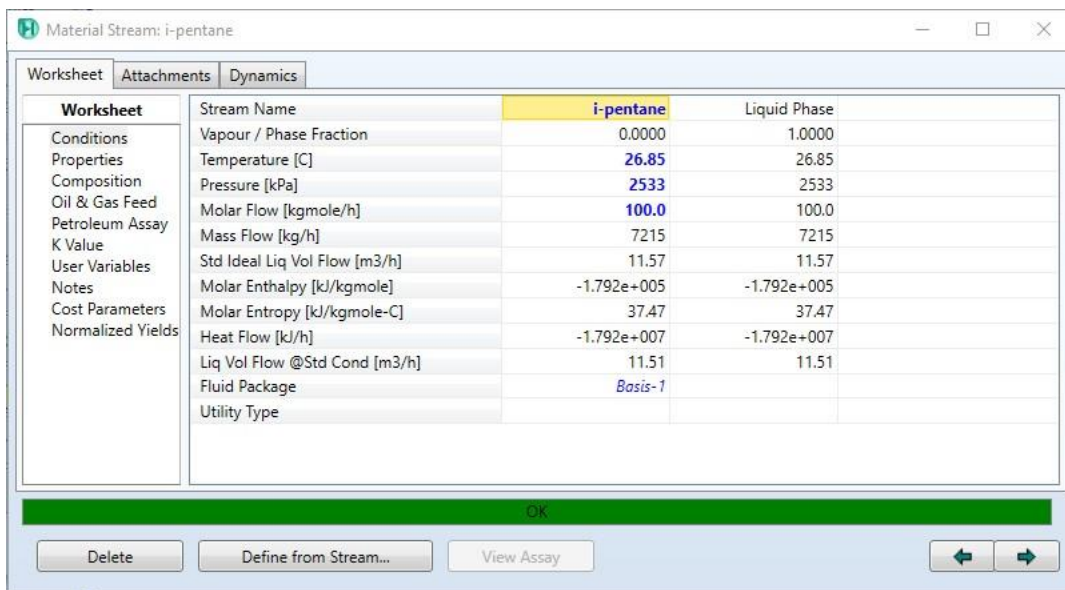
- Create new material stream:
  1. Select simulation.
  2. Object palette.
  3. Select the material stream icon.

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

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

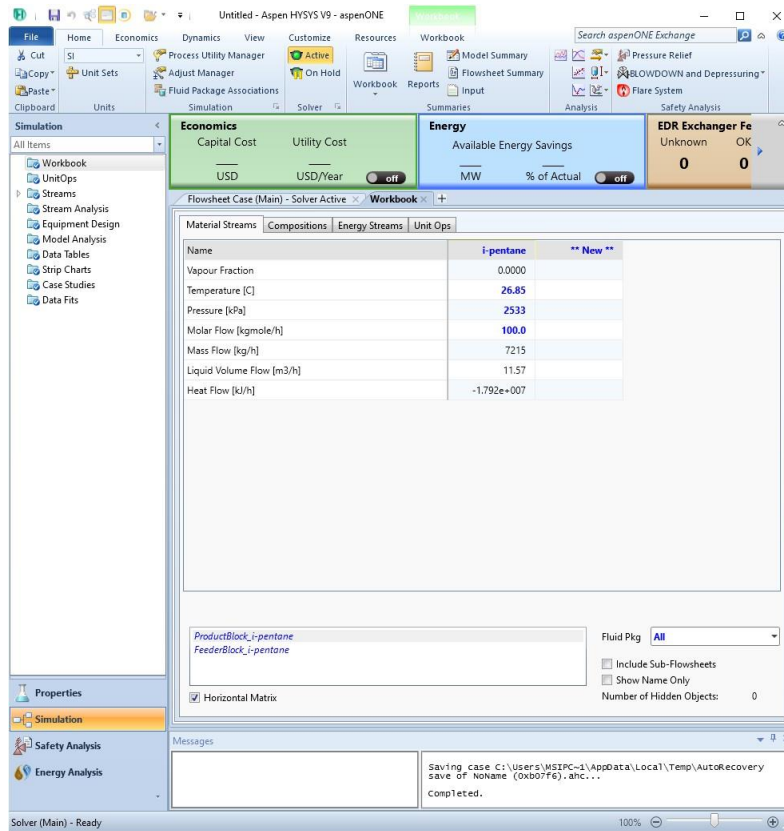
Name	i-pentane
Conditions	
Temperature	300 k
Pressure	25 atm
Molar flow	100 kgmole/h
Composition	
i-pentane	1

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



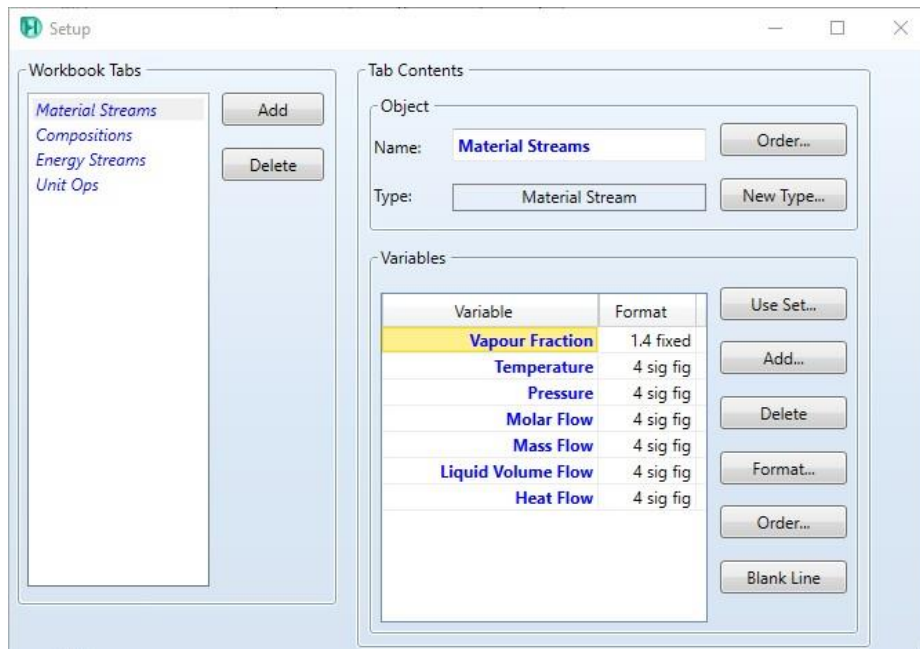
- Working with Workbook:
  1. From the Home toolbar, click on workbook

Alternatively, press Ctrl+w

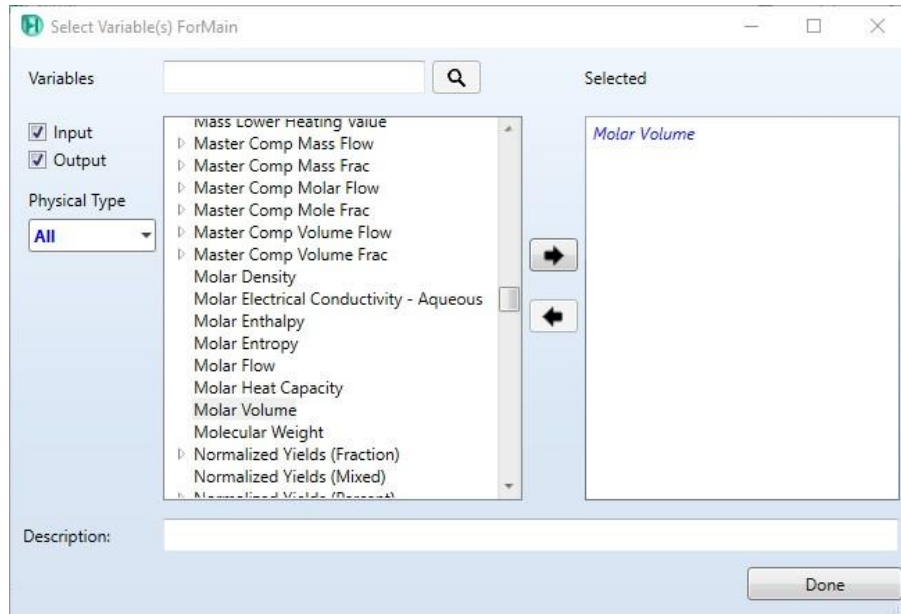


There is no molar volume in the workbook.

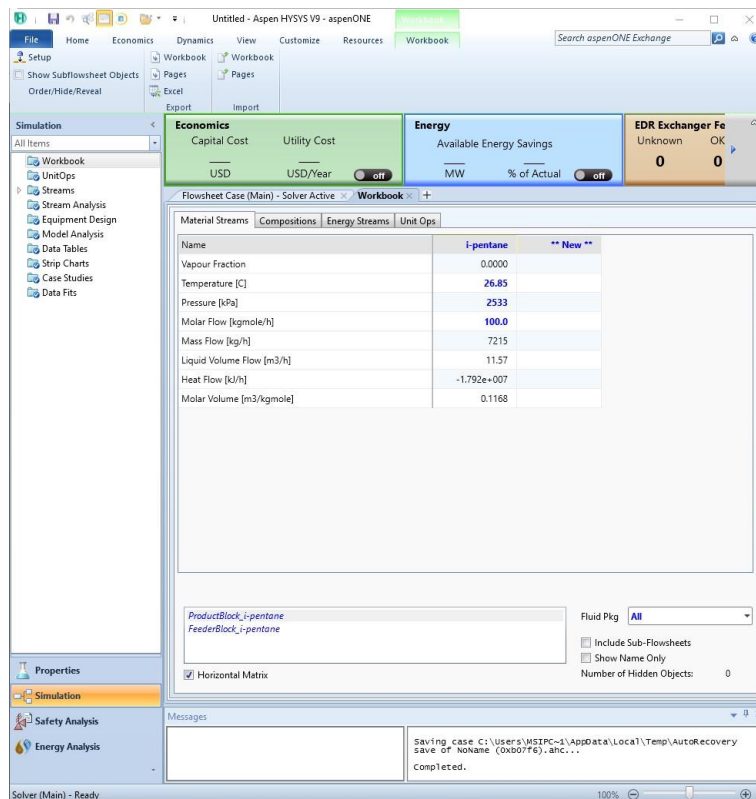
2. From the workbook toolbar, click on Setup



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



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





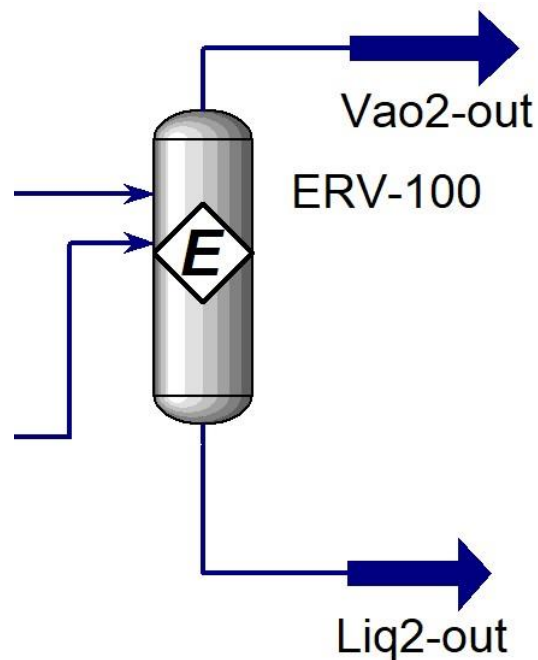
- Save the case:
  1. File menu
  2. Select save as
  3. Give the name (equation of State)

**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 H<sub>2</sub> 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 Equilibrium reactor with its inlet and outlet streams using Aspen HYSYS V.9.

### **Example:**

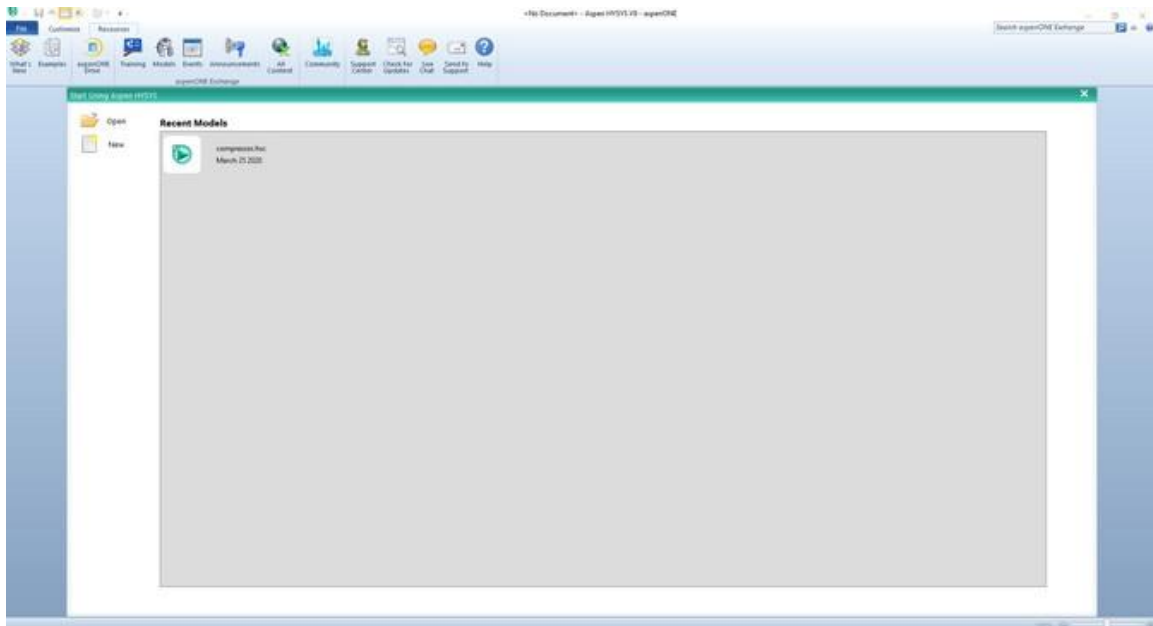
It is possible to improve the efficiency of Hydrogen production by reducing the CO levels. Water Gas Shift (WGS) reaction is an optimum purification process for increasing H<sub>2</sub> yield and decreasing CO concentration. The following reaction:



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

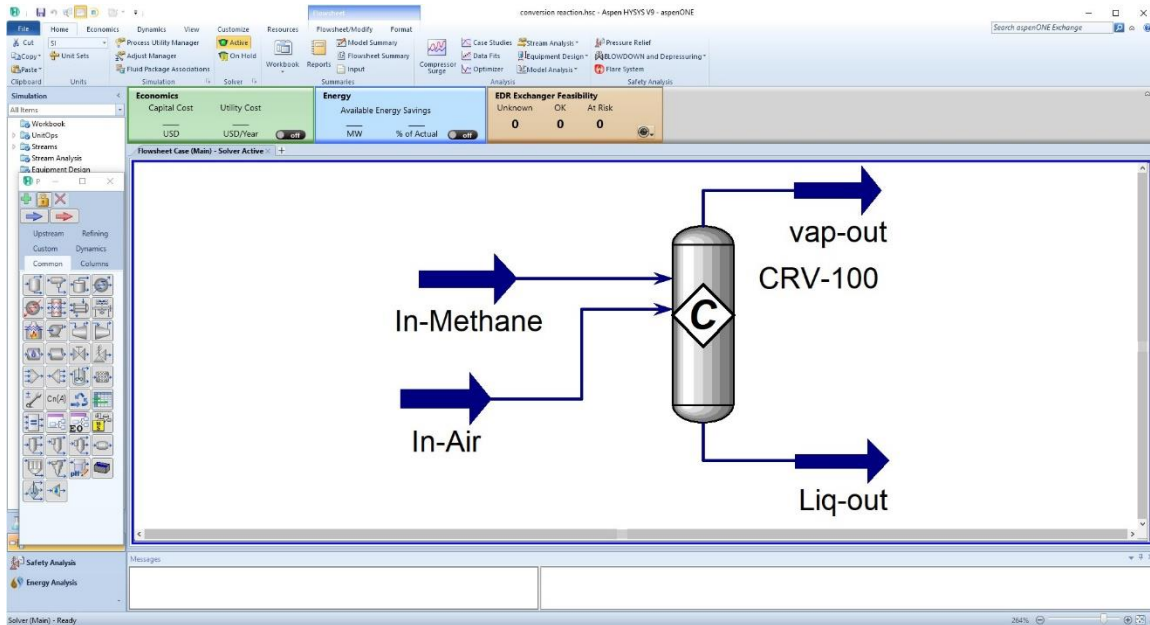
### **Solution:**

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

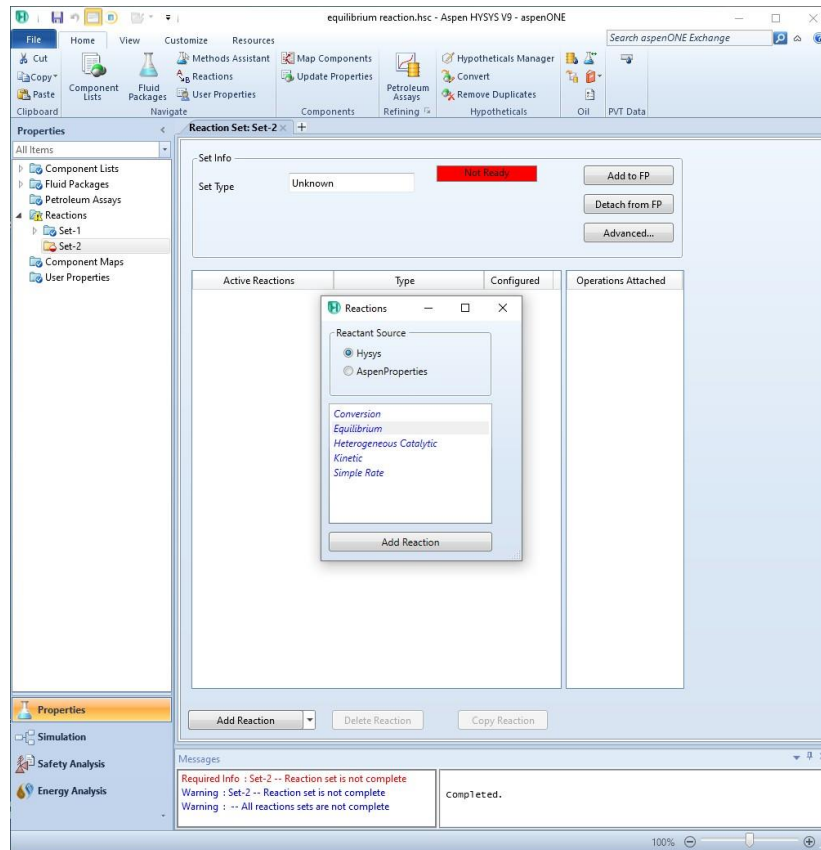


The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.

- Open the previous case of conversion reaction:
  1. File menu
  2. Open \ conversion reaction



- Modify the component list:
  1. Properties
  2. Double click on (Component list)
  3. Component List-1
  4. Add H<sub>2</sub>O 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.

Equilibrium Reaction: Rxn-3

Stoichiometry   Keq   Approach   Library

Stoichiometry

Component	Mole Weight	Stoich Coeff
CO	28.011	-1.000
H2O	18.015	-1.000
CO2	44.010	1.000
Hydrogen	2.016	1.000
**Add Comp**		

Balance

Balance Error: 0.00000  
Reaction Heat (25 C): -4.1e+04 kJ/kgmole

Basis

Basis	Activity
Phase	VapourPhase
Min Temperature	-273.1 C
Max Temperature	3000 C

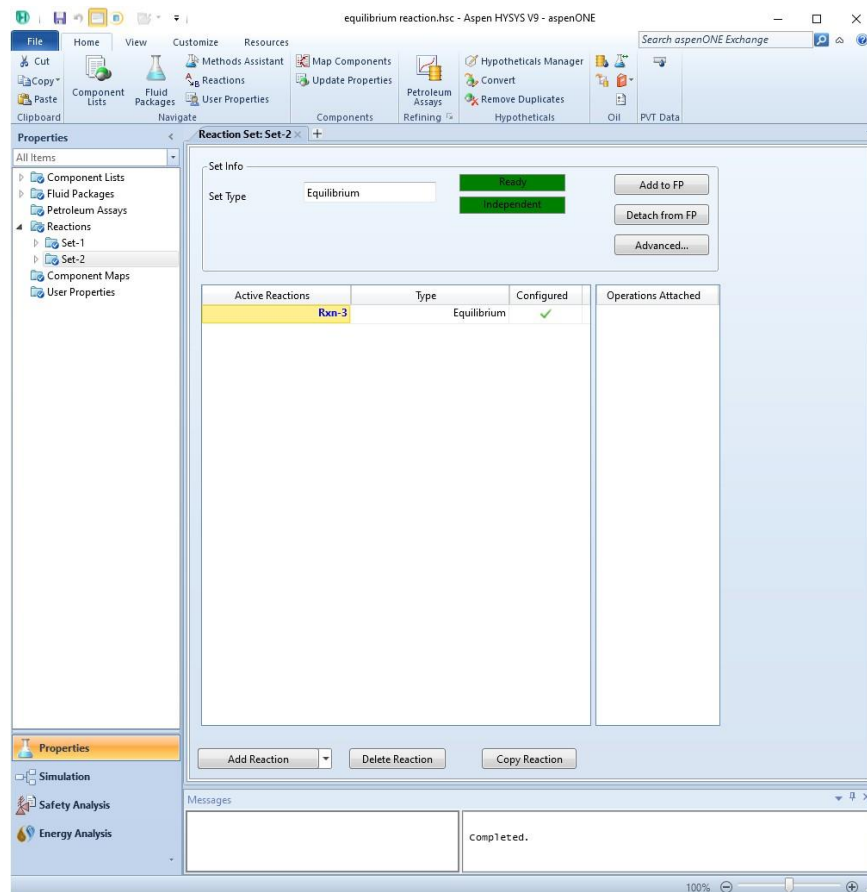
Basis Units:

Ready   Gibbs

- 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 <sup>o</sup> C
Pressure	3 bar
Molar flow	100 kgmole/h
Composition	
H <sub>2</sub> O	1

Input Composition for Stream: Material Stream: Water

	MoleFraction
Methane	<empty>
Nitrogen	<empty>
CO	<empty>
CO2	<empty>
Hydrogen	<empty>
Oxygen	<empty>
H2O	1.0000

Composition Basis:

- ☒ Mole Fractions
- ☐ Mass Fractions
- ☐ Liq Volume Fractions
- ☐ Mole Flows
- ☐ Mass Flows
- ☐ Liq Volume Flows

Composition Controls:

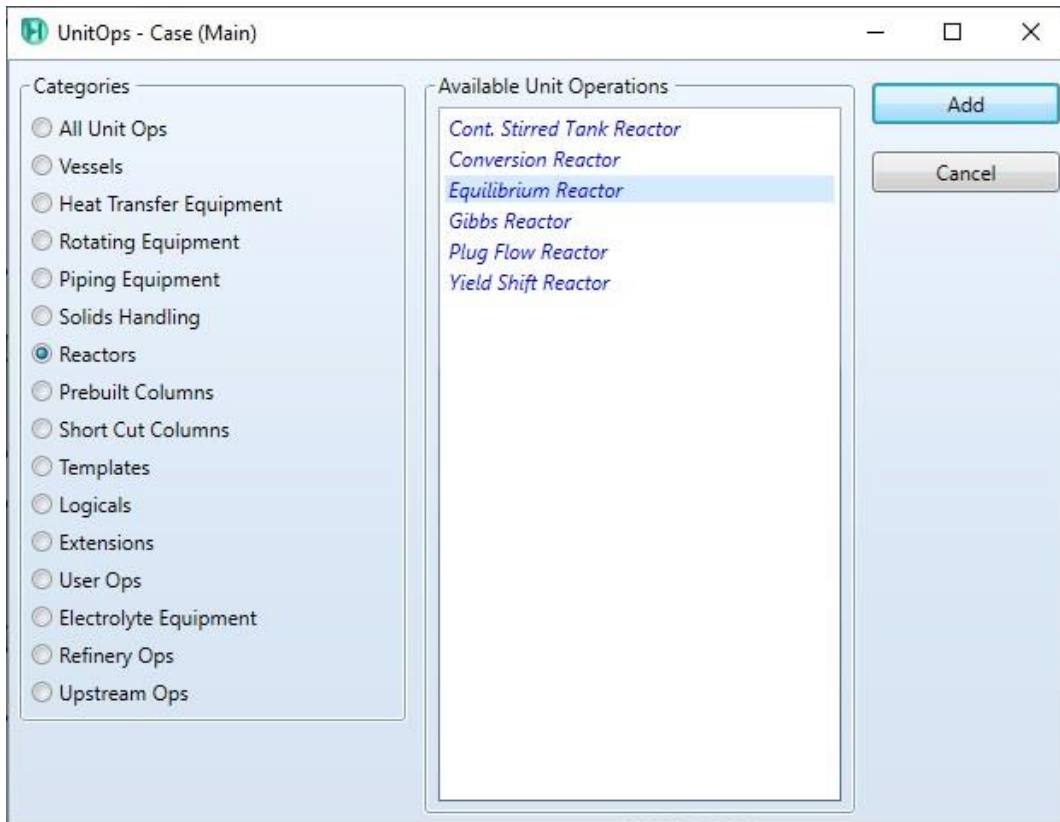
Erase

Equalize Composition

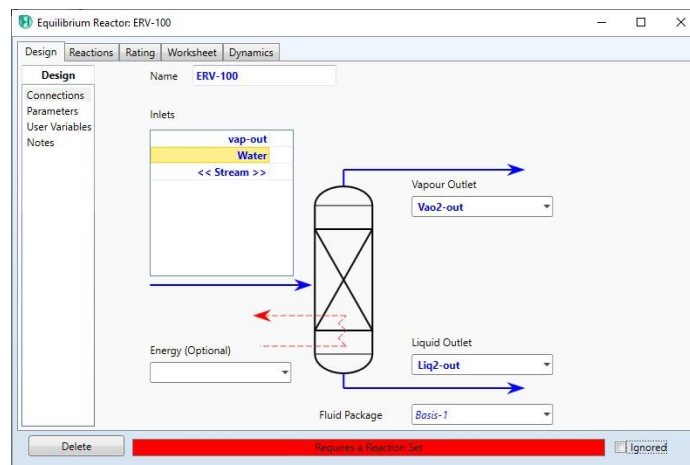
Cancel

Normalize Total 1.0000 OK

- 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)

Equilibrium Reactor: ERV-100 - Set-2

Design Reactions Rating Worksheet Dynamics

**Reactions**

Equilibrium Reaction Details

Reaction Set: **Set-2** Reaction: **Rxn-4**

☒ Stoichiometry ☐ Basis ☐ Keq ☐ Approach [View Rxn...](#)

Stoichiometry Info

Component	Mole Wt.	Stoich Coeff
CO	28.011	-1.000
H2O	18.015	-1.000
CO2	44.010	1.000
Hydrogen	2.016	1.000
**Add Comp**		

Balance Error: 0.00000  
Reaction Heat (25 C): -4.1e+04 kJ/kgmole

Delete OK Ignored

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

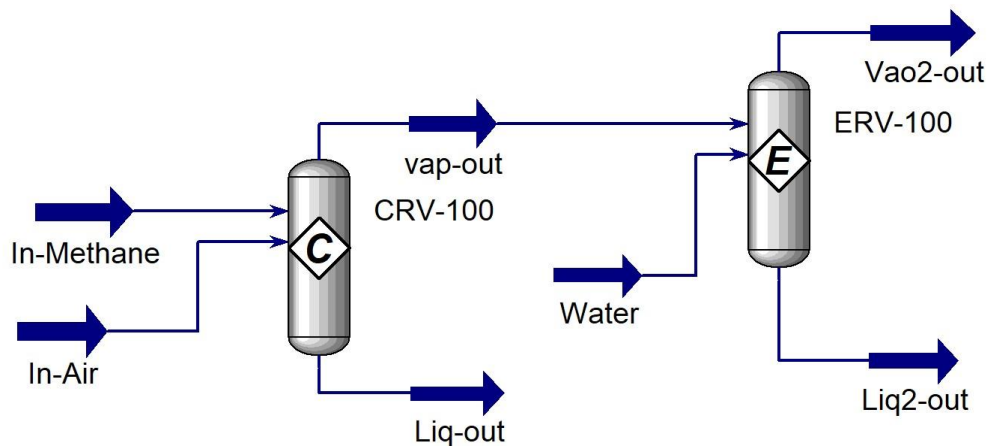
Equilibrium Reactor: ERV-100 - Set-2

Design Reactions Rating Worksheet Dynamics

**Worksheet**

Name	vap-out	Water	Liq2-out	Vao2-out
Vapour	1.0000	0.0000	0.0000	1.0000
Temperature [C]	817.1	110.0	511.1	511.1
Pressure [kPa]	300.0	300.0	300.0	300.0
Molar Flow [kgmole/h]	442.5	100.0	0.0000	542.5
Mass Flow [kg/h]	8817	1802	0.0000	1.062e+004
Std Ideal Liq Vol Flow [m3/h]	15.65	1.805	0.0000	18.01
Molar Enthalpy [kJ/kgmole]	-1.708e+004	-2.796e+005	-6.546e+004	-6.546e+004
Molar Entropy [kJ/kgmole-C]	189.1	73.34	184.1	184.1
Heat Flow [kJ/h]	-7.556e+006	-2.796e+007	-0.0000	-3.551e+007

Delete OK Ignored



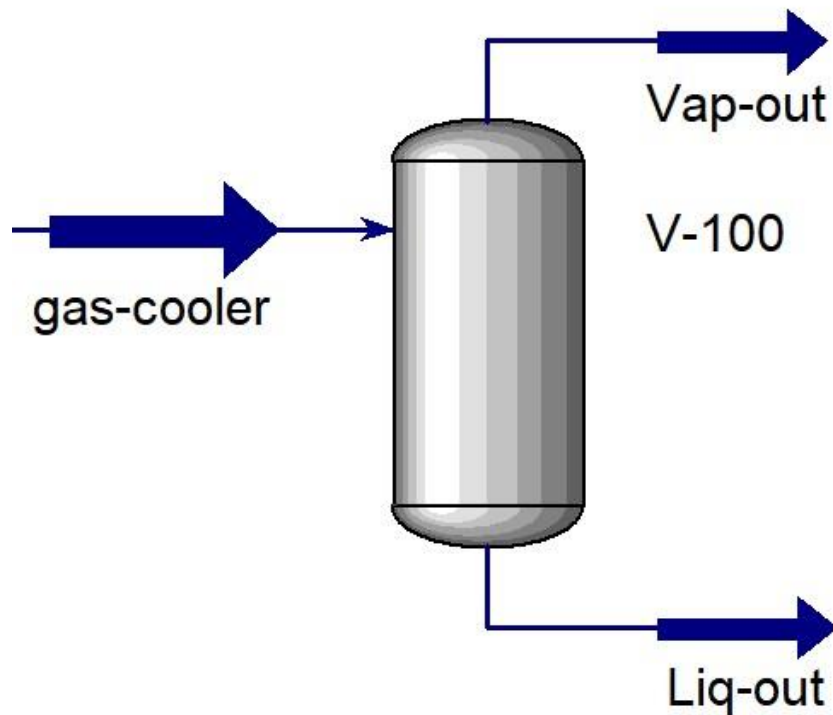
- Save the case:
  1. File menu
  2. Select save as
  3. Give the name (equilibrium Reaction)

### **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 separator 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° 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° 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:

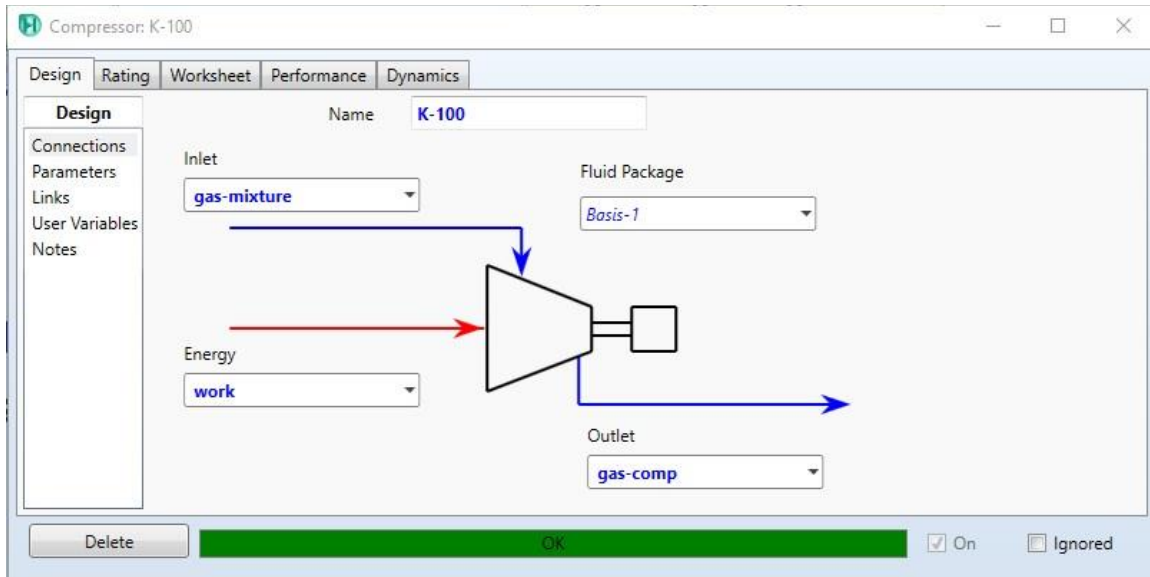
Name	Gas-Mixture
Conditions	
Temperature	40 <sup>o</sup> F
Pressure	1 atm
Molar flow	100 lbmole/hr
Composition	
i-C4, C2, C3	0.3, 0.4, 0.3

- 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

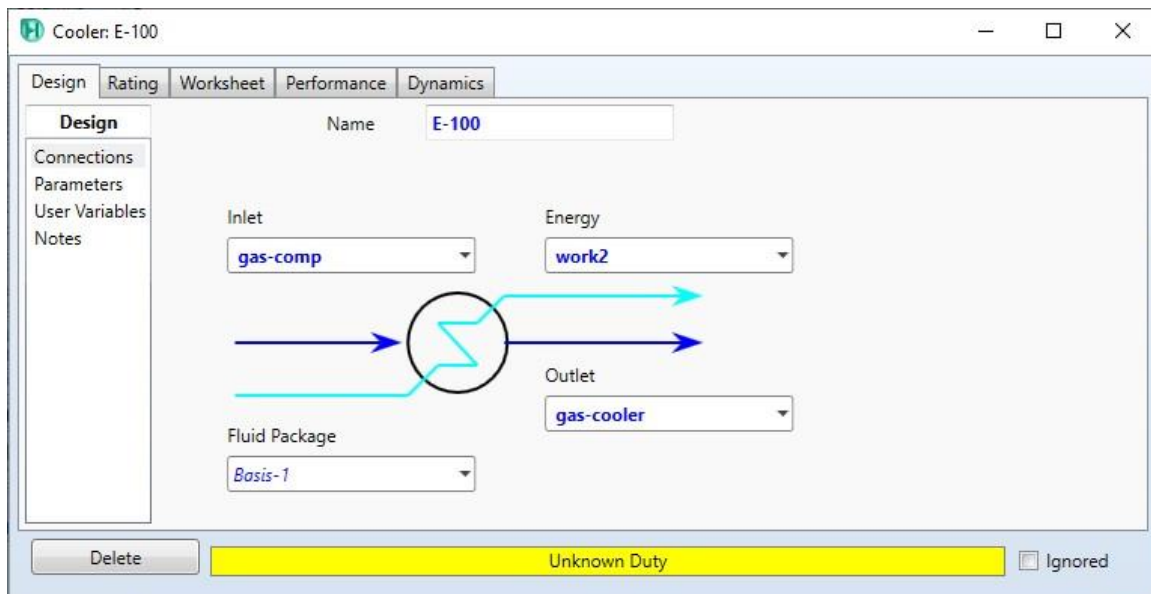
7. In the outlet field, type (gas-comp). [ a new material stream will be created and connected to the heat exchanger]
8. In the Energy field, type (work). [ a new energy stream will be created and connected to the heat exchanger]



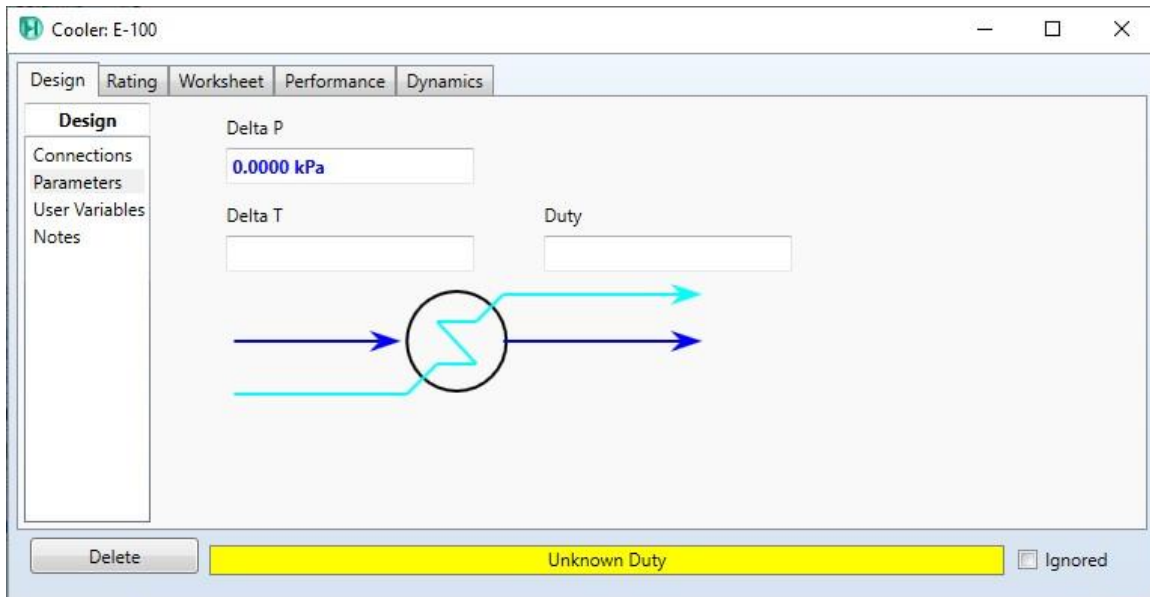
9. Worksheet\ gas-comp
10. Change the pressure to 60 psia

	gas-mixture	gas-comp	work
Name	gas-mixture	gas-comp	work
Vapour	1.0000	1.0000	<empty>
Temperature [C]	4.444	68.55	<empty>
Pressure [kPa]	101.3	413.7	<empty>
Molar Flow [kgmole/h]	45.36	45.36	<empty>
Mass Flow [kg/h]	1937	1937	<empty>
LiqVol Flow [m3/h]	4.126	4.126	<empty>
Molar Enthalpy [kJ/kgmole]	-1.070e+005	-1.024e+005	<empty>
Molar Entropy [kJ/kgmole-C]	178.7	182.2	<empty>
Heat Flow [kJ/h]	-4.854e+006	-4.647e+006	2.070e+005

- 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 35° F

The screenshot shows the 'Cooler: E-100' window with the 'Worksheet' tab selected. The 'Worksheet' sidebar is active. The main area displays a table with the following data:

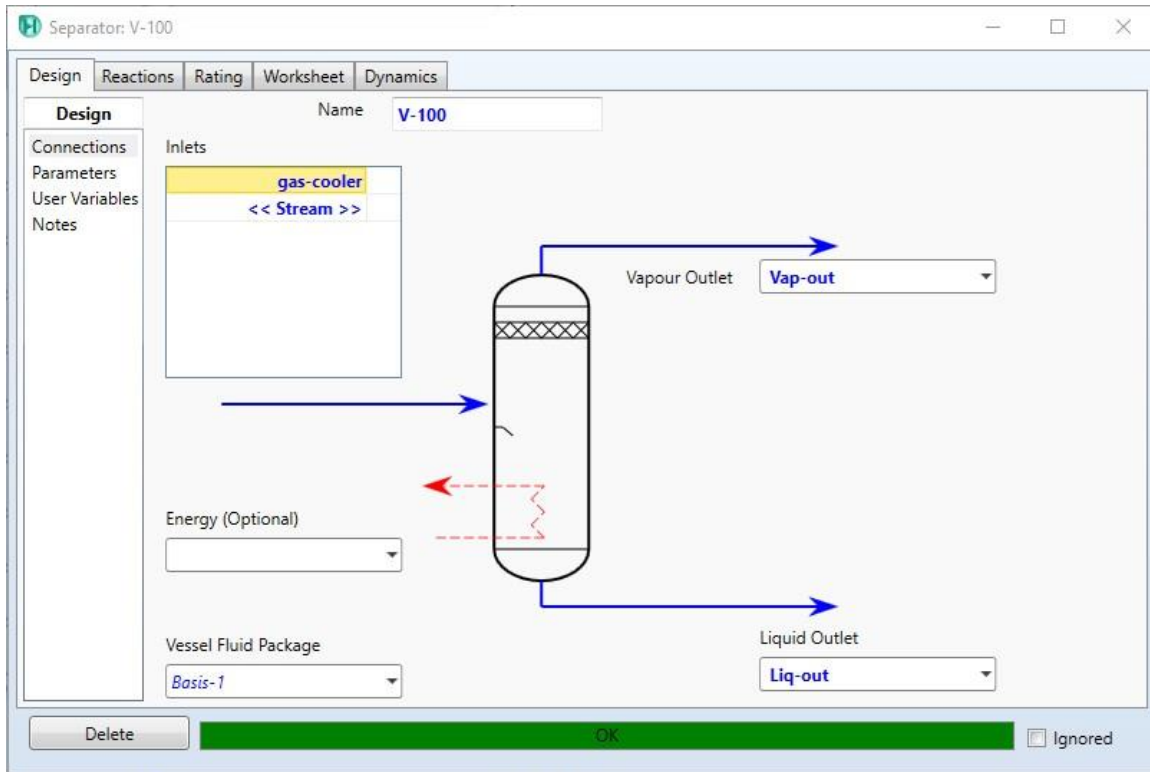
Name	gas-comp	gas-cooler	work2
Vapour	1.0000	0.9656	<empty>
Temperature [C]	68.55	1.667	<empty>
Pressure [kPa]	413.7	413.7	<empty>
Molar Flow [kgmole/h]	45.36	45.36	<empty>
Mass Flow [kg/h]	1937	1937	<empty>
Std Ideal Liq Vol Flow [m3/h]	4.126	4.126	<empty>
Molar Enthalpy [kJ/kgmole]	-1.024e+005	-1.082e+005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

The status bar at the bottom shows 'OK'.

- 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.

Separator: V-100

Design Reactions Rating Worksheet Dynamics

**Worksheet**

	gas-cooler	Liq-out	Vap-out
Name	0.9656	0.0000	1.0000
Vapour			
Temperature [C]	1.667	1.667	1.667
Pressure [kPa]	413.7	413.7	413.7
Molar Flow [kgmole/h]	45.36	1.561	43.80
Mass Flow [kg/h]	1937	81.37	1855
Std Ideal Liq Vol Flow [m3/h]	4.126	0.1524	3.973
Molar Enthalpy [kJ/kgmole]	-1.082e+005	-1.436e+005	-1.070e+005
Molar Entropy [kJ/kgmole-C]	163.1	86.90	165.9
Heat Flow [kJ/h]	-4.909e+006	-2.241e+005	-4.685e+006

Delete OK Ignored

11. Select compositions

12. Read the compositions of the outlet streams

Separator: V-100

Design Reactions Rating Worksheet Dynamics

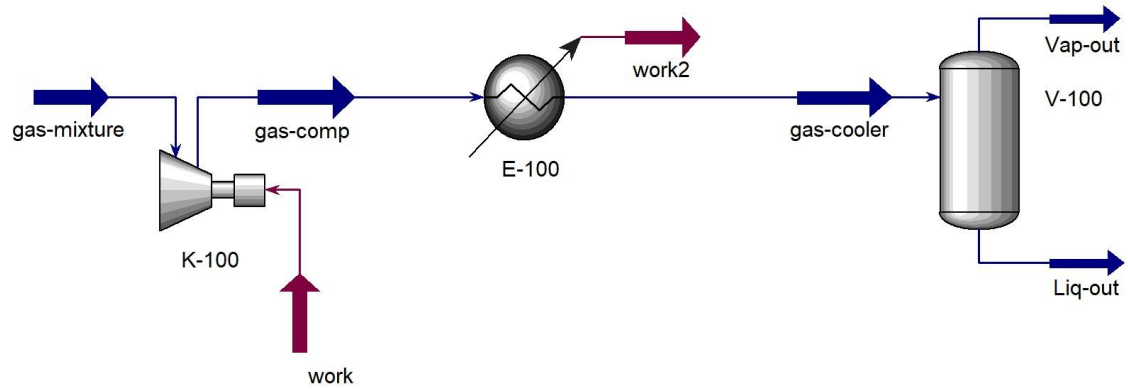
**Worksheet**

	gas-cooler	Liq-out	Vap-out
Ethane	0.4000	0.0865	0.4112
Propane	0.3000	0.2548	0.3016
i-Butane	0.3000	0.6587	0.2872

Delete OK Ignored

- Save the case:

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

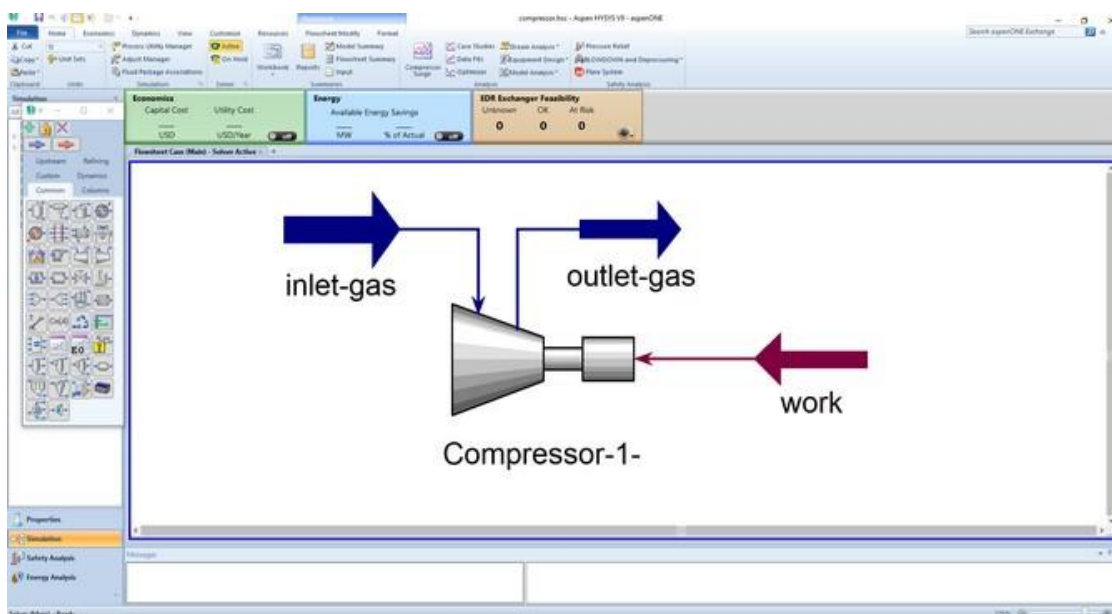


### **References:**

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.



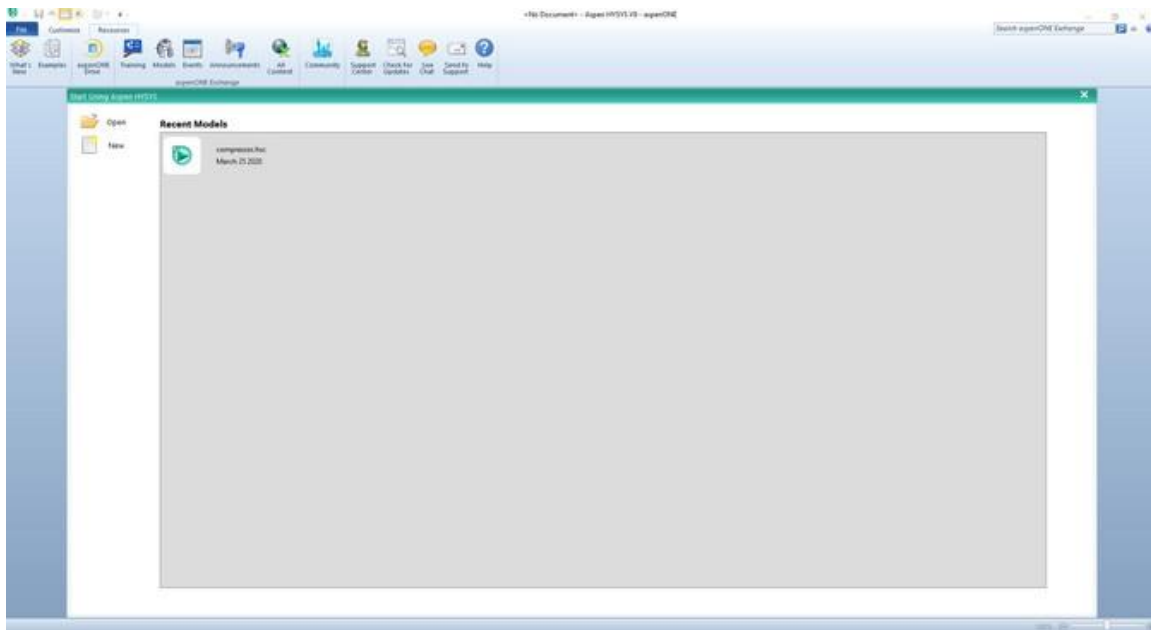
The figure above shows a simple model containing the compressor with inlet, outlet and energy streams using Aspen HYSYS V.9.

### **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.

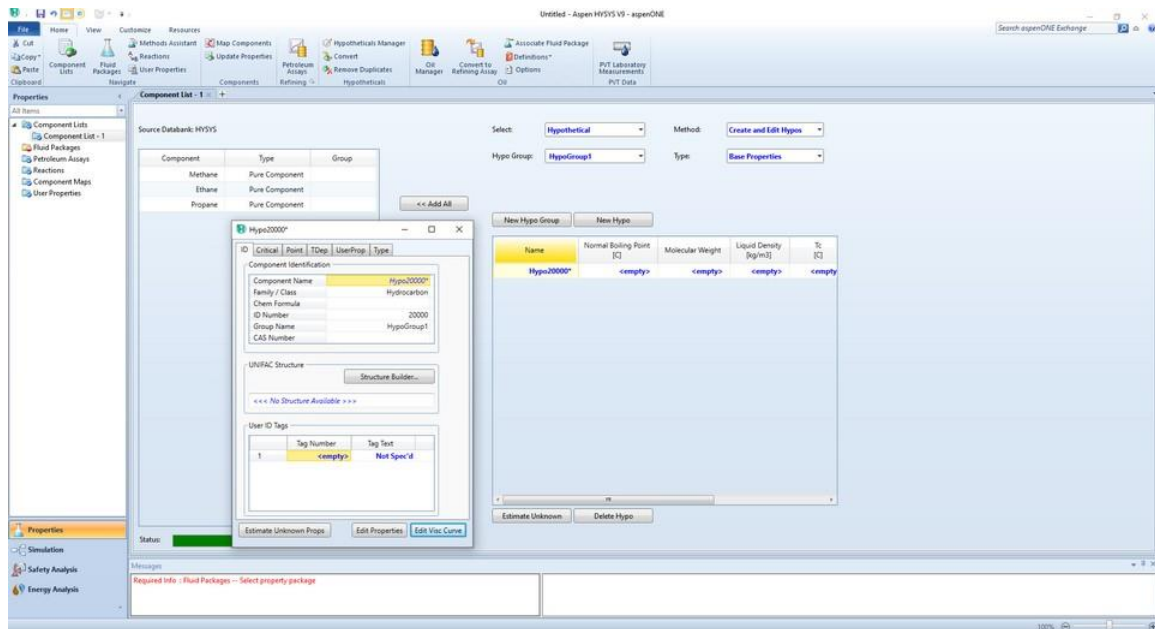


The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new window.

- 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 method field, select (create and edit hypos)
  3. Click New Hypo
  4. Double- Click on the added new component



5. Change the component name to : C-Hypo
6. Select critical
7. Change the Normal Boiling point to : (150° C). [ the value of the normal Boiling 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

C-hypo\*

ID Critical Point TDep UserProp Type

Base Properties

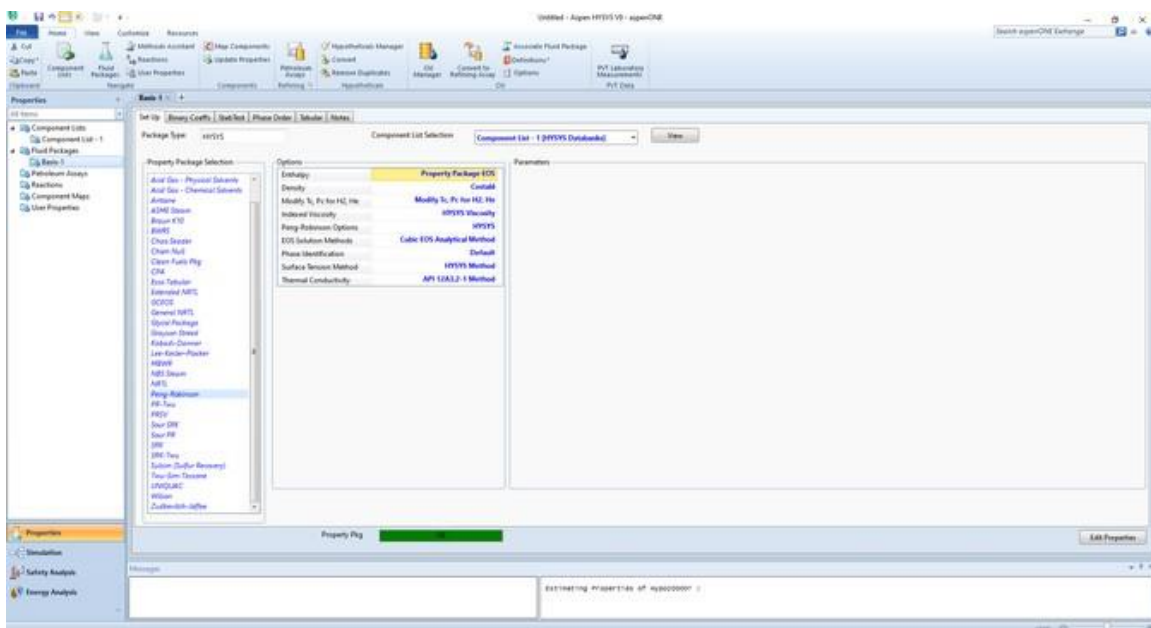
Molecular Weight	127.5
Normal Boiling Pt [C]	150.0
Ideal Liq Density [kg/m3]	768.1

Critical Properties

Temperature [C]	336.7
Pressure [kPa]	2591
Volume [m3/kgmole]	0.5020
Acentricity	0.3659

Estimate Unknown Props Edit Properties Edit Visc Curve

- 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 <sup>o</sup> 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.

Material Stream: inlet-gas

Worksheet Attachments Dynamics

**Worksheet**

Stream Name	inlet-gas	Vap
Vapour / Phase Fraction	1.0000	
Temperature [C]	120.0	
Pressure [kPa]	200.0	
Molar Flow [kgmole/h]	100.0	
Mass Flow [kg/h]	5377	
Std Ideal Liq Vol Flow [m3/h]	9.874	
Molar Enthalpy [kJ/kgmole]	-1.118e+005	-1
Molar Entropy [kJ/kgmole-C]	236.1	
Heat Flow [kJ/h]	-1.118e+007	-1
Liq Vol Flow @Std Cond [m3/h]	9.272	
Fluid Package	Basis-compressor	
Utility Type		

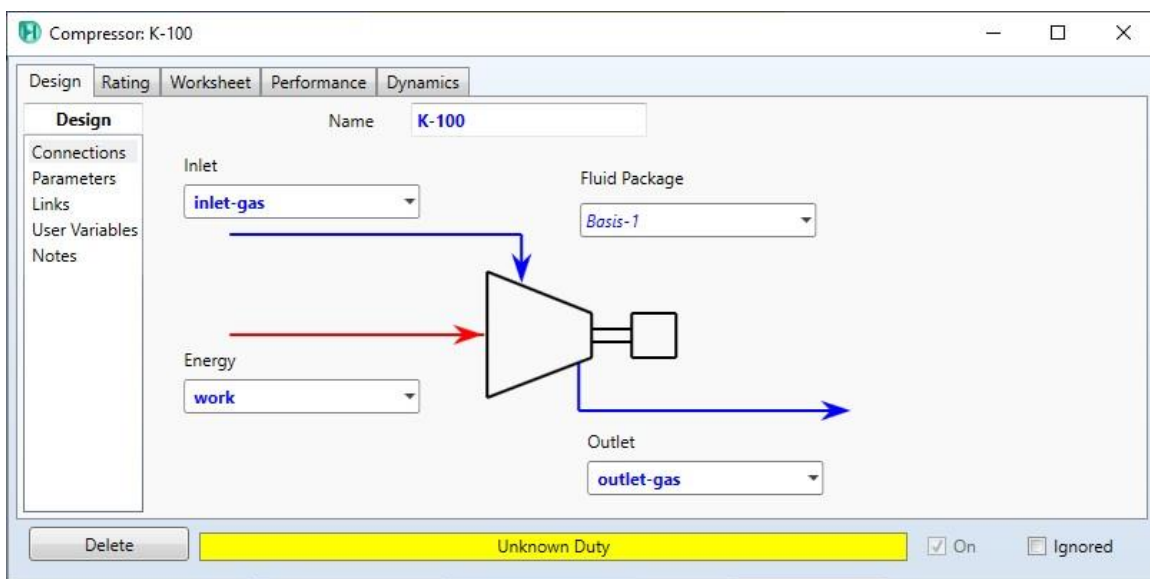
OK

Delete Define from Stream... View Assay

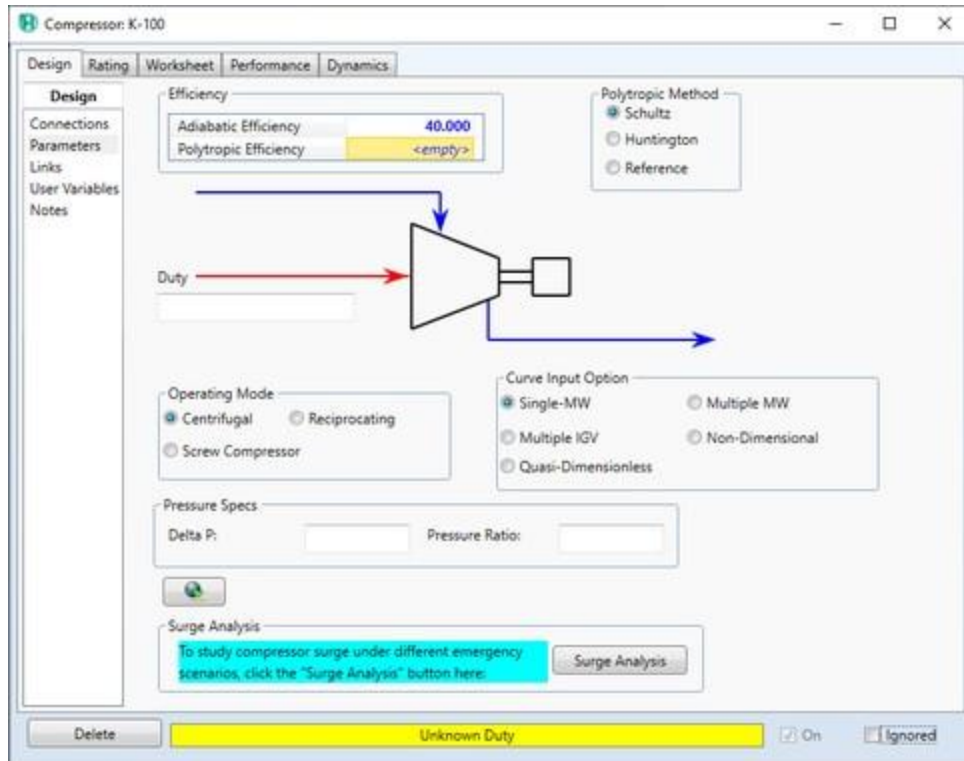
- Adding Compressor:
  1. Object palette.
  2. Select compressor
  3. Place the selected unit in the desired position.

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.

Compressor: K-100

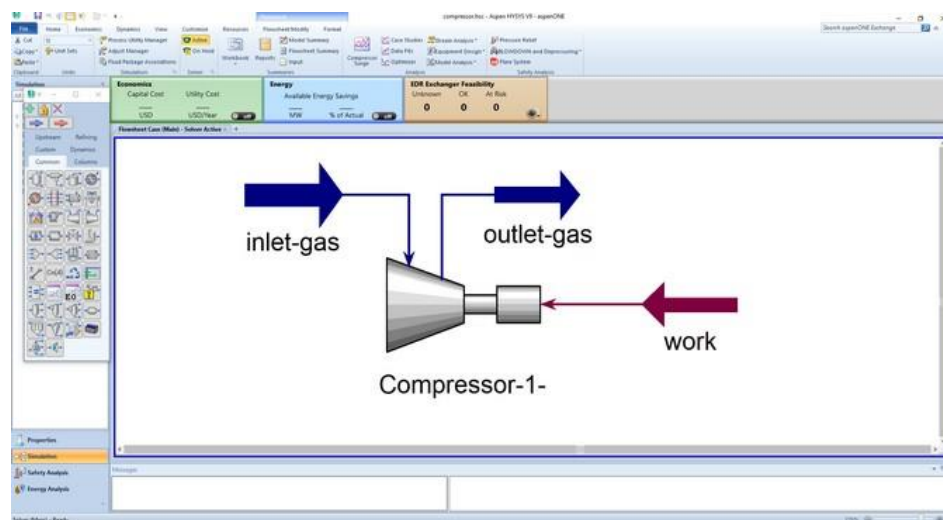
Design Rating Worksheet Performance Dynamics

Worksheet

	Name	inlet-gas	outlet-gas	work
Conditions	Vapour	1.0000	1.0000	<empty>
Properties	Temperature [C]	120.0	209.4	<empty>
Composition	Pressure [kPa]	200.0	700.0	<empty>
PF Specs	Molar Flow [kgmole/h]	100.0	100.0	<empty>
	Mass Flow [kg/h]	5377	5377	<empty>
	LiqVol Flow [m3/h]	9.874	9.874	<empty>
	Molar Enthalpy [kJ/kgmole]	-1.118e+005	-1.014e+005	<empty>
	Molar Entropy [kJ/kgmole-C]	236.1	249.7	<empty>
	Heat Flow [kJ/h]	-1.118e+007	-1.014e+007	1.037e+006

Delete On Ignored

- Save the case:
  1. File menu
  2. Select save as
  3. Give the name (compressor)

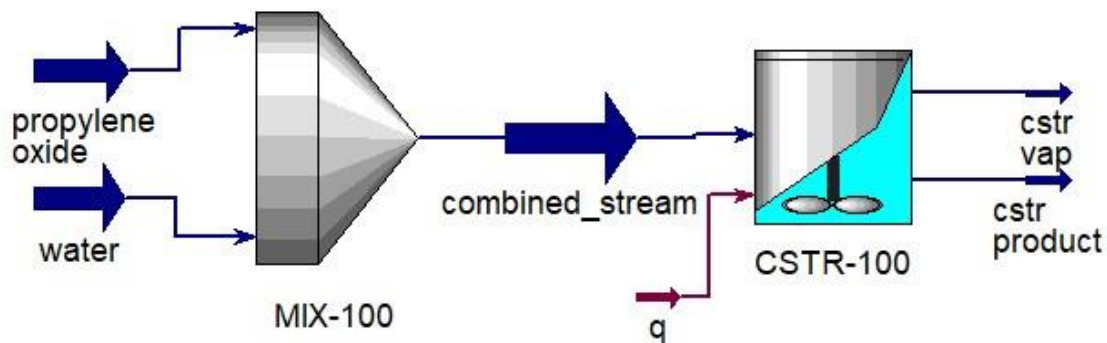


**References:**

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

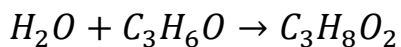
## Modeling of CSTR Using HYSYS V9

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:



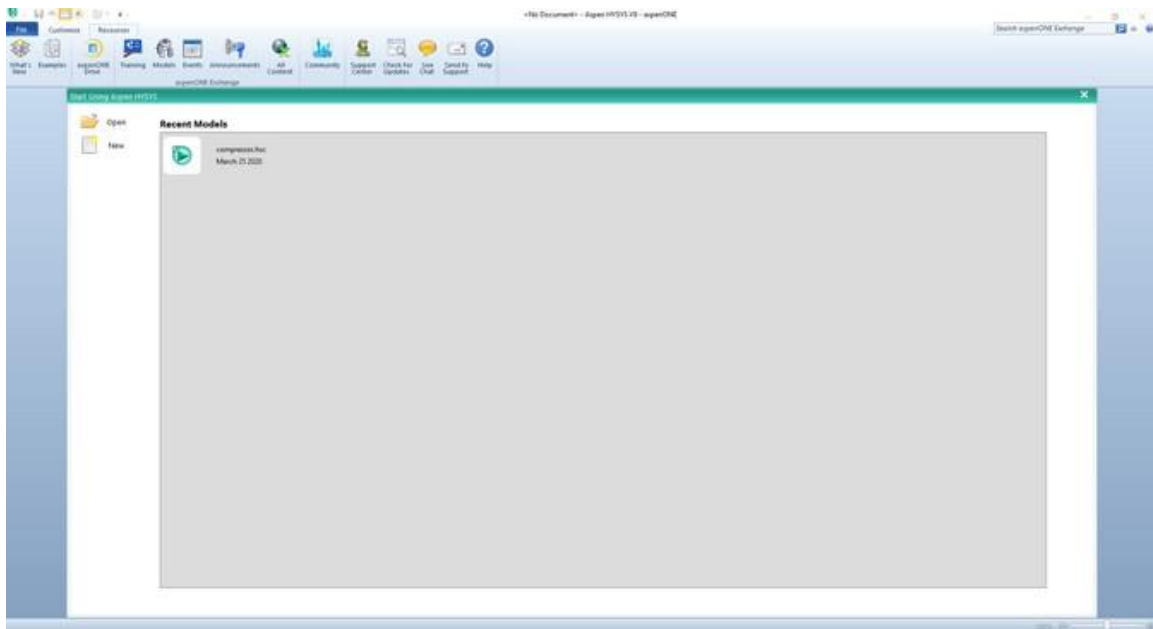
The forward reaction arrhenius parameters:

Frequency factor:  $1.7 \times 10^{13}$ , Activation Energy:  $3.24 \times 10^4$

(fluid Package: UNIQUAC) [1]

## **Solution:**

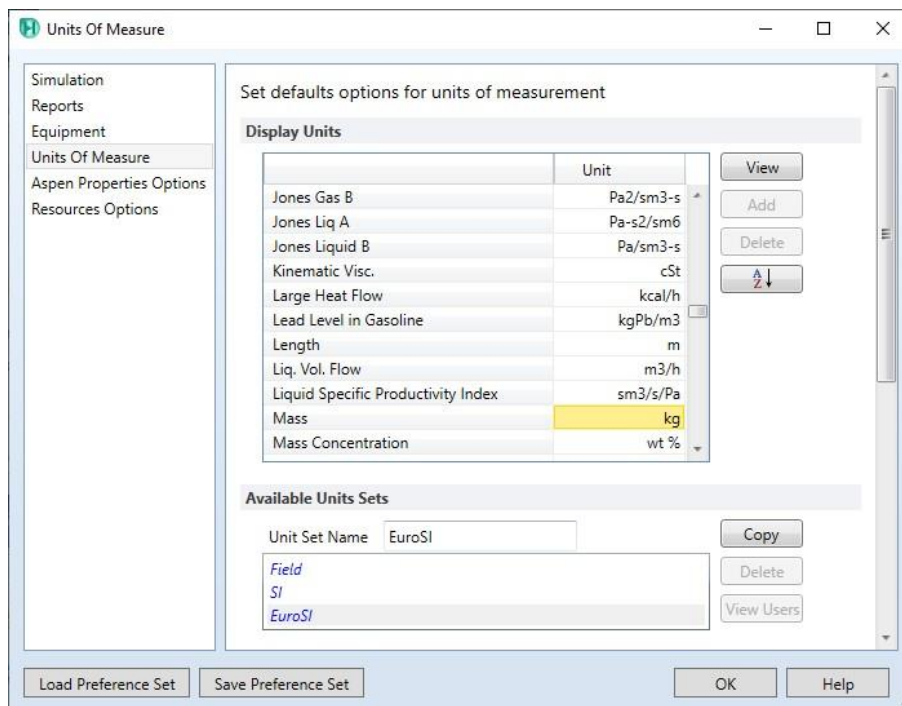
- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



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

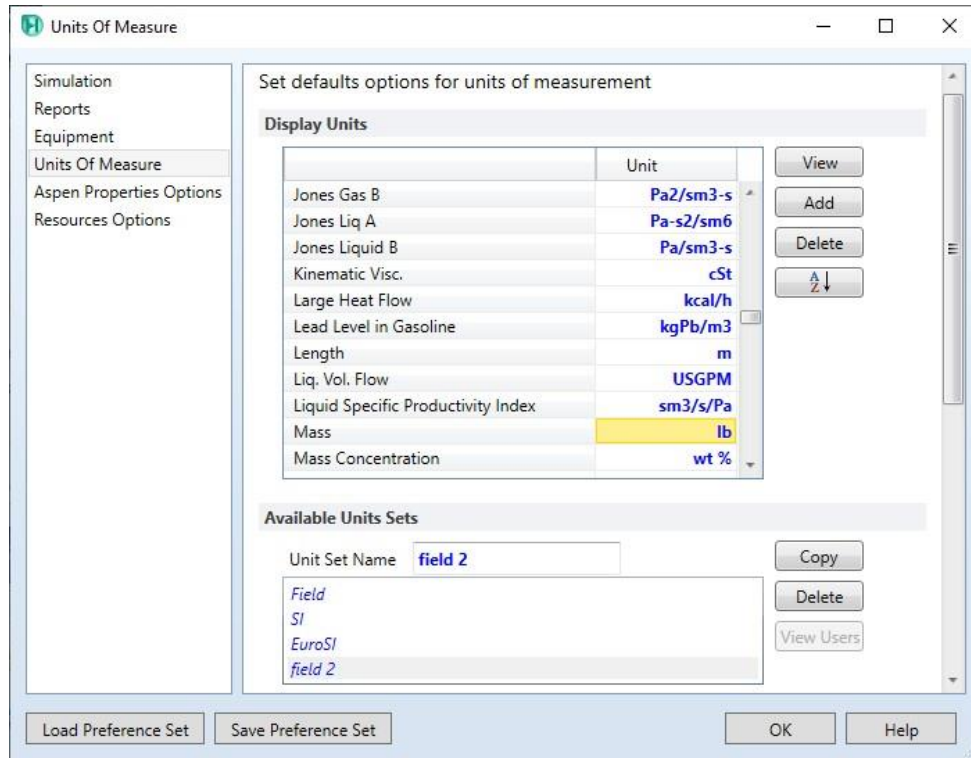
- There are two main necessary information have to be given in the properties tab before starting the simulation:
  1. Property package : UNIQUAC
  2. Components: Propylene\_Glycol, H<sub>2</sub>O, PropyleneOxide
- Preference Set:
  1. File
  2. Options
  3. Click (unit of measure)



4. Available unit set \ click (copy) : new unit set is given.
5. Change 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).

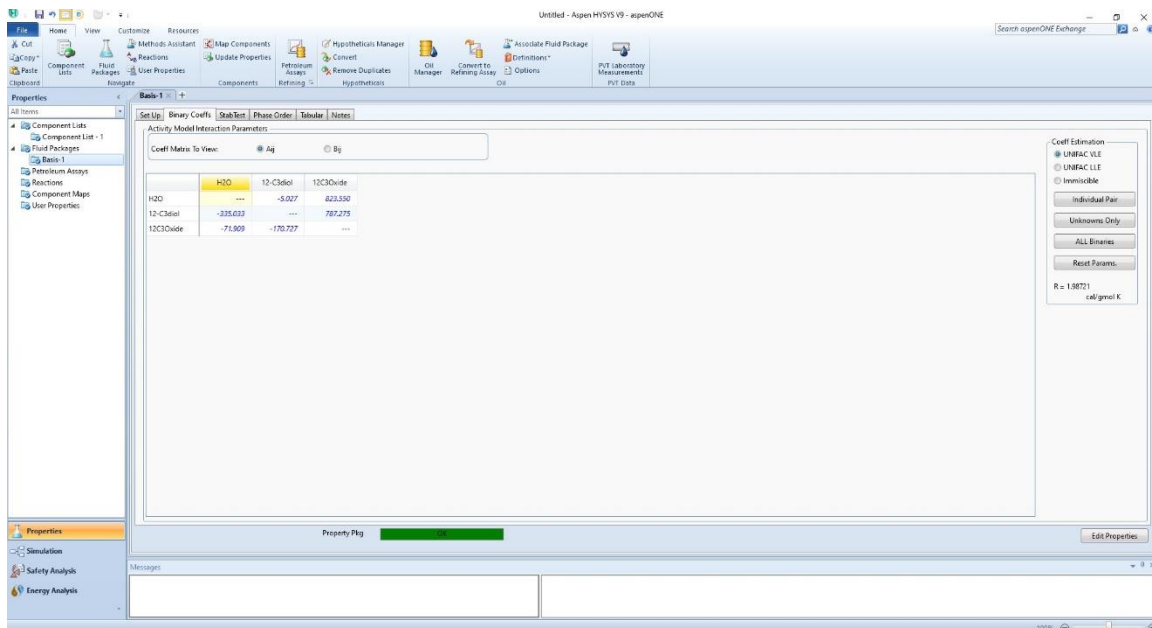


9. Click (save preference set) in order to save the set as a separate file. It is possible to use this preference set in another simulation case by clicking (load preference set).
10. Click ok

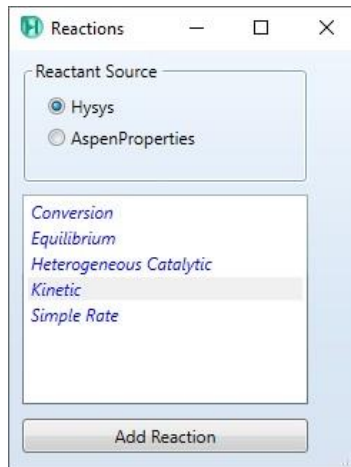


- Adding Component list:
  1. Properties
  2. Component lists \ Add
  3. Select: Pure components
  4. Type in the search field Propylene\_Glycol
  5. Select Propylene\_Glycol \ add
  6. Repeat the steps (4,5) for PropyleneOxide and water

- 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<sub>2</sub>O 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:  $1.7 \times 10^{13}$  as given above. [1.7e+13]
14. Set (E) to the value of the Activation Energy:  $3.24 \times 10^4$  as given above. [3.24e+4]

**Stoichiometry and Rate Info**

Component	Mole Wt.	Stoich Coeff	Fwd Order	Rev Order
H2O	18.015	-1.000	0.00	0.00
12C3Oxide	58.080	-1.000	1.00	0.00
12-C3diol	76.096	1.000	0.00	1.00
**Add Comp**				

**Basis**

Basis	Molar Conc
Base Component	12C3Oxide
Rxn Phase	CombinedLiquid
Min. Temperature	-273.1 C
Max Temperature	3000 C

Basis Units:   
Rate Units:

**Forward Reaction**

A	1.7000e+013
E	32400
b	<empty>

**Reverse Reaction**

A'	<empty>
E'	<empty>
b'	<empty>

**Equation Help**

$r = k \cdot f(\text{Basis}) - k' \cdot f(\text{Basis})$   
 $k = A \cdot \exp \{ -E / RT \} \cdot T^b$   
 $k' = A' \cdot \exp \{ -E' / RT \} \cdot T^{b'}$   
T in Kelvin

Balance Error: 0.00000  
Reaction Heat (25 C): -2.1e+04 kcal/kgmole

Ready

- 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° F
PRESSURE	1.1 atm
Molar flow	150 lbmole/h
Composition	
Propylene Oxide	1

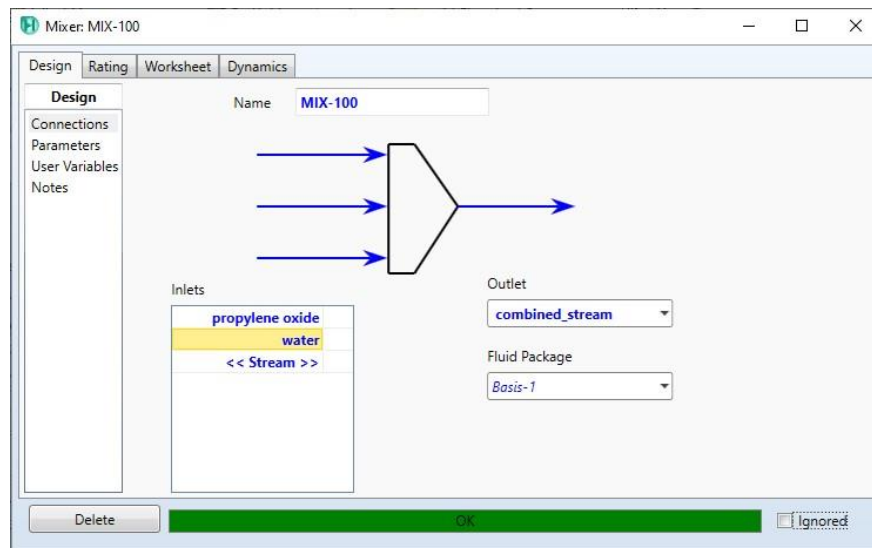
6. Repeat step 5 to add another stream and give the following information:

Name	Water
Conditions	
Temperature	75° F
PRESSURE	1.1 atm
Molar flow	1.1e+4 lb/hr
Composition	
Water	1

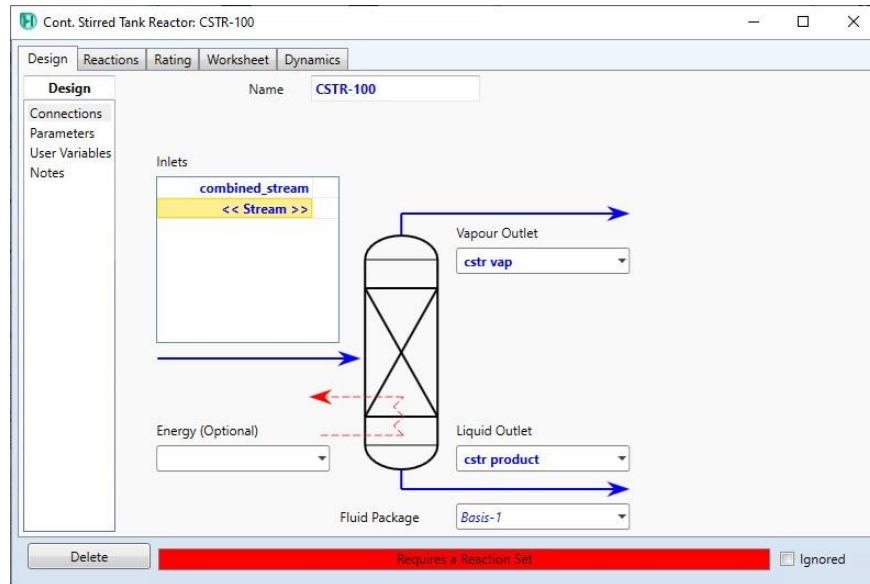
- Adding Mixer:
  1. Object palette.
  2. Select mixer
  3. Place the selected unit in the desired position.

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

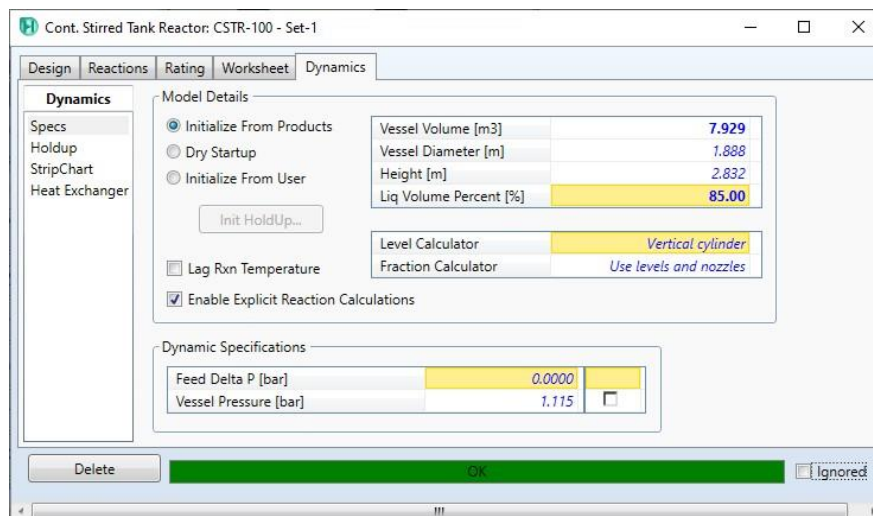
9. In Reaction Set field , select Set-1

10. Dynamics

11. Model details

12. Set the vessel Volume to :280 ft<sup>3</sup>

13. Set the Liq Volume Percent [%] to 85%



14. Design \connection

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

16. Worksheet

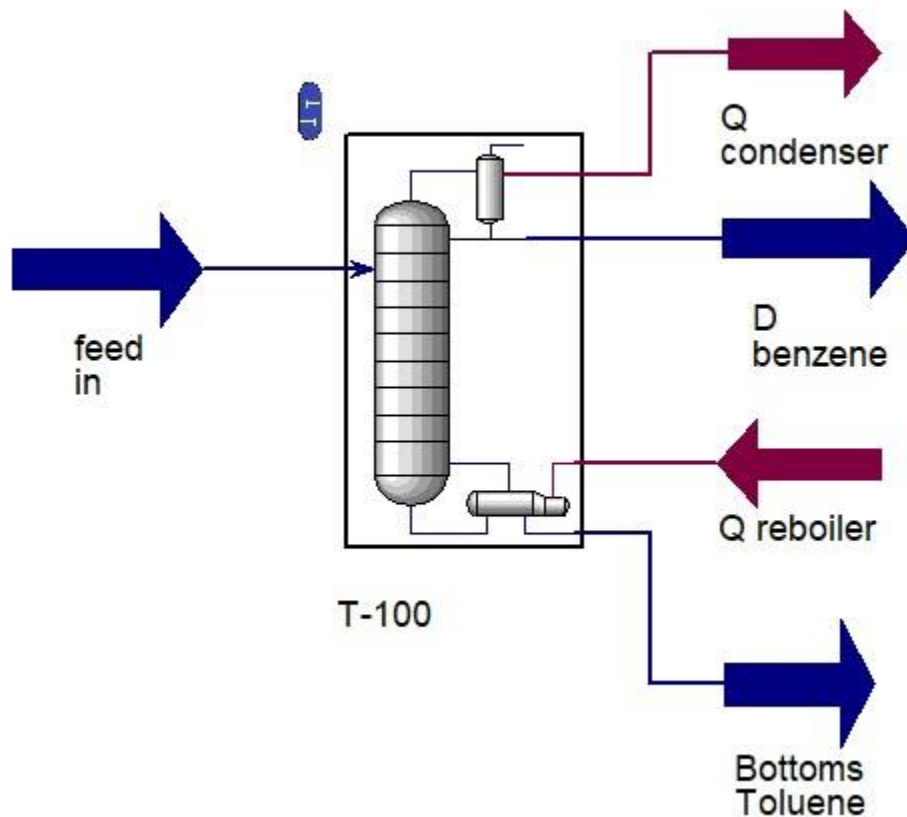
17. Set the temperature in cstr product to 75°F.

- 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.

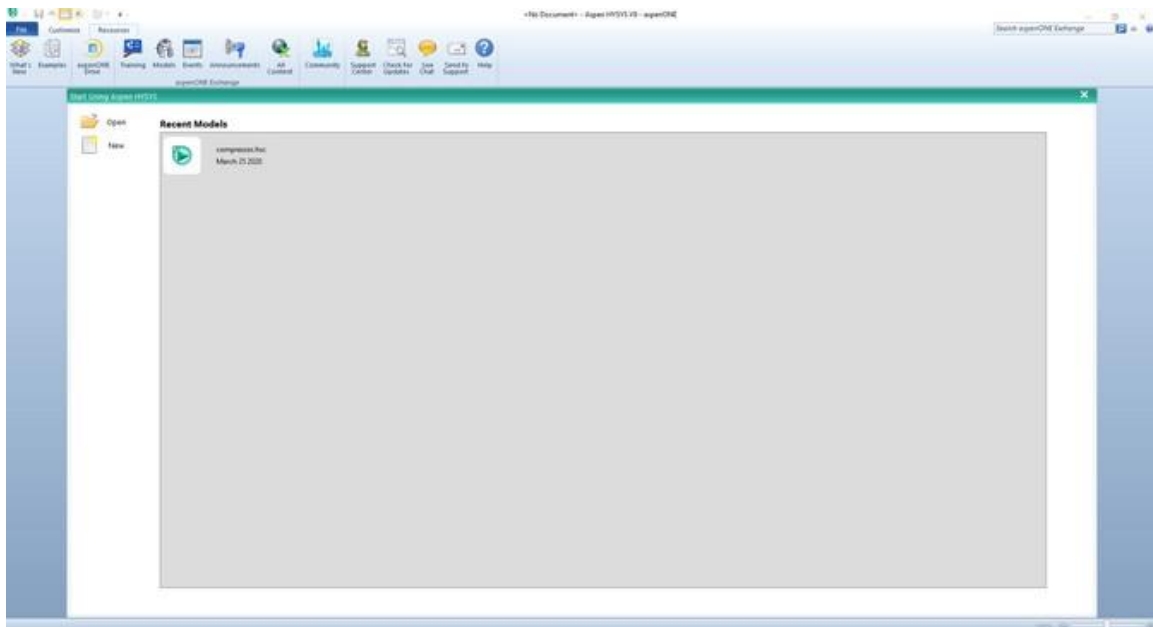
### Example:

A material stream consists of 40% Benzyn and 60% Toluene with temperature of 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 using (distillation column subflowsheet).



## **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)

Shortcut Column: distillation column

Design Rating Worksheet Performance Dynamics

**Design**

Connections  
Parameters  
User Variables  
Notes

Components

Component	Mole Fraction
Light Key in Bottoms	Benzene 0.0300
Heavy Key in Distillate	Toluene 0.0200

Pressures

Condenser Pressure	111.457 kPa
Reboiler Pressure	115.000 kPa

Reflux Ratios

External Reflux Ratio	2.300
Minimum Reflux Ratio	1.545

Delete OK Ignored

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

Shortcut Column: distillation column

Design Rating Worksheet Performance Dynamics

**Performance**

Trays

Minimum Number of Trays	7.933
Actual Number of Trays	14.846
Optimal Feed Stage	8.685

Temperatures

Condenser [C]	82.28
Reboiler [C]	113.7

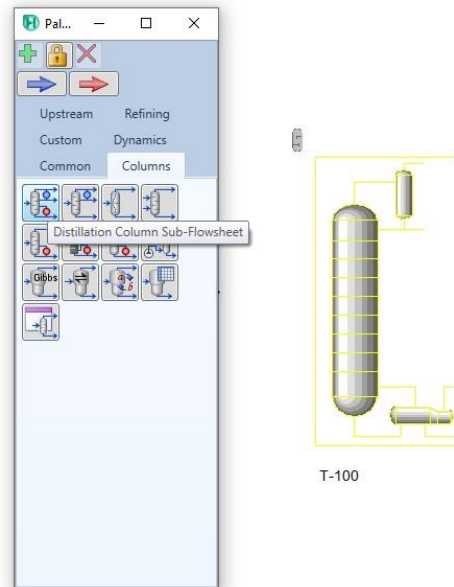
Flows

Rectify Vapour [kgmole/h]	192.789
Rectify Liquid [kgmole/h]	134.368
Stripping Vapour [kgmole/h]	192.789
Stripping Liquid [kgmole/h]	284.368
Condenser Duty [kJ/h]	-5945847.712
Reboiler Duty [kJ/h]	7540780.626

Delete OK Ignored

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

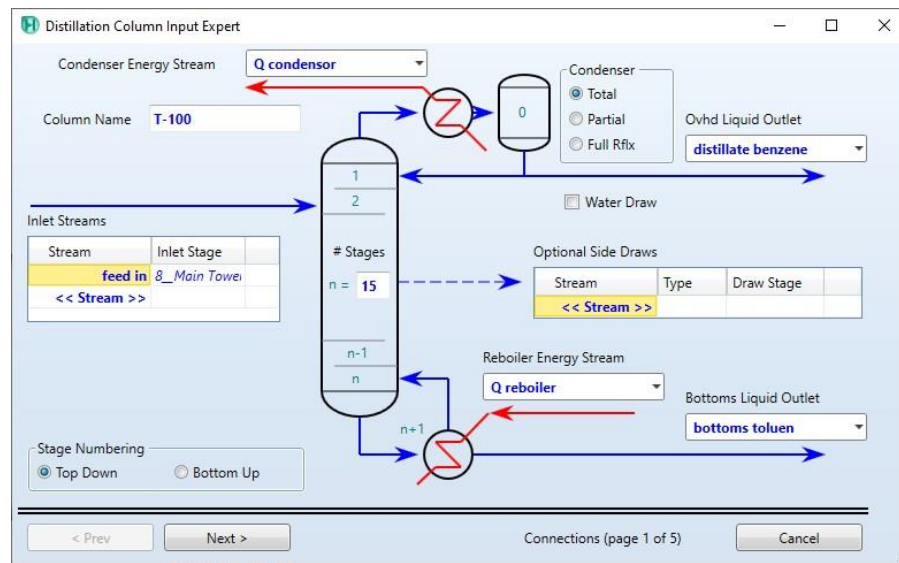
- Adding (distillation column sub-flowsheet)
1. Simulation
  2. Object palette \ columns
  3. Select (distillation column sub-flowsheet)
  4. Place the selected unit in the desired location inside the flowsheet



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 distillation 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]

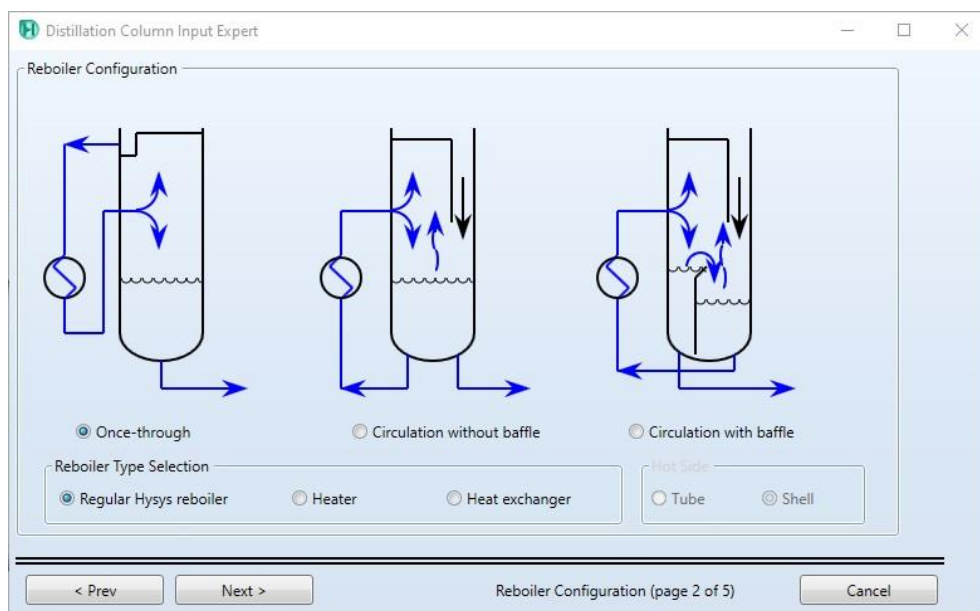
12. In Bottoms Liquid Outlet field, type (Bottoms toluene). [ a new material stream will be created and connected to the distillation column]

13. Click (Next)



14. In reboiler configuration select (once through)

15. Click (Next)

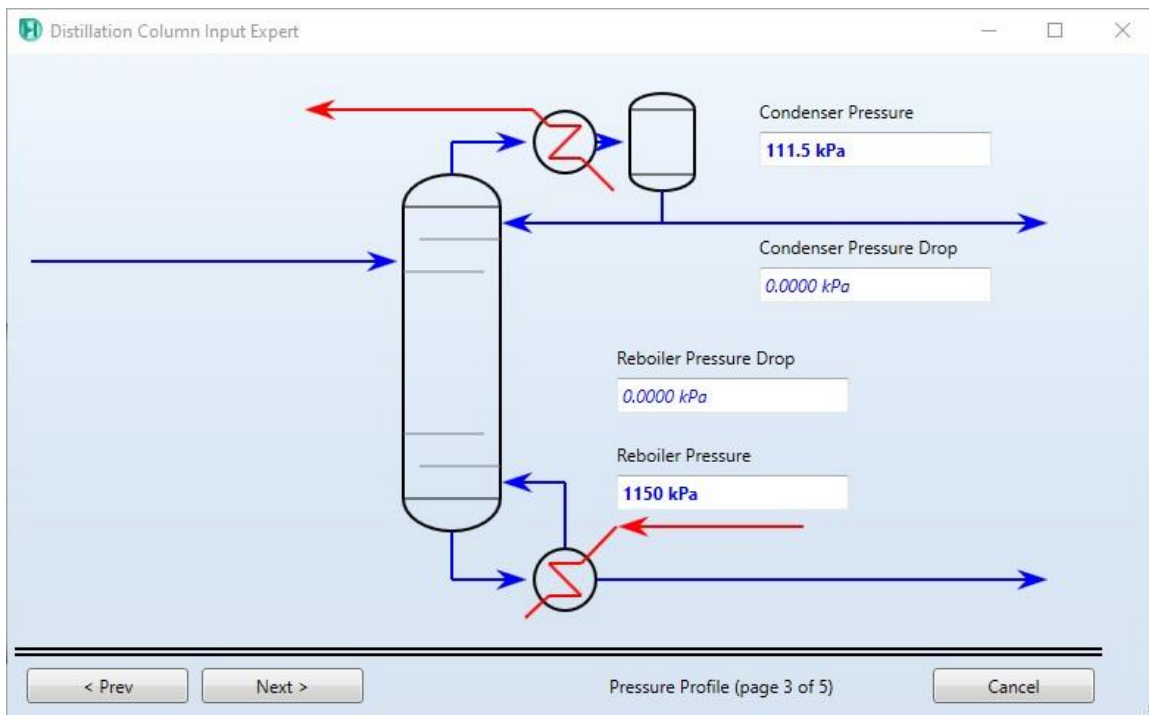


16. Set the condenser pressure to 1.1 atm

17. Set the reboiler pressure to 115 KPa

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

19. Click (Next)

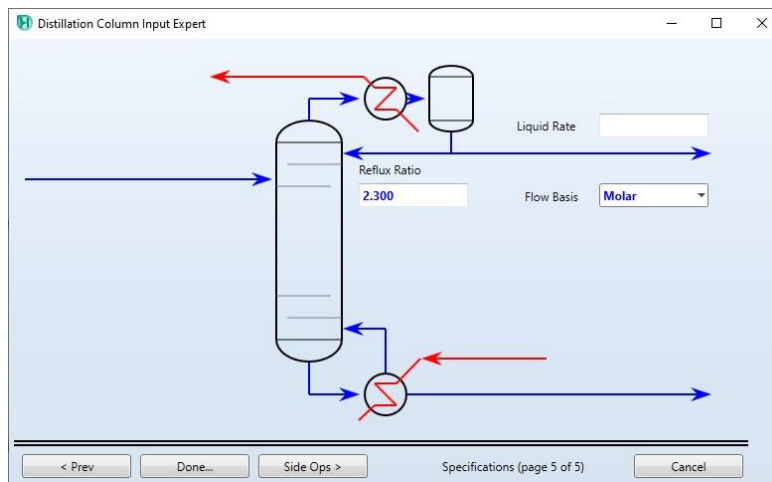


The screenshot shows the 'Distillation Column Input Expert' window, specifically the 'Pressure Profile' page (page 3 of 5). The diagram illustrates a distillation column with a condenser at the top and a reboiler at the bottom. The condenser pressure is set to 111.5 kPa, and the reboiler pressure is set to 1150 kPa. Both the condenser and reboiler pressure drops are set to 0.0000 kPa. The interface includes a schematic of the column and heat exchangers, with blue arrows indicating flow directions. At the bottom, there are navigation buttons: '< Prev', 'Next >', 'Cancel', and a status bar indicating 'Pressure Profile (page 3 of 5)'.

20. In optional estimates page click (Next)

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

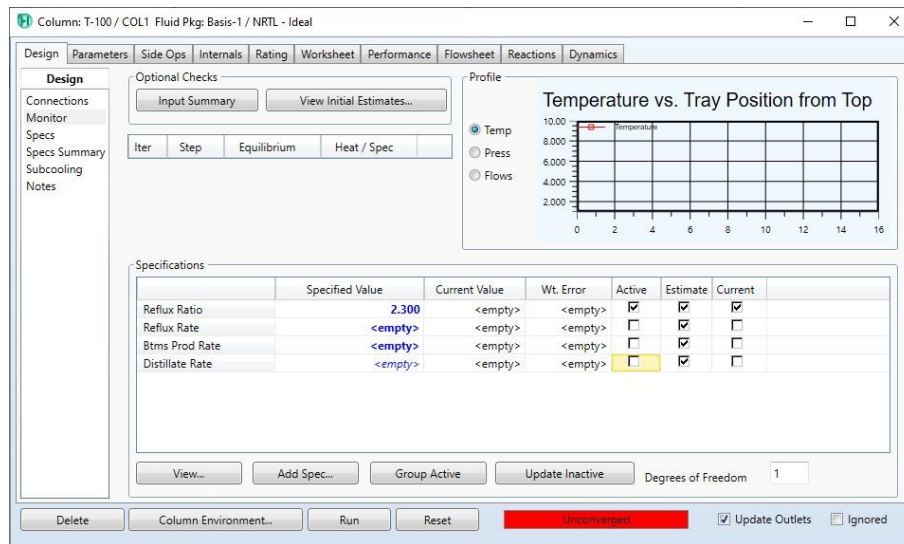
22. Click (Done)



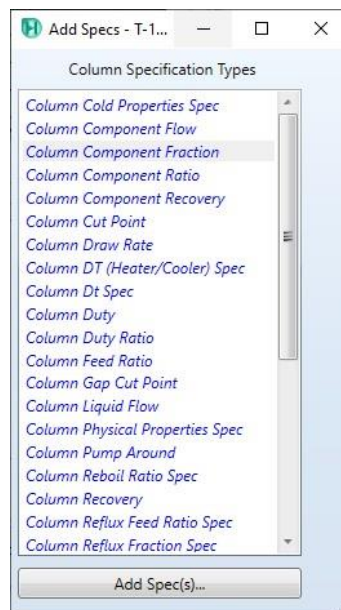
The screenshot shows the 'Distillation Column Input Expert' window, specifically the 'Specifications' page (page 5 of 5). The diagram is the same as the previous page, but the 'Reflux Ratio' is set to 2.300. The 'Flow Basis' is set to 'Molar'. The 'Liquid Rate' field is empty. The interface includes the same schematic of the column and heat exchangers. At the bottom, there are navigation buttons: '< Prev', 'Done...', 'Side Ops >', 'Cancel', and a status bar indicating 'Specifications (page 5 of 5)'.

- 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)

Parameters	
Name	Comp Fraction
Stage	Condenser
Flow Basis	Mole Fraction
Phase	Liquid
Spec Value	0.9800

Components:

Benzene
<< Component >>

Target Type: ☐ Stream ☒ Stage

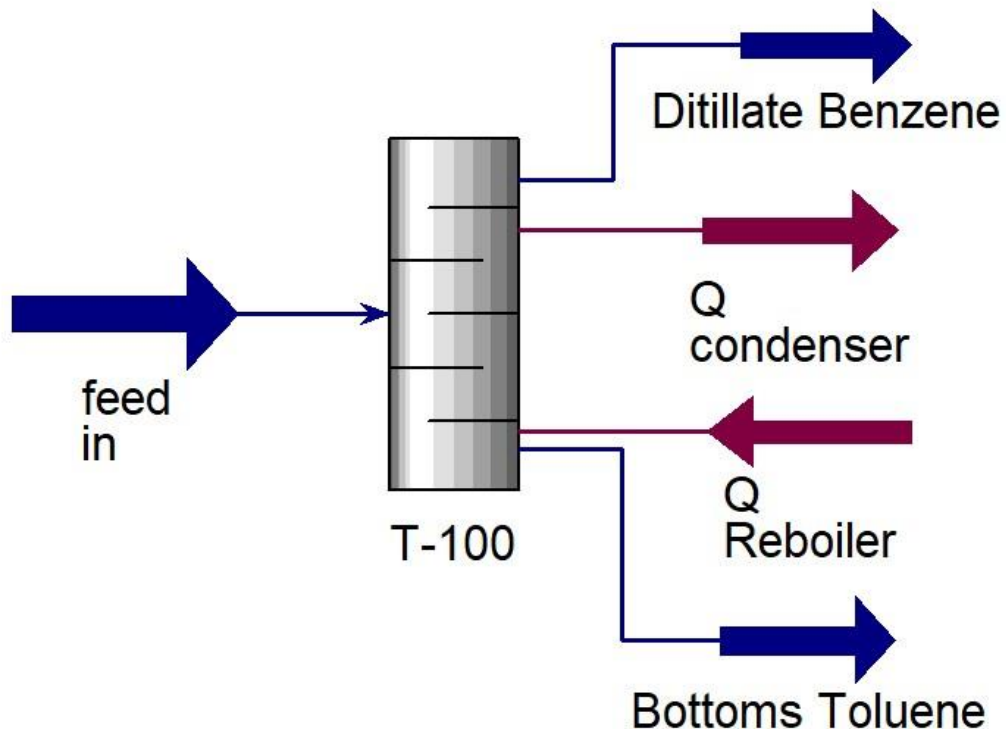
Delete

- 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.

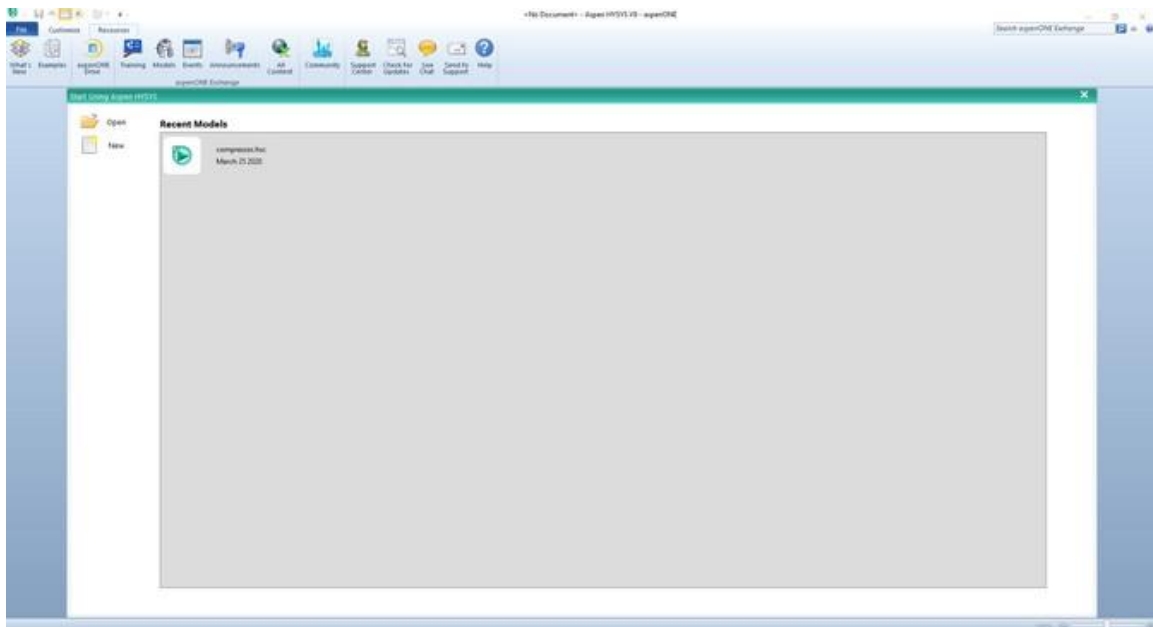
### Example:

A material stream consists of 40% Benzyn and 60% Toluene with temperature of 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:**

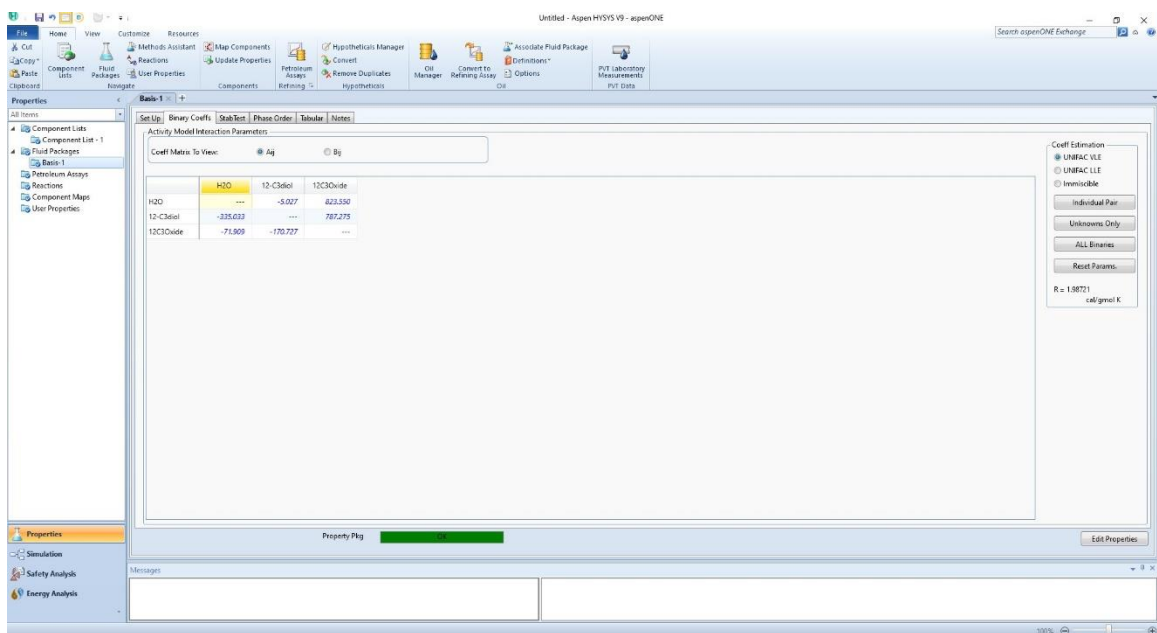
- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



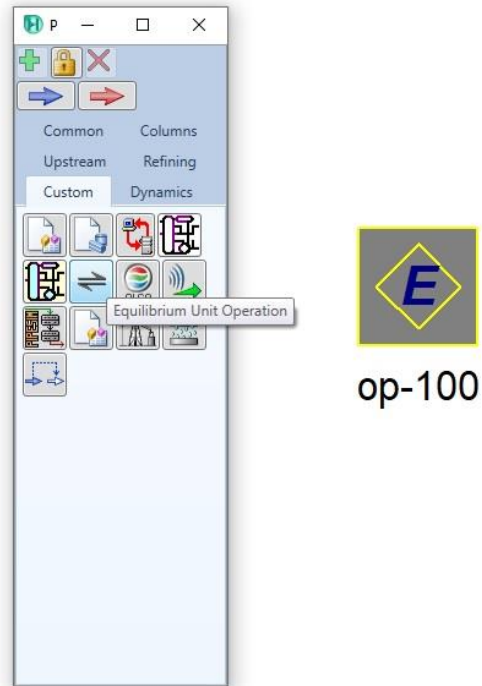
The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new window.

- 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

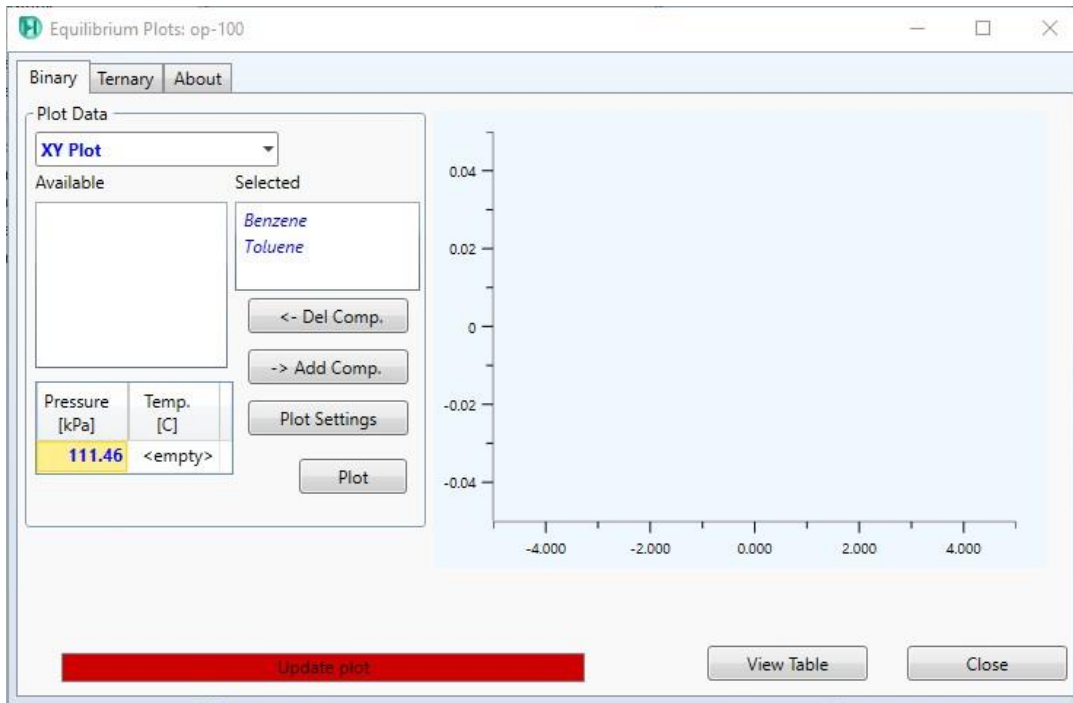
- Adding Component list:
  1. Properties
  2. Component lists \ Add
  3. Select: Pure components
  4. Type in the search field Benzyn
  5. Select Benzyn \ add
  6. Repeat the steps (4,5) for Toluen
  
- Add fluid package:
  1. Properties
  2. Select Fluid package
  3. Click Add
  4. Select (NRTL)
  5. 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.



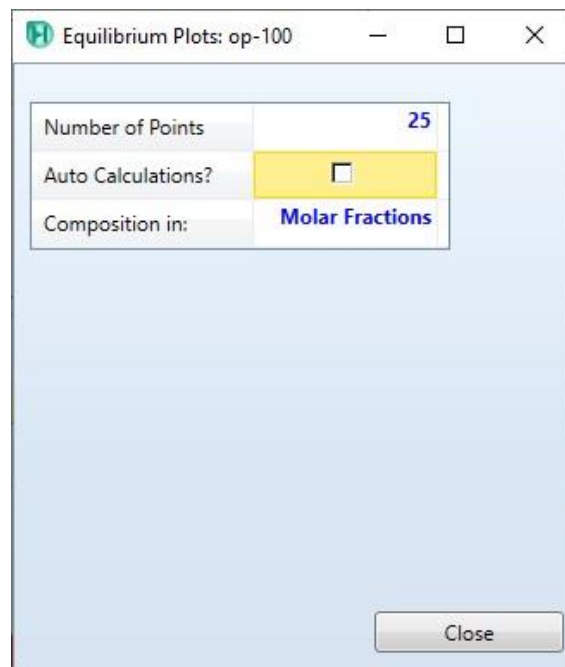
5. Double click on the added unit
6. Binary
7. Available
8. Select Benzene
9. Click (Add Comp.)
10. Select Toluene
11. Click (Add Comp.)
12. Set the pressure to 1.1 atm
13. Data plot
14. Select (XY plot)



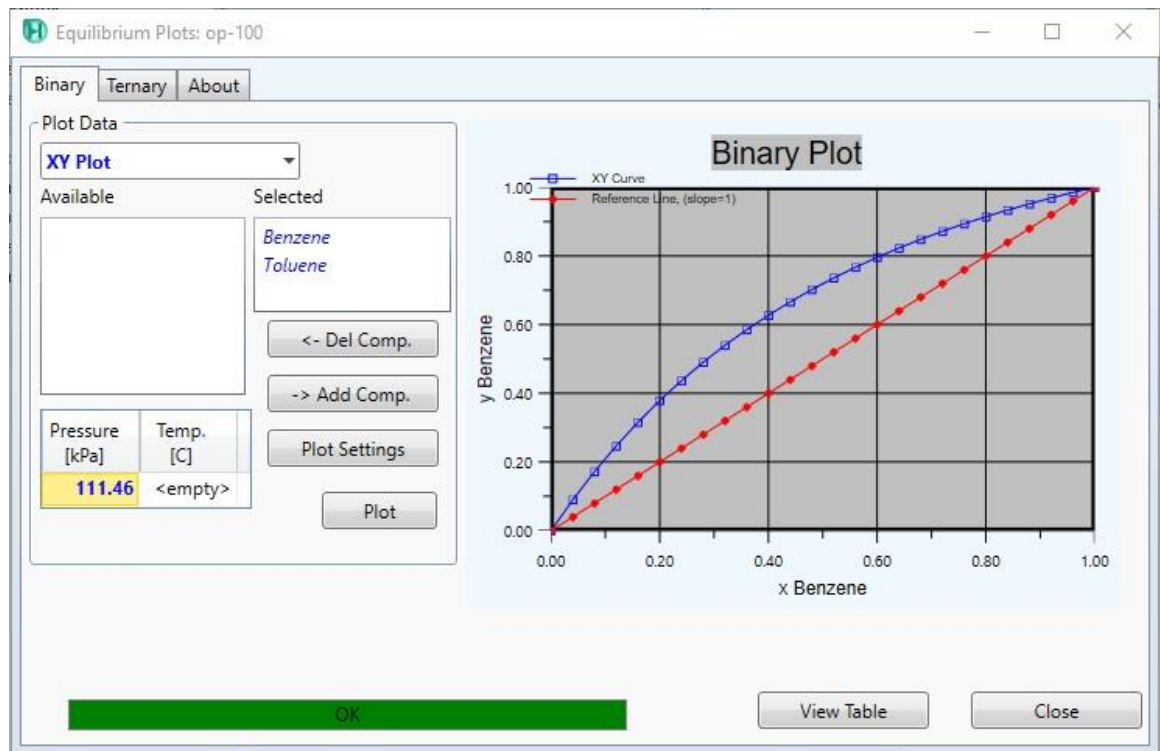
15. Click plot settings

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.

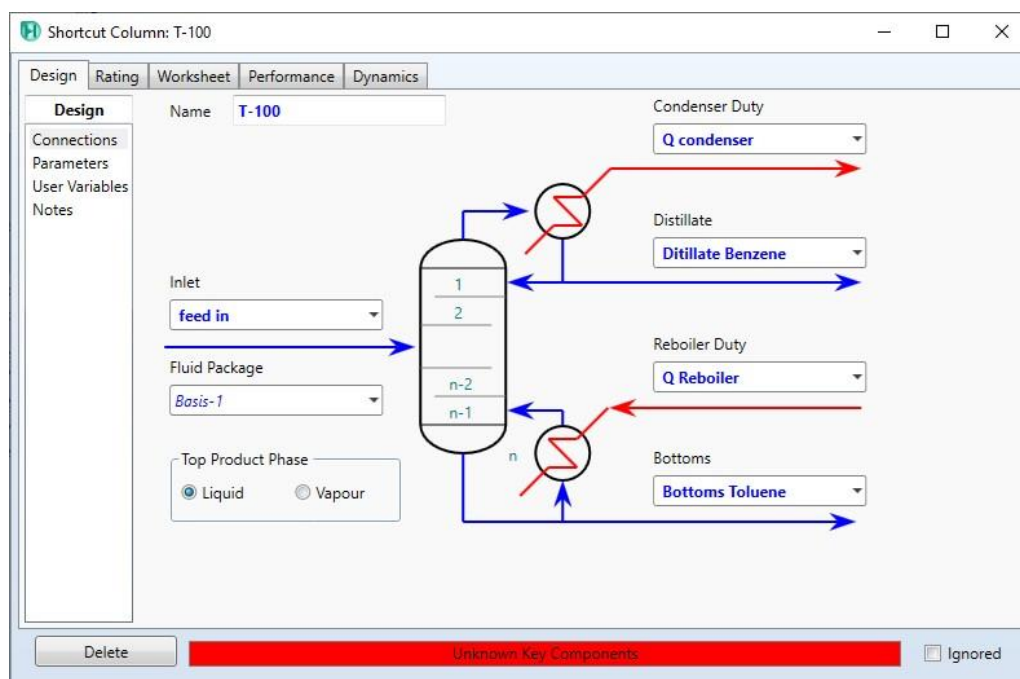
4. Double click on the added material stream
5. Give the below information:

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

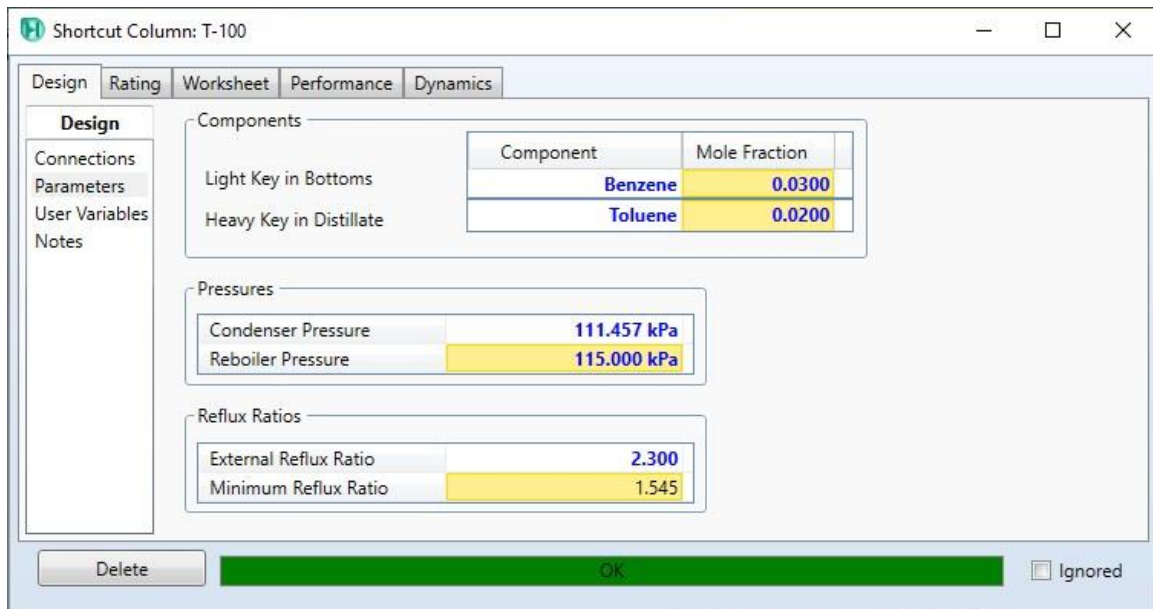
- Adding distillation column:
6. Object palette\ column
  7. Select (short cut distillation)
  8. Place the selected unit in the desired position.

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 Distillate 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 Bottoms 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



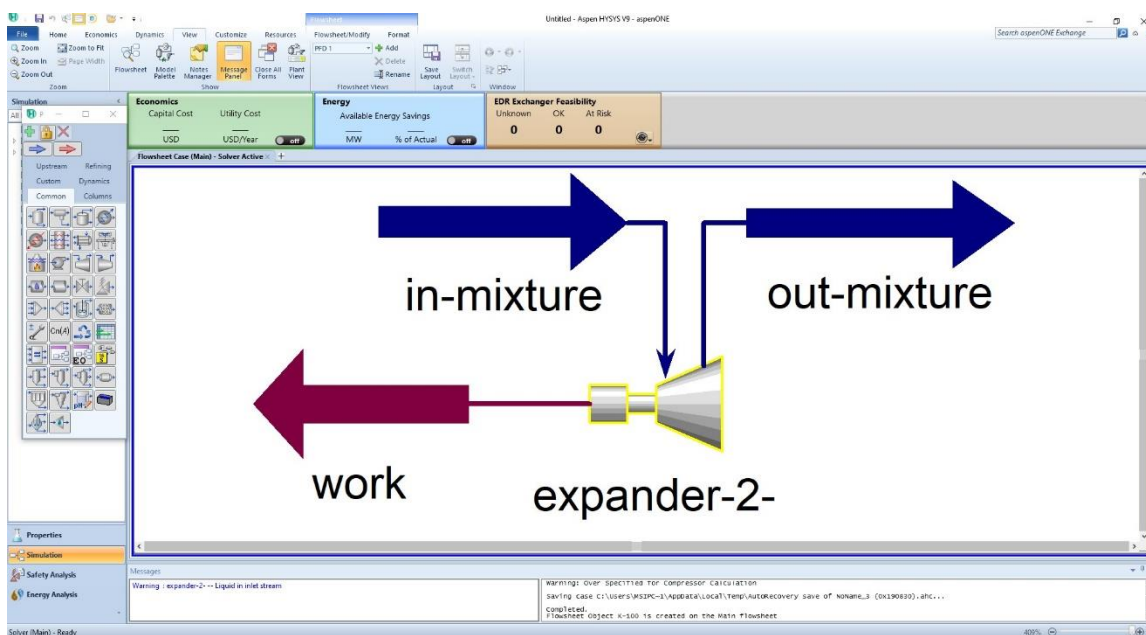
- Save the case:
  1. File menu
  2. Select save as
  3. Give the name (Distillation)

### 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.

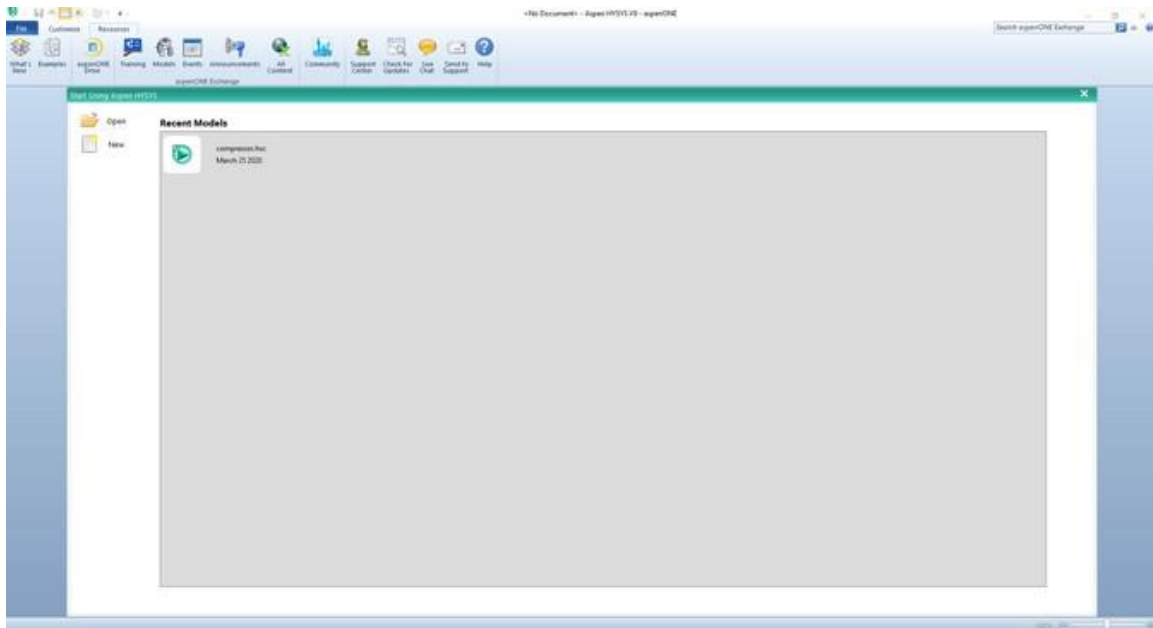


### **Example:**

A mixture of (Methane, Ethane, Propane, and i-Butane ) at 30° 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:**

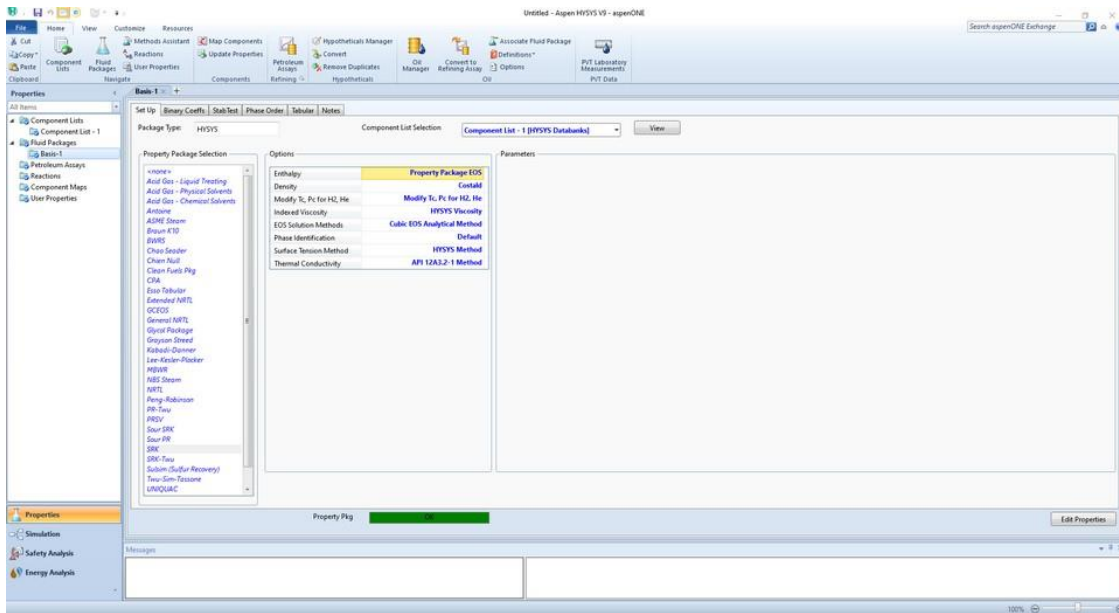
- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



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.

- 
- The screenshot displays the Aspen HYSYS V5 - AspenONE software interface. The top menu bar includes File, Home, Database, Resources, and Search. The left sidebar contains icons for various functions: Get, Get/Save, Paste, Properties, Component List, Fluid Packages, Reaction, Component Maps, and User Properties. The main window is divided into several panes. The 'Component List' pane on the left shows a table with columns for Component, Type, and Group. The 'Simulation Basis' pane on the right shows a table with columns for Simulation Name, Full Name / Synonym, and Formula. The 'Properties' pane at the bottom left shows the 'Simulation' tab selected. The 'Messages' pane at the bottom right displays a message: 'Request Info - Fluid Packages -- Select property package'.
- | Component | Type           | Group |
|-----------|----------------|-------|
| Methane   | Pure Component |       |
| Ethane    | Pure Component |       |
| Propane   | Pure Component |       |
| i-Butane  | Pure Component |       |
- | Simulation Name | Full Name / Synonym | Formula                         |
|-----------------|---------------------|---------------------------------|
| n-Butane        | n-C4                | C <sub>4</sub> H <sub>10</sub>  |
| i-Butane        | i-C4                | C <sub>4</sub> H <sub>10</sub>  |
| n-Pentane       | n-C5                | C <sub>5</sub> H <sub>12</sub>  |
| i-Pentane       | i-C5                | C <sub>5</sub> H <sub>12</sub>  |
| n-Hexane        | n-C6                | C <sub>6</sub> H <sub>14</sub>  |
| n-Heptane       | n-C7                | C <sub>7</sub> H <sub>16</sub>  |
| n-Octane        | n-C8                | C <sub>8</sub> H <sub>18</sub>  |
| n-Nonane        | n-C9                | C <sub>9</sub> H <sub>20</sub>  |
| n-Decane        | n-C10               | C <sub>10</sub> H <sub>22</sub> |
| n-Undecane      | n-C11               | C <sub>11</sub> H <sub>24</sub> |
| n-Dodecane      | n-C12               | C <sub>12</sub> H <sub>26</sub> |
| n-Tridecane     | n-C13               | C <sub>13</sub> H <sub>28</sub> |
| n-Tetradecane   | n-C14               | C <sub>14</sub> H <sub>30</sub> |
| n-Pentadecane   | n-C15               | C <sub>15</sub> H <sub>32</sub> |
| n-Hexadecane    | n-C16               | C <sub>16</sub> H <sub>34</sub> |
| n-Heptadecane   | n-C17               | C <sub>17</sub> H <sub>36</sub> |
| n-Octadecane    | n-C18               | C <sub>18</sub> H <sub>38</sub> |
| n-Nonadecane    | n-C19               | C <sub>19</sub> H <sub>40</sub> |
| n-Eicosane      | n-C20               | C <sub>20</sub> H <sub>42</sub> |
| n-Heneicosane   | n-C21               | C <sub>21</sub> H <sub>44</sub> |
| n-Docosane      | n-C22               | C <sub>22</sub> H <sub>46</sub> |
| n-Tricosane     | n-C23               | C <sub>23</sub> H <sub>48</sub> |
| n-Tetracosane   | n-C24               | C <sub>24</sub> H <sub>50</sub> |
- Request Info - Fluid Packages -- Select property package

- 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° C
Pressure	25 bar
Molar flow	100 kgmole/h
Composition	
C1	0.3
C2	0.4
C3	0.2
i-C4	0.1

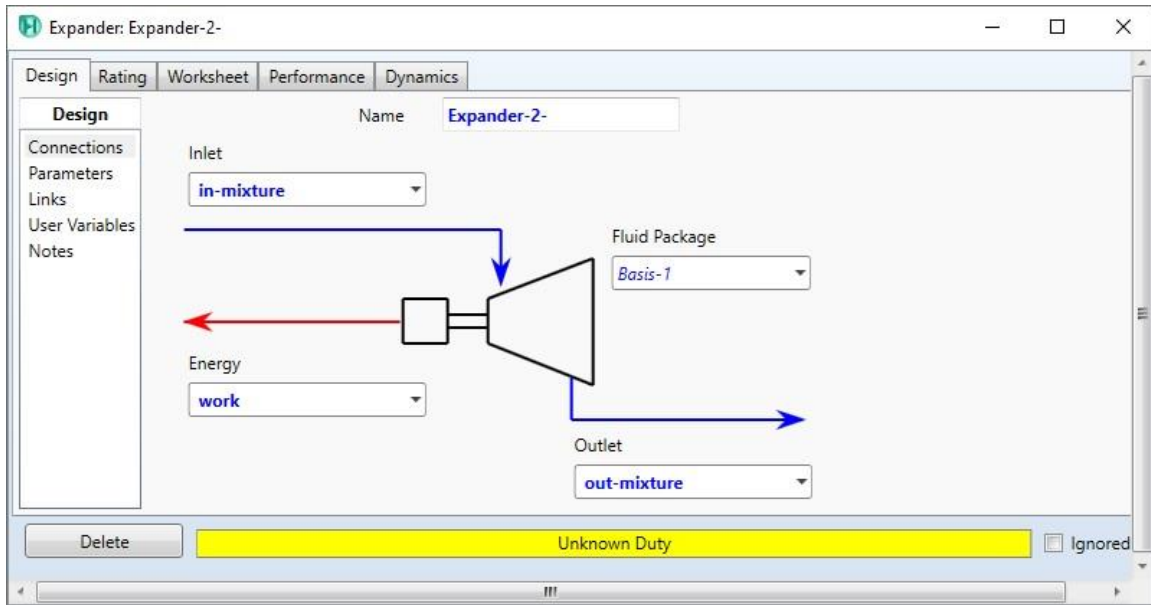
The above information should be given according to the application or example.

Worksheet	Stream Name	in-mixture	Vapour Phase	Liquid Phase
Conditions	Vapour / Phase Fraction	0.9694	0.9694	0.0306
Properties	Temperature [C]	30.00	30.00	30.00
Composition	Pressure [kPa]	2500	2500	2500
Oil & Gas Feed	Molar Flow [kgmole/h]	100.0	96.94	3.063
Petroleum Assay	Mass Flow [kg/h]	3147	3014	132.8
K Value	Std Ideal Liq Vol Flow [m3/h]	7.764	7.489	0.2753
User Variables	Molar Enthalpy [kJ/kgmole]	-9.236e+004	-9.144e+004	-1.217e+005
Notes	Molar Entropy [kJ/kgmole-C]	161.5	163.0	114.2
Cost Parameters	Heat Flow [kJ/h]	-9.236e+006	-8.863e+006	-3.726e+005
Normalized Yields	Liq Vol Flow @Std Cond [m3/h]	751.1	1022	0.2694
	Fluid Package	Basis-1		
	Utility Type			

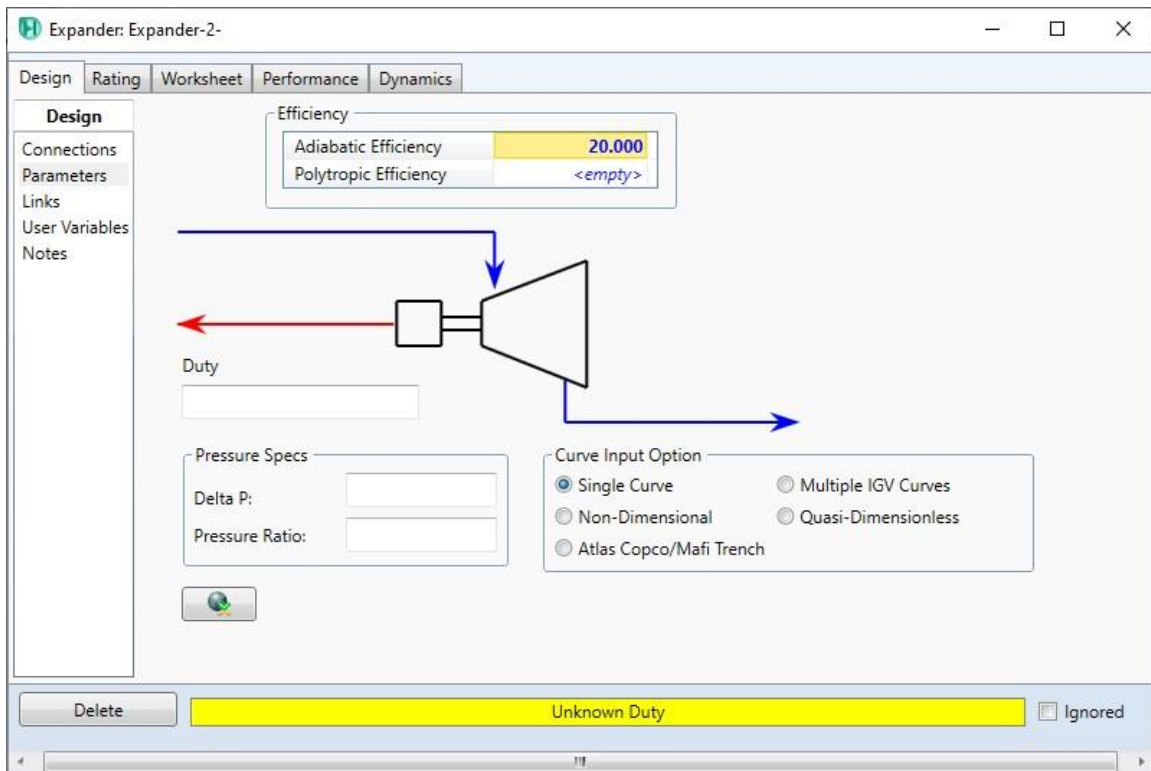
- Adding Expander:
  1. Object palette.
  2. Select expander
  3. Place the selected unit in the desired position.

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



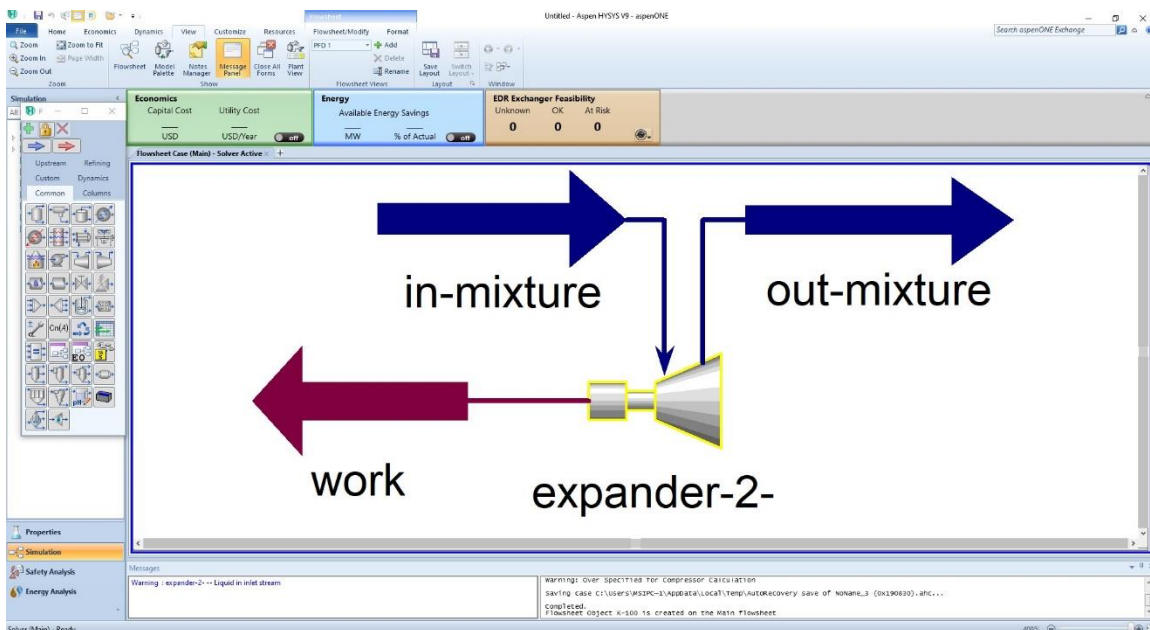
12. Change the outlet-gas pressure to 10 bar.
13. Read the temperature of the outlet-gas.

The temperature of the outlet stream is 2.384° C.

Expander: expander-2-

Design	Rating	Worksheet	Performance	Dynamics
<b>Worksheet</b>				
Conditions	Name	in-mixture	out-mixture	work
Properties	Vapour	0.9694	0.9907	<empty>
Composition	Temperature [C]	30.00	2.384	<empty>
PF Specs	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)

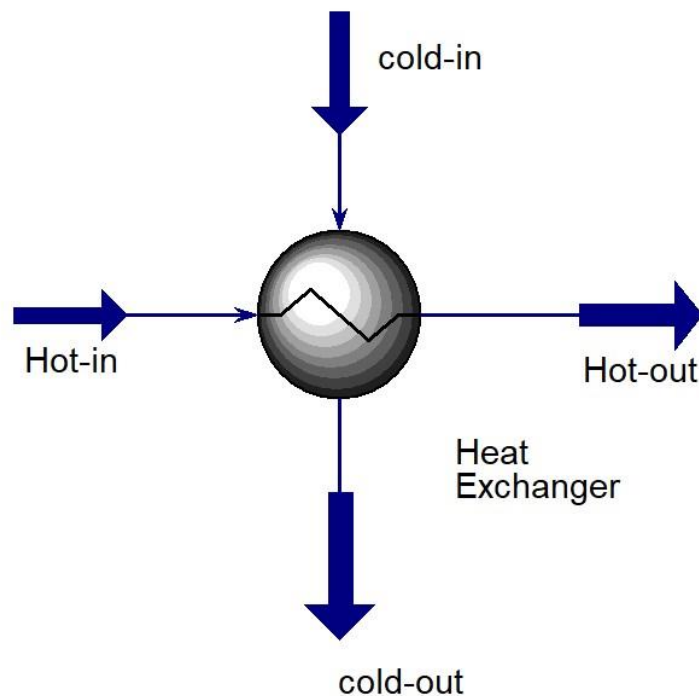


**References:**

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° C and 110 psig via a hot water stream at 300° C and 1100 psig. The temperatures of the outlet cold and hot streams are 135° C and 220° C. The flow rate of the hot stream is 100 kg/h. using Peng-Robinson as a fluid package, determine the mass flow 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<sub>2</sub>O
- Create list of components
  1. Properties
  2. Component lists \ Add
  3. Select: Pure components
  4. Type in the search field H<sub>2</sub>O
  5. Select H<sub>2</sub>O \ 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° C
Pressure	1100 psig
Mass flow	100 kg/h
Composition	
H <sub>2</sub> O	1

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

Name	Cold-in
Conditions	
Temperature	20° C
Pressure	110 psig
Composition	
H <sub>2</sub> O	1

Material Stream: Hot-in

Worksheet Attachments Dynamics

Worksheet	Stream Name	Hot-in	Vapour Phase
Conditions	Vapour / Phase Fraction	1.0000	1.0000
Properties	Temperature [C]	300.0	300.0
Composition	Pressure [kPa]	790.8	790.8
Oil & Gas Feed	Molar Flow [kgmole/h]	5.551	5.551
Petroleum Assay	Mass Flow [kg/h]	100.0	100.0
K Value	Std Ideal Liq Vol Flow [m3/h]	0.1002	0.1002
User Variables	Molar Enthalpy [kJ/kgmole]	-2.326e+005	-2.326e+005
Notes	Molar Entropy [kJ/kgmole-C]	178.9	178.9
Cost Parameters	Heat Flow [kJ/h]	-1.291e+006	-1.291e+006
Normalized Yields	Liq Vol Flow @Std Cond [m3/h]	9.854e-002	9.854e-002
	Fluid Package	Basis-1	
	Utility Type		

OK

Delete Define from Stream... View Assay

Material Stream: cold-in

Worksheet Attachments Dynamics

Worksheet	Stream Name	cold-in	Aqueous Phase
Conditions	Vapour / Phase Fraction	0.0000	1.0000
Properties	Temperature [C]	25.00	25.00
Composition	Pressure [kPa]	859.7	859.7
Oil & Gas Feed	Molar Flow [kgmole/h]	5.551	5.551
Petroleum Assay	Mass Flow [kg/h]	100.0	100.0
K Value	Std Ideal Liq Vol Flow [m3/h]	0.1002	0.1002
User Variables	Molar Enthalpy [kJ/kgmole]	-2.862e+005	-2.862e+005
Notes	Molar Entropy [kJ/kgmole-C]	53.69	53.69
Cost Parameters	Heat Flow [kJ/h]	-1.589e+006	-1.589e+006
Normalized Yields	Liq Vol Flow @Std Cond [m3/h]	9.854e-002	9.854e-002
	Fluid Package	Basis-1	
	Utility Type		

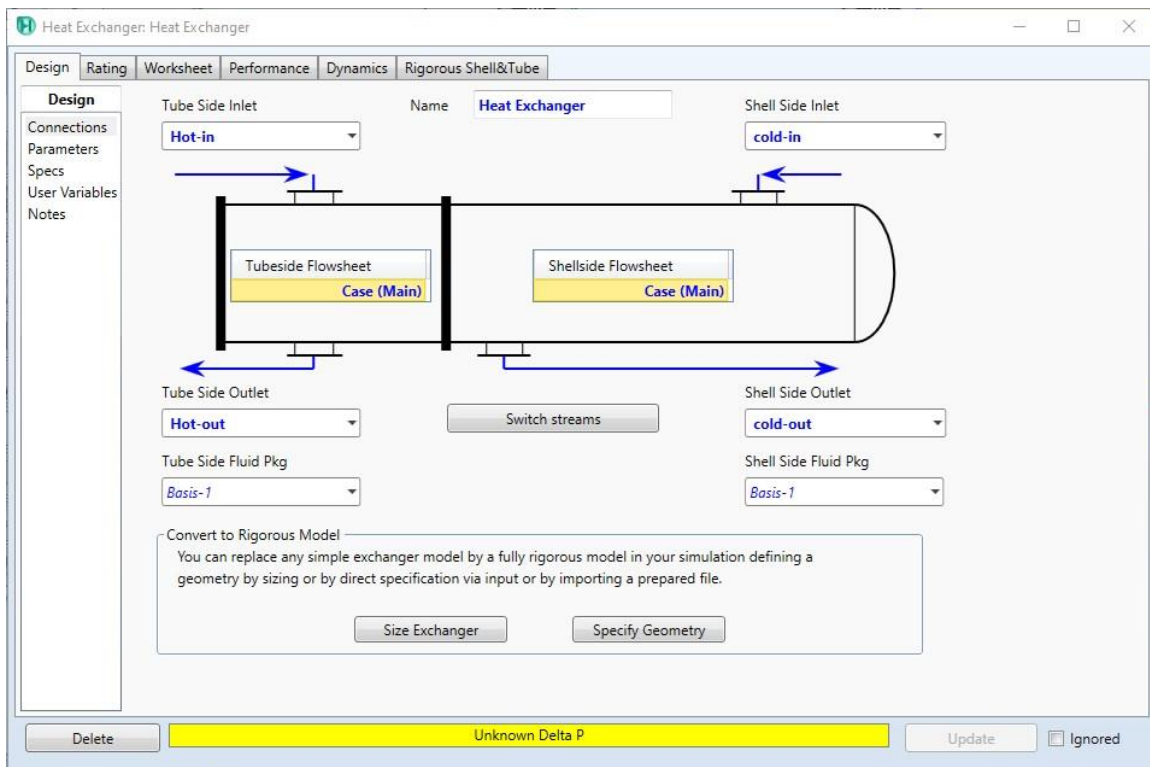
OK

Delete Define from Stream... View Assay

- 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.

Heat Exchanger: Heat Exchanger

Design Rating Worksheet Performance Dynamics Rigorous Shell&Tube

**Design**

Connections  
Parameters  
Specs  
User Variables  
Notes

Heat Exchanger Model: **Simple End Point**

Heat Leak/Loss: ☒ None ☐ Extremes ☐ Proportional

End Point Model

Overall UA [kJ/C-h]: **<empty>**

Specified Pressure Drop [kPa]: SHELL-SIDE **0.0000** TUBE-SIDE **0.0000**

Use Ft	Tube Passes	Shell Passes	Shells In Series	First Pass	Shell Type
<input checked="" type="checkbox"/>	2	1	1	Counter	E

Convert to Rigorous Model

You can replace any simple exchanger model by a fully rigorous model in your simulation defining a geometry by sizing or by direct specification via input or by importing a prepared file.

Delete Under Specified Update Ignored

12. Select worksheet

13. Change the temperature in hot-out to 200° C

14. Change the temperature in cold-out to 135° C

Heat Exchanger: Heat Exchanger

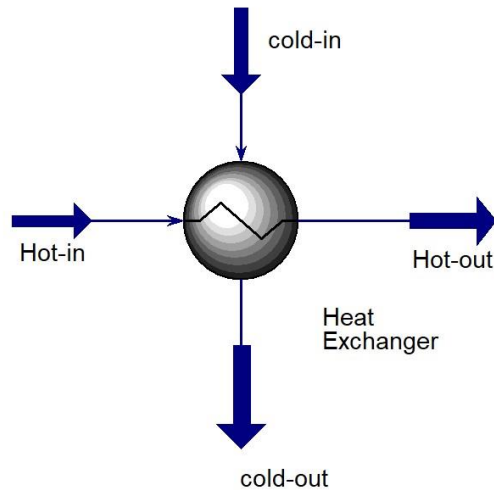
Design Rating **Worksheet** Performance Dynamics Rigorous Shell&Tube

	Hot-in	Hot-out	cold-in	cold-out
Name	1.0000	1.0000	0.0000	0.0000
Vapour	300.0	200.0	25.00	135.0
Temperature [C]	790.8	790.8	859.7	859.7
Pressure [kPa]	5.551	5.551	2.346	2.346
Molar Flow [kgmole/h]	100.0	100.0	42.26	42.26
Mass Flow [kg/h]	0.1002	0.1002	4.234e-002	4.234e-002
Std Ideal Liq Vol Flow [m3/h]	-2.326e+005	-2.362e+005	-2.862e+005	-2.775e+005
Molar Enthalpy [kJ/kgmole]	178.9	171.8	53.69	78.41
Molar Entropy [kJ/kgmole-C]	-1.291e+006	-1.311e+006	-6.713e+005	-6.510e+005
Heat Flow [kJ/h]				

Delete OK Update Ignored

15. Read the mass flow of the cold stream.

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



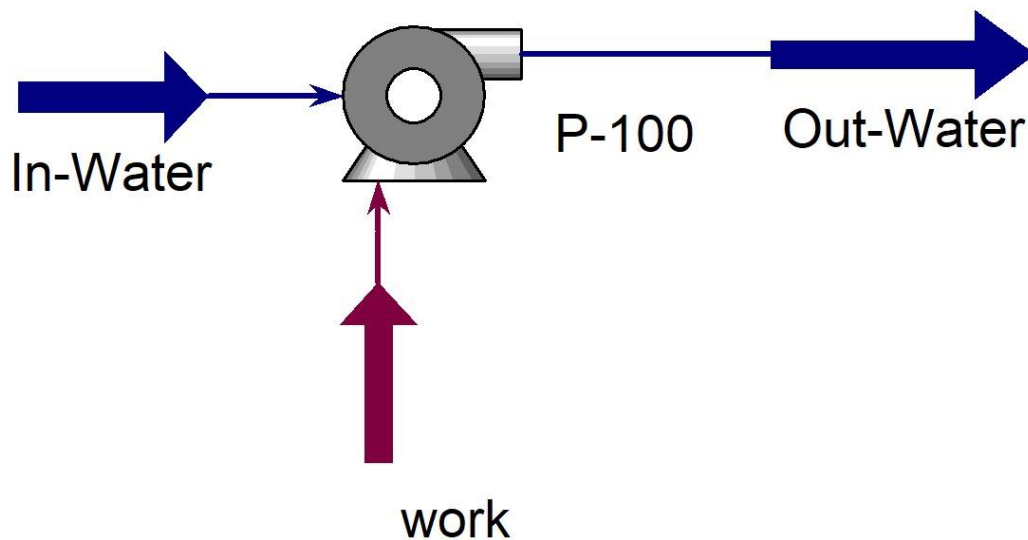
- Save the case:
  1. File menu
  2. Select save as
  3. Give the name (expander)

### **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.



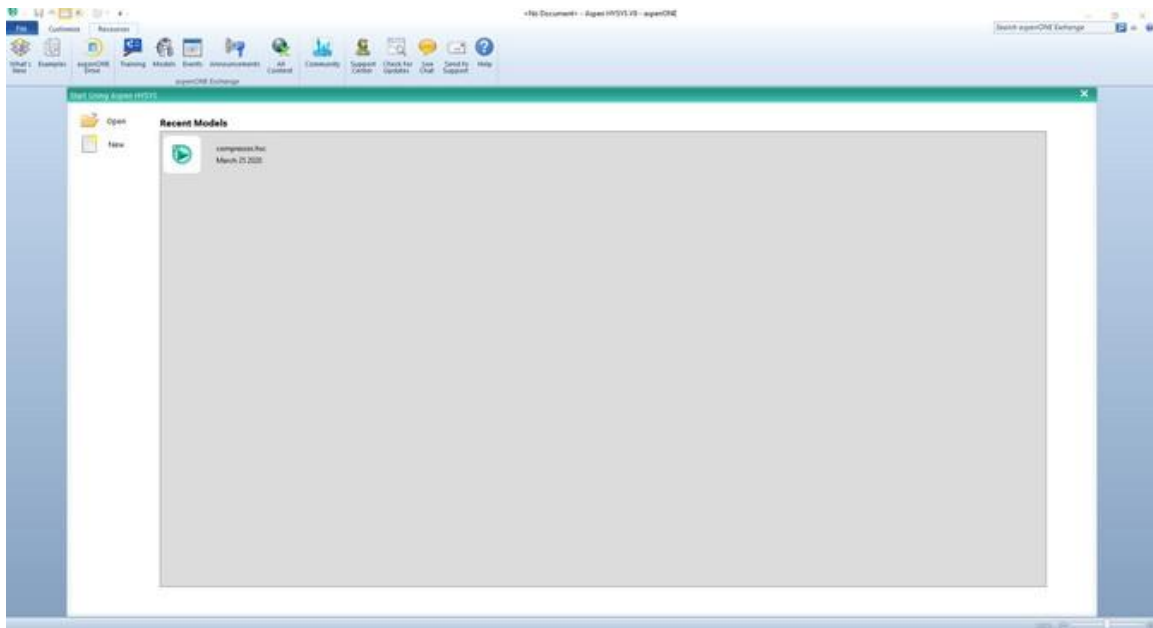
The figure above shows a simple model containing the Pump with inlet, outlet and energy streams using Aspen HYSYS V.9.

### **Example:**

Material stream of Water at 130°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. Determine the outlet temperature of the water using Peng-Robinson equation [1].

### **Solution:**

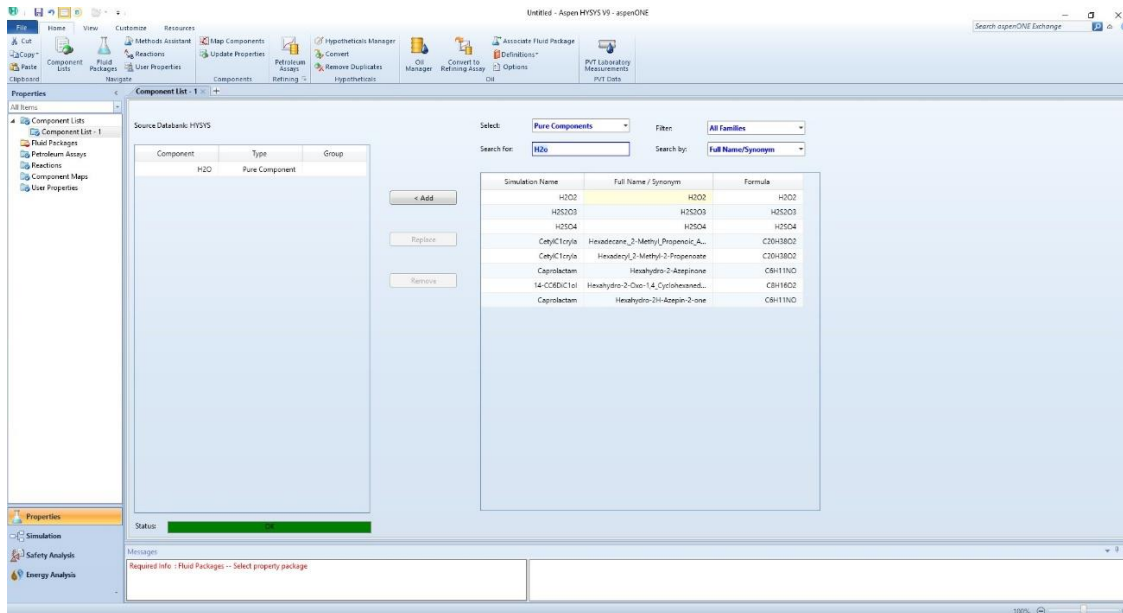
- Starting HYSYS:
  1. Start menu.
  2. Type in the search field: Aspen HYSYS V9.
  3. Select open.



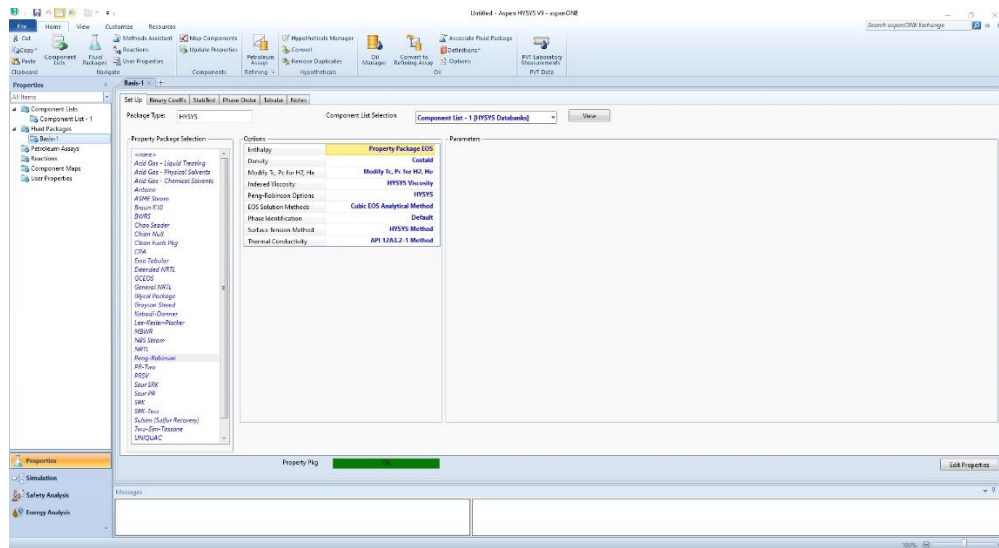
The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.



- 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<sub>2</sub>O
- 1. Properties
- 2. Component lists \ Add
- 3. Select: Pure components
- 4. Type in the search field H<sub>2</sub>O



- 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 <sup>o</sup> C
Pressure	4 bar
Molar flow	100 kgmole/h
Composition	
H <sub>2</sub> O	1

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

Material Stream: In-Water

Worksheet	Attachments	Dynamics
<b>Worksheet</b>		
Conditions	Stream Name	In-Water
Properties	Vapour / Phase Fraction	0.0000
Composition	Temperature [C]	130.0
Oil & Gas Feed	Pressure [kPa]	400.0
Petroleum Assay	Molar Flow [kgmole/h]	100.0
K Value	Mass Flow [kg/h]	1802
User Variables	Std Ideal Liq Vol Flow [m3/h]	1.805
Notes	Molar Enthalpy [kJ/kgmole]	-2.780e+005
Cost Parameters	Molar Entropy [kJ/kgmole-C]	77.42
Normalized Yields	Heat Flow [kJ/h]	-2.780e+007
	Liq Vol Flow @Std Cond [m3/h]	1.775
	Fluid Package	Basis-1
	Utility Type	

OK

Delete Define from Stream... View Assay

- 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].

Pump: P-100

Design	Rating	Worksheet	Performance	Dynamics
<b>Design</b>				
Connections				
Parameters				
Curves				
Links				
User Variables				
Notes				

Name: P-100

Inlet: In-Water

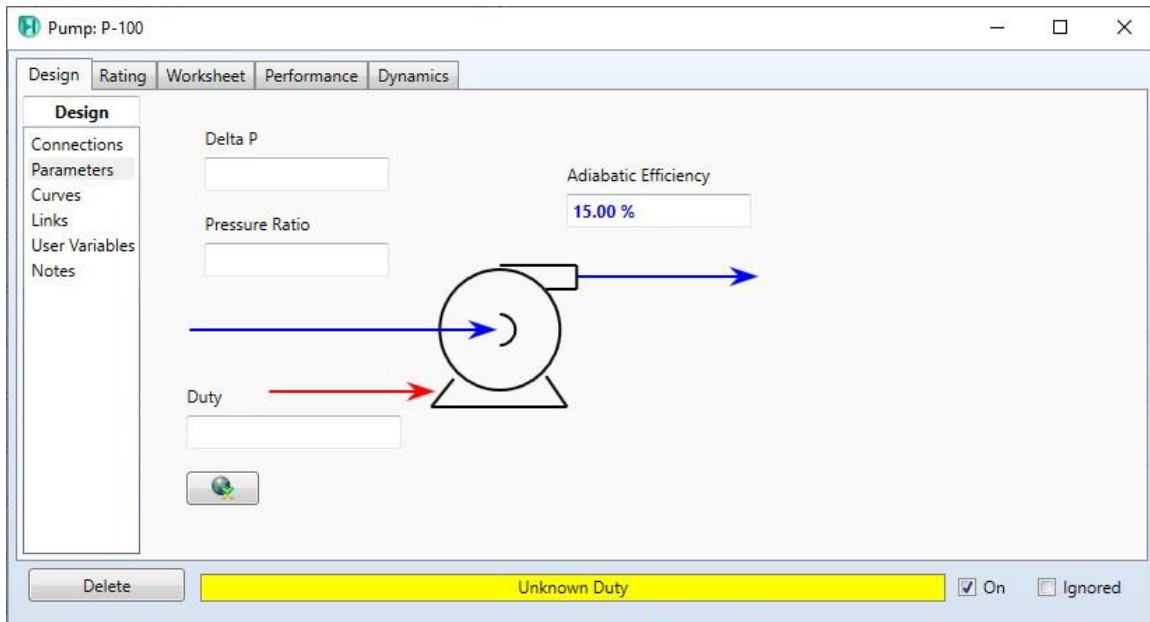
Outlet: Out-Water

Energy: work

Fluid Package: Basis-1

Delete Unknown Duty On Ignored

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



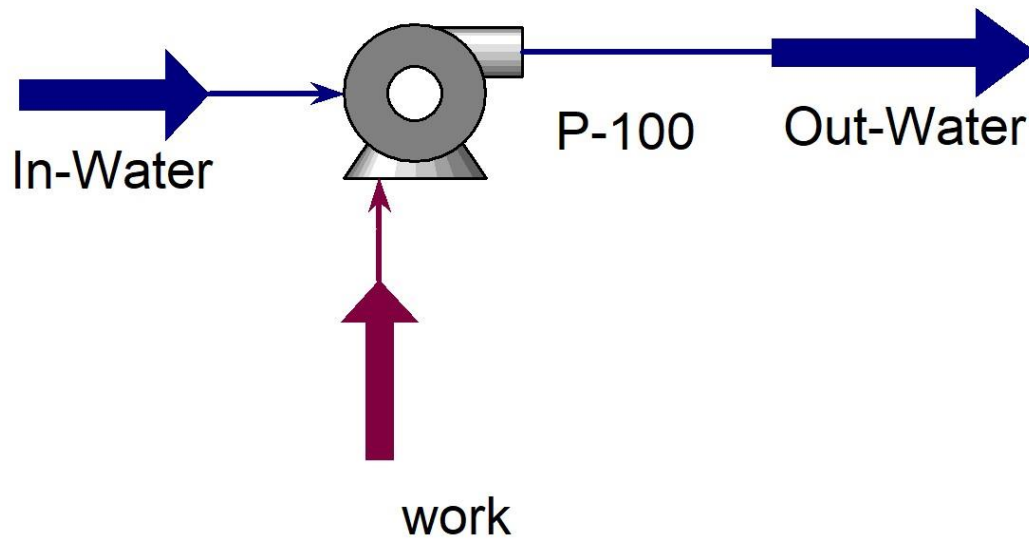
11. Select worksheet
12. Change the outlet-stream pressure to 90 bar.
13. Read the temperature of the outlet-stream.

The temperature of the outlet stream is 142.4° C.

The screenshot shows the 'Worksheet' tab for 'Pump: P-100'. The table below contains the data shown in the interface:

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:**

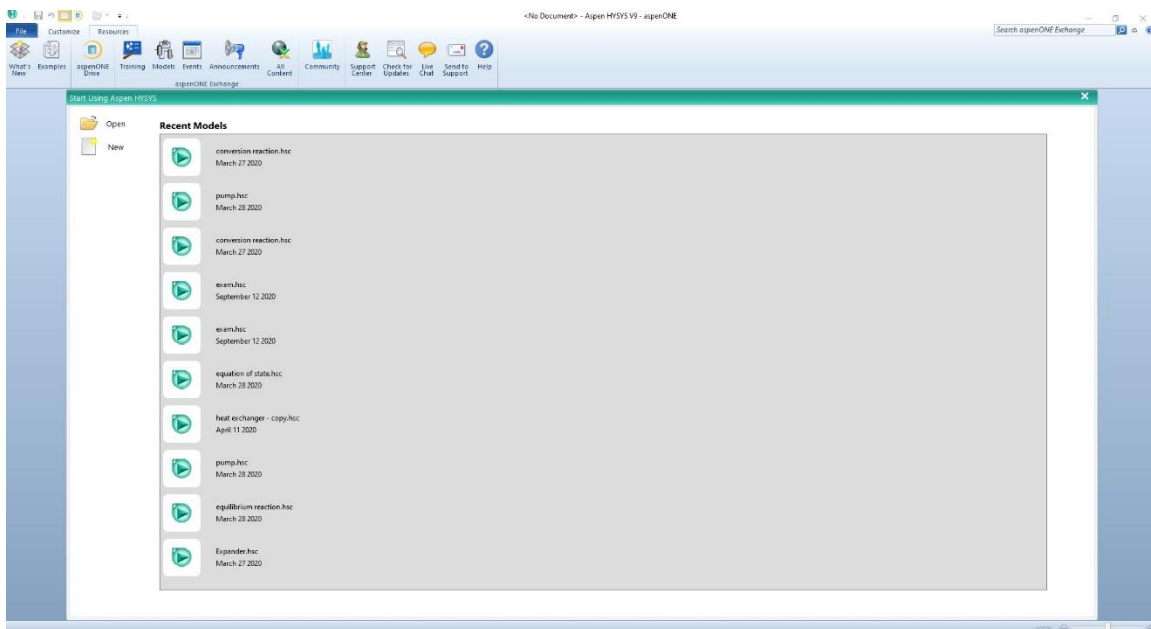
1. Hamid, M. K. A. "Hysys: An introduction to chemical engineering simulation." *Apostila de Hamid* (2007).

## **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:

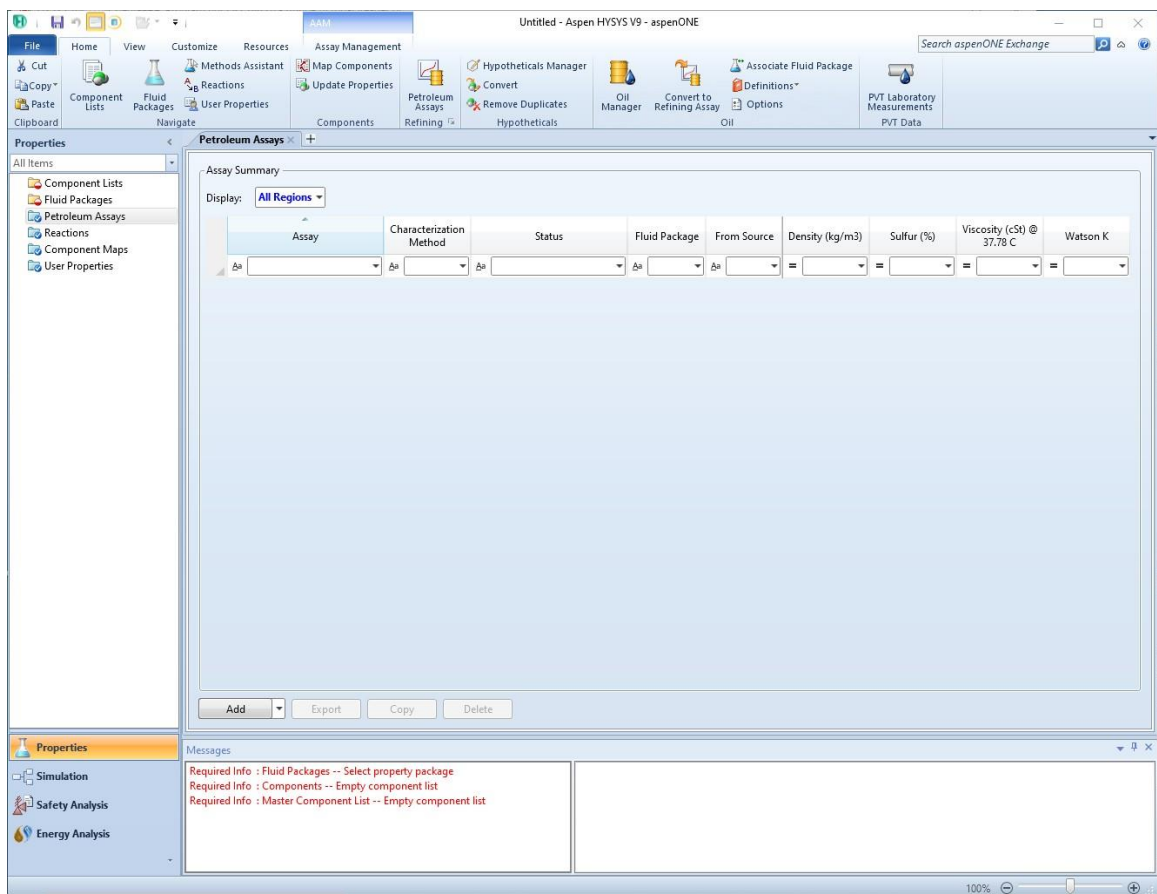
- **Open**: Enables the user to work with the models and projects which have been created previously. If (open) is chosen, it will be possible to browse your computer and select the desired project. However, it can be seen in the above figure that there are shortcuts for recently opened files that have 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 necessary to define the main properties 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 window for a new simulation case. The properties tab exists on the left down corner. It is possible to access and edit the related 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 separately in order to use them with other projects.

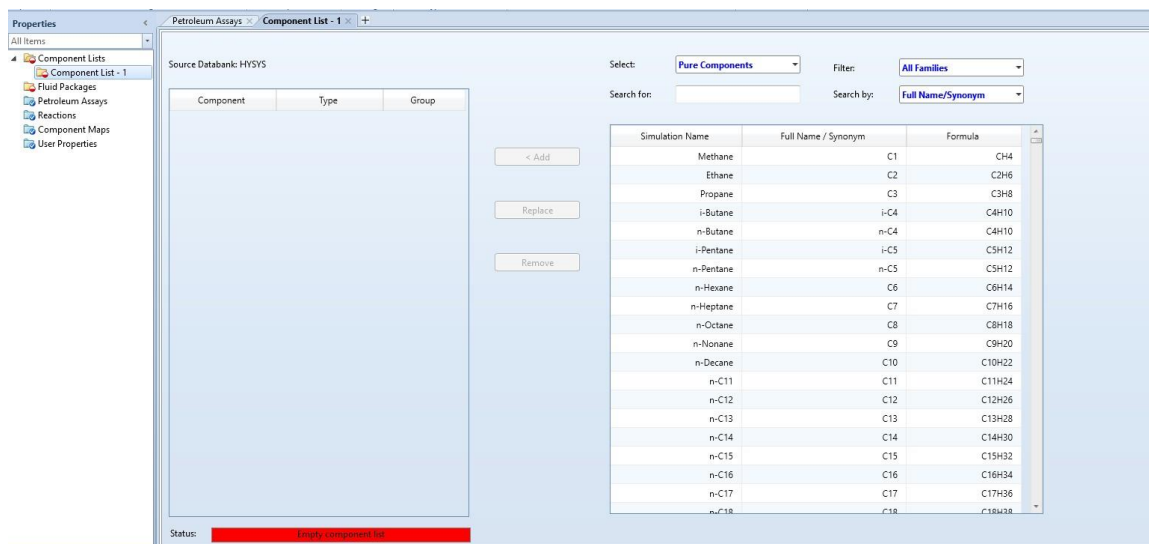


### **Adding component lists:**

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.

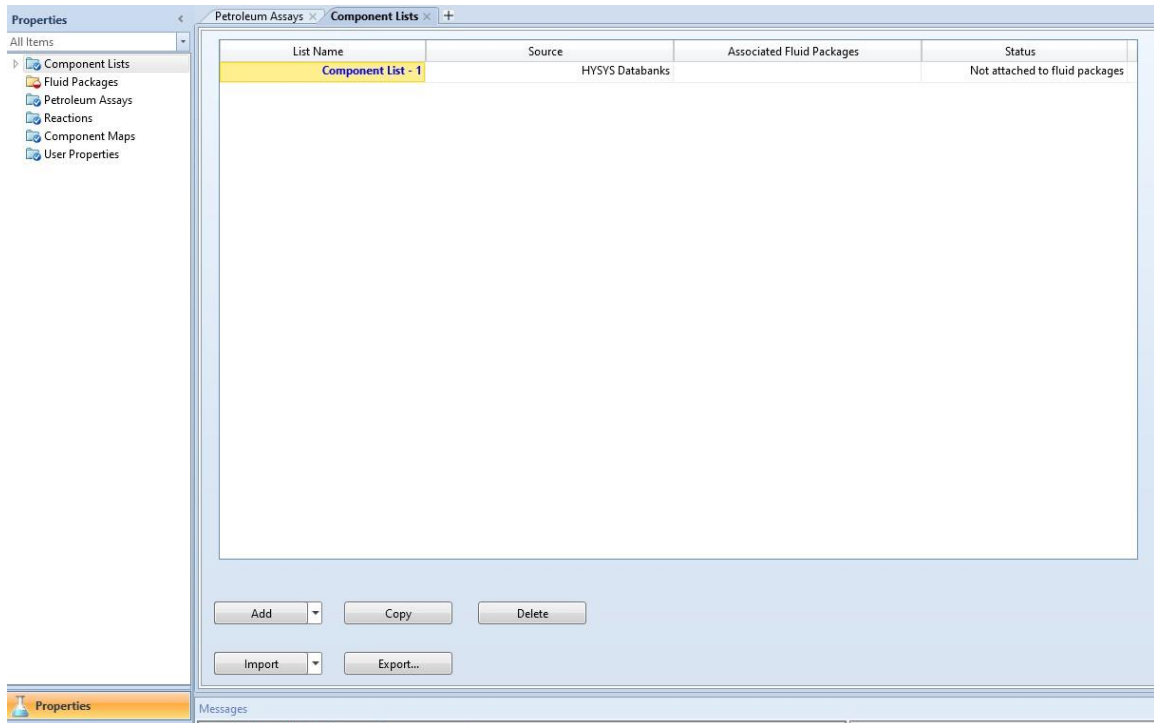
[Choose the (Full name/Synonym) and write (water) in search for field. Select water]

4. Add

A new component list is created (component List – 1) with single component (H<sub>2</sub>O). 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**

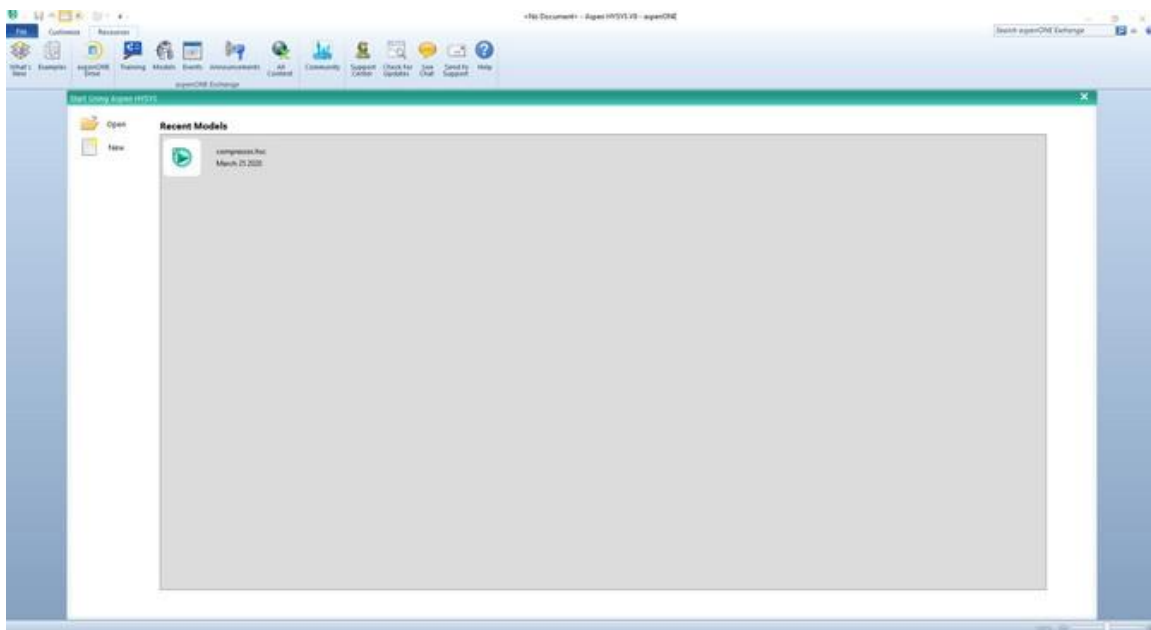
We can analyze the molar volume with a range of temperature values using the case study utility in Aspen HYSYS V9.

### **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].

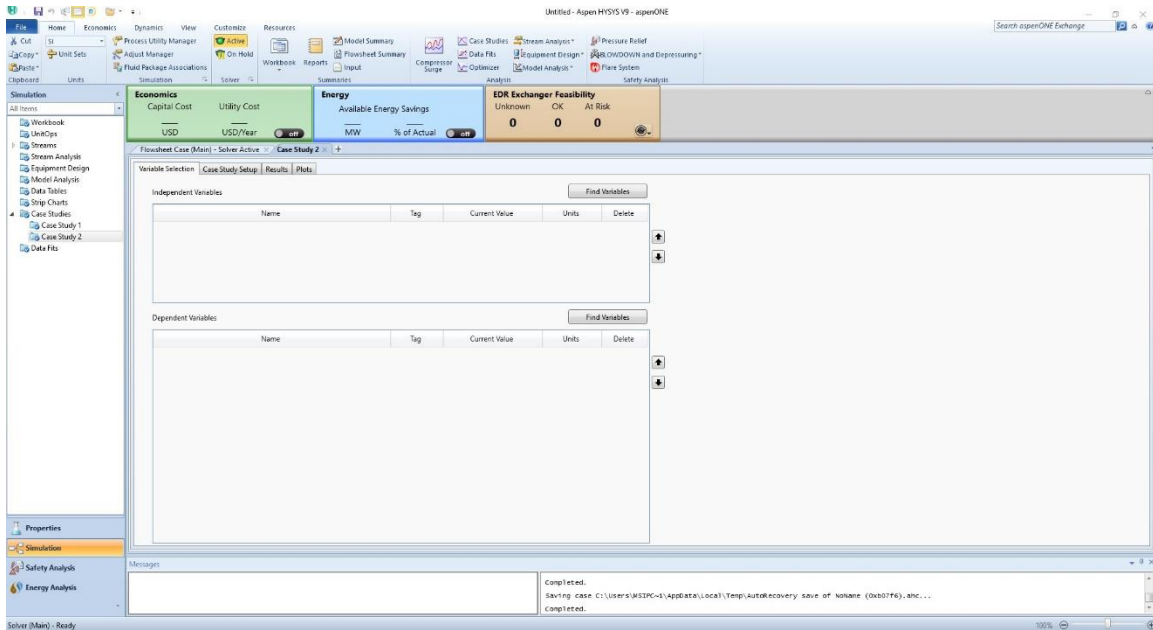
### **Solution:**

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

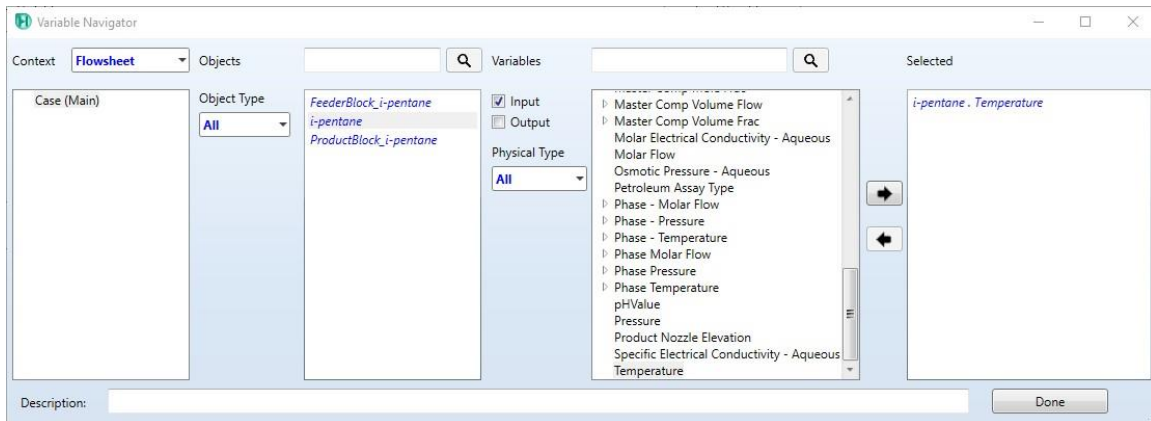


The above window will pop up once you start HYSYS. It is possible by the Aspen HYSYS start window to open previous cases or create a new case.

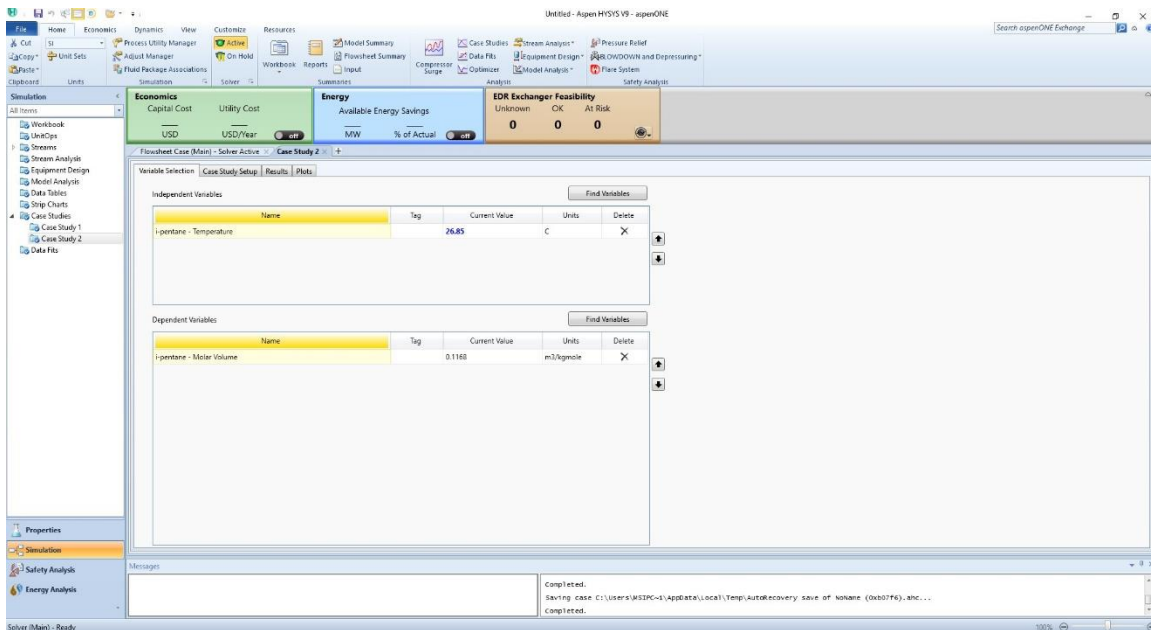
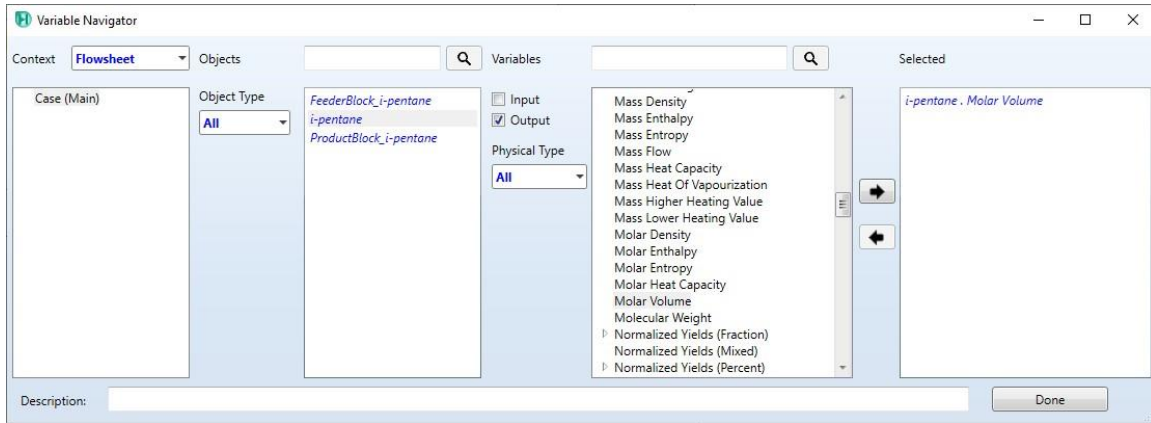
- Open the case of the previous example:
  1. File menu
  2. Open \ equation of state
- Working with databook:
  1. From the Home toolbar, click on case studies
  2. Add



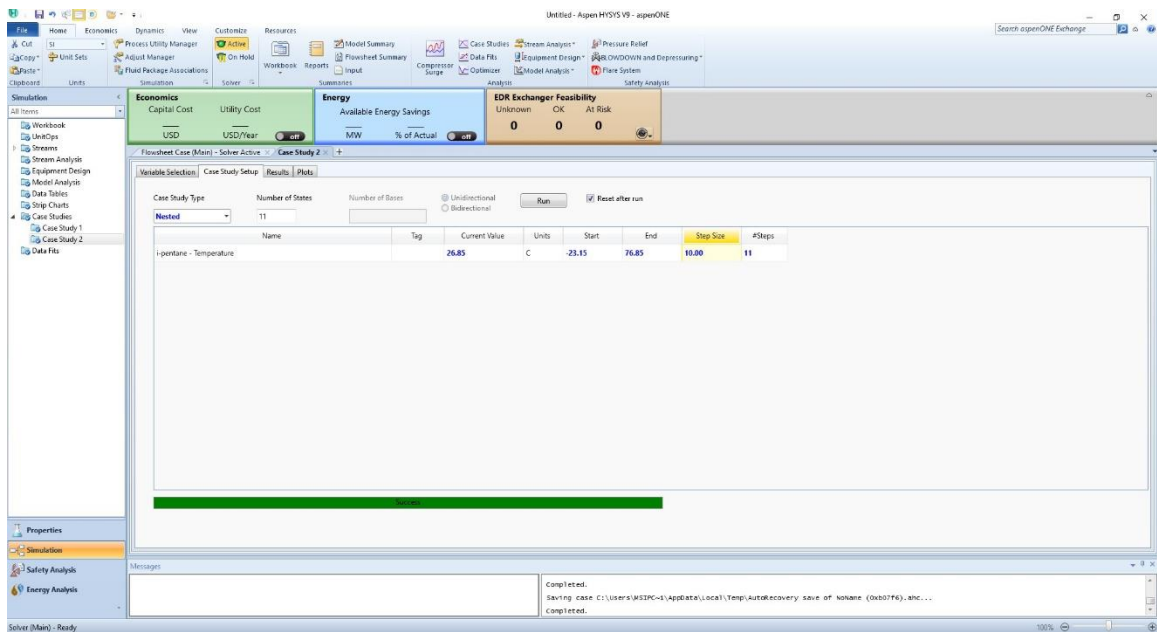
3. Variable selection
4. In Independent Variable click on Find variables
5. Highlight the desired material stream
6. Select the desired variable (temperature) \ Add
7. Done



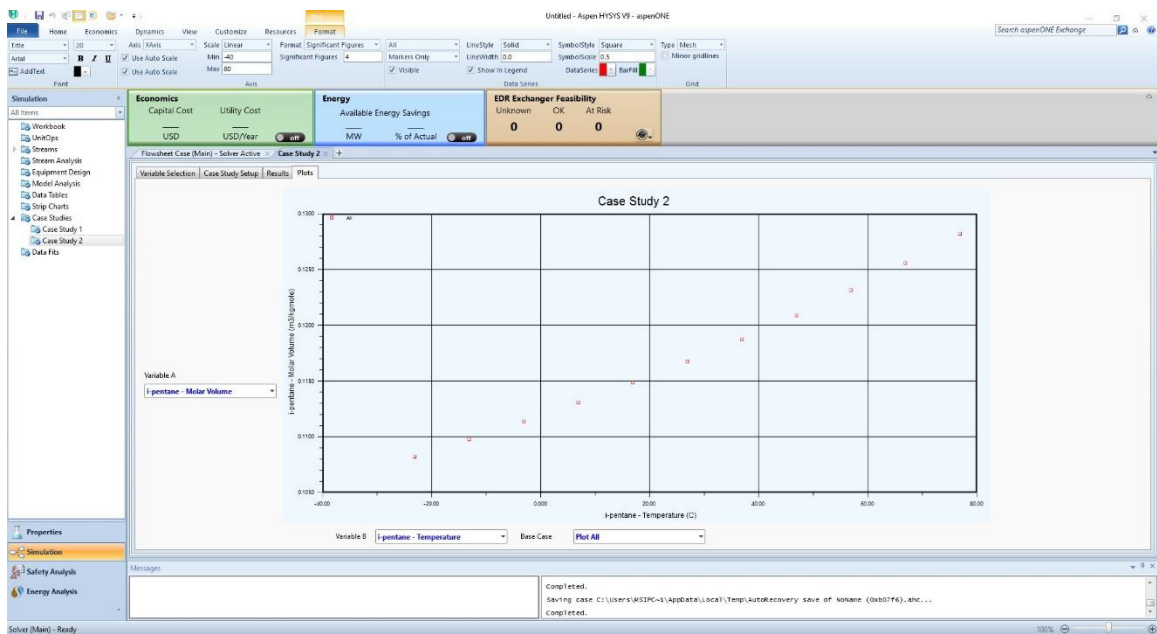
8. In Dependent Variable click on Find variables
9. Highlight the desired material stream
10. Select the desired variable (Molar Volume) \ Add
11. Done



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).