

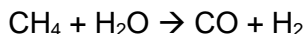


Equilibrium Reactors Simulation

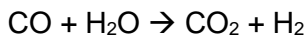




Example: Methane steam reforming is the heart of hydrogen, ammonia, and methanol plants. In such fired heaters, methane with steam reacts and as a result, CO and H₂ is produced.



Alongside the reaction, another reaction named water-gas shift reaction occurs at the same time and are in a state of equilibrium.



Here is the K table versus temperature for the first reaction.

Temperature	K _{eq}
595C	0.5
650C	3
705C	14
760C	63
815C	243
870C	817

In this example, 800 kg/hr. of methane with operating condition of 20 C, 520 kPa reacts with the steam with operating condition of 900 kPa and 180C. The Steam molar flowrate is always 2.5 times the methane molar flowrate. The inlet temperature is 760C and also consider the outlet temperature to be 760C. Determine the amount of hydrogen in the outlet of the reactor.

As might have noticed, we have not specified the flowrate of steam. It is typical for ammonia and methanol plants to adjust the steam flowrate in a way that steam/carbon mole ration is between 1.5-3. For this example we consider S/C = 2.5



How to simulate:

1. Add the reactants and the products to the component list:

Source Databank: HYSYS

Select: **Pure Components** Filter: **All Families**

Search for: Search by: **Full Name/Synonym**

Component	Type	Group
Methane	Pure Component	
CO	Pure Component	
CO2	Pure Component	
H2O	Pure Component	
Hydrogen	Pure Component	

< Add

Replace

Remove

Simulation Name	Full Name / Synonym	Formula
Ethane	C2	C2H6
Propane	C3	C3H8
i-Butane	i-C4	C4H10
n-Butane	n-C4	C4H10
i-Pentane	i-C5	C5H12
n-Pentane	n-C5	C5H12
n-Hexane	C6	C6H14
n-Heptane	C7	C7H16
n-Octane	C8	C8H18
n-Nonane	C9	C9H20
n-Decane	C10	C10H22
n-C11	C11	C11H24

Status: OK

2. Select PRSV as the Fluid Package.

Set Up | Binary Coeffs | Stab Test | Phase Order | Tabular | Notes

Package Type: HYSYS Component List Selection: **Component List - 1 [HYSYS Databanks]** View

Property Package Selection

- Grayson Streed
- IAPWS-IF97
- Kabadi-Danner
- Lee-Kesler-Plöcker
- MBWR
- NBS Steam
- NRTL
- Peng-Robinson
- PR-Twu
- PRSV**
- Sour PR
- Sour SRK
- Sour Water
- SRK
- SRK-Twu
- Sulsim (Sulfur Recovery)
- Twu-Sim-Tassone
- UNIQUAC

Options

Enthalpy	Peng-Robinson Equation
Density Method	Costald
Surface Tension Method	HYSYS Method

PRSV Component Parameters

	Kappa
Methane	-0.0193
CO	-0.2150
CO2	0.1430
H2O	-0.0767
Hydrogen	-0.5018

Property Pkg: OK Edit Properties



3. Under Properties/Reaction, Add a set, Add Rxn-1 and Rxn-2. For Rxn-1, add the first reaction. Select Equilibrium for both reactions.

Name	Type	Associated Fluid Packages
Set-1	Equilibrium	Basis-1

Buttons: Add, Delete Set, Copy Set, Add to FP, Detach from FP, Import Set, Export Set

Equilibrium Reaction: Rxn-1

Stoichiometry | Keq | Approach | Library

Stoichiometry

Component	Mole Weight	Stoich Coeff
Methane	16.043	-1.000
H2O	18.015	-1.000
CO	28.011	1.000
Hydrogen	2.016	3.000
Add Comp		

Balance

Balance Error: 0.00000
Reaction Heat (25 C): 2.1e+05 kJ/kgmole

Basis

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

Basis Units: [Dropdown]

Ready K Table



4. Under Keq, add K for different temperatures. By default, Hysys selects Gibbs Free Energy but this source is selected when we don't have that much information but here, we have K table and thus select the last source. Simply add T versus K in the table.

Equilibrium Reaction: Rxn-1

Stoichiometry Keq Approach Library

Keq Source

- ☐ Ln(Keq) Equation
- ☐ Gibbs Free Energy
- ☐ Fixed Keq
- ☒ Keq vs T Table

☐ Auto Detect

A	-2.7e+02
B	-9.0e+02
C	4.1e+01
D	-1.5e-02
E	0.0e-01
F	0.0e-01
G	0.0e-01
H	0.0e-01
R2	0.999926
T Hi	<empty>
T Lo	<empty>

K Table

T	Keq	KCalc	% Error
595.0	0.5000	0.5038	-0.8
650.0	3.000	2.917	2.8
705.0	14.00	14.47	-3.4
760.0	63.00	62.64	0.6
815.0	243.0	239.8	1.3

☒ Active Erase Table

Only A, B, C and D coefficients used in Aspen Properties

Ready K Table

5. Now for second reaction, click on library, and select the second reaction from the library. Yes, Aspen has it!

Equilibrium Reaction: Rxn-2

Stoichiometry Keq Approach Library

Library Equilibrium Rxns

- CO + H2O = CO2 + H2
- CH4 + H2O = CO + 3H2
- 1/2N2 + 3/2H2 = NH3
- Ethylbenzene = Styrene + H2
- COS + H2 = H2S + CO
- COS + H2O = H2S + CO2
- CO2 + 3H2 = CH3OH + H2O
- CO + 2H2 = CH3OH

Add Library Rxn

Not Ready Gibbs



Now if you check the Keq tab, you should see the following:

Equilibrium Reaction: Rxn-2

Stoichiometry **Keq** Approach Library

Keq Source

- ☐ Ln(Keq) Equation
- ☐ Gibbs Free Energy
- ☐ Fixed Keq
- ☒ Keq vs T Table

☒ Auto Detect

A	-1.2e+01
B	5.3e+03
C	1.0e+00
D	1.1e-04
E	0.0e-01
F	0.0e-01
G	0.0e-01
H	0.0e-01
R2	0.999972
T Hi	<empty>
T Lo	<empty>

☒ Active

Erase Table

Only A, B, C and D coefficients used in Aspen Properties

T	Keq	KCalc	% Error
93.3	4523	4547	-0.5
148.9	783.6	781.3	0.3
204.4	206.8	205.7	0.5
232.2	119.0	118.5	0.4
260.0	72.75	72.52	0.3

Ready

K Table

Finally click add to FP.

6. Now enter Simulation Environment and define the stream named Methane and Steam.

Material Stream: Methane

Worksheet Attachments Dynamics

Worksheet

- Conditions
- Properties
- Composition
- Oil & Gas Feed
- Petroleum Assay
- K Value
- User Variables
- Notes
- Cost Parameters
- Normalized Yields
- ▶ Emissions

Stream Name	Methane	Vapour Phase
Vapour / Phase Fraction	1.0000	1.0000
Temperature [C]	20.00	20.00
Pressure [kPa]	520.0	520.0
Molar Flow [kgmole/h]	49.87	49.87
Mass Flow [kg/h]	800.0	800.0
Std Ideal Liq Vol Flow [m3/h]	2.672	2.672
Molar Enthalpy [kJ/kgmole]	-7.518e+004	-7.518e+004
Molar Entropy [kJ/kgmole-C]	169.1	169.1
Heat Flow [kJ/h]	-3.749e+006	-3.749e+006
Liq Vol Flow @Std Cond [m3/h]	<empty>	<empty>
Fluid Package	Basis-1	
Utility Type		

OK

Delete Define from Stream... View Assay



Material Stream: Steam

Worksheet Attachments Dynamics

Worksheet

Conditions
Properties
Composition
Oil & Gas Feed
Petroleum Assay
K Value
User Variables
Notes
Cost Parameters
Normalized Yields
Emissions

Stream Name	Steam	Vapour Phase
Vapour / Phase Fraction	1.0000	1.0000
Temperature [C]	180.0	180.0
Pressure [kPa]	900.0	900.0
Molar Flow [kgmole/h]	<empty>	<empty>
Mass Flow [kg/h]	<empty>	<empty>
Std Ideal Liq Vol Flow [m3/h]	<empty>	<empty>
Molar Enthalpy [kJ/kgmole]	-2.370e+005	-2.370e+005
Molar Entropy [kJ/kgmole-C]	169.1	169.1
Heat Flow [kJ/h]	<empty>	<empty>
Liq Vol Flow @Std Cond [m3/h]	<empty>	<empty>
Fluid Package	Basis-1	
Utility Type		

Unknown Flow Rate

Delete Define from Stream... View Assay

Since we always want the S/C to be 2.5 without changing the flowrate of steam, we can use Set tool in Aspen Plus. The reason we want to happen this way stems from the fact that for methanol or ammonia fired heater, if we deviate from such ratio, coking happens. So, when the methane flowrate changes, the flowrate of steam should be changed correspondingly by controllers in FCS in monitoring system. How to simulate it in Hysys? We use Set.

7. Select Set from Model Palette and put it in the flowsheet.

SET-1

Connections Parameters User Variables Notes

Name SET-1

Target Variable

Object: Select Var...

Variable:

Source

Object: Select Obj...

Requires a Target connection

Delete Ignored



Target Variable in our example is mole flowrate of steam while source is the flowrate of the methane.

Select Target Object and Variable

Context: Case (Main)

Objects: Object Type: All

- 4
- 5
- 23
- E-100
- ERV-100
- FeederBlock_Methane
- FeederBlock_Steam
- L
- Methane
- MIX-100
- ProductBlock_L
- ProductBlock_V
- Steam
- V

Variables: Input, Output, Physical Type: All

- BO Water Oil Ratio
- BO Watson K
- Cost Factor
- Feed Nozzle Elevation
- Liq Vol Flow @Std Cond
- Mass Flow
- Molar Enthalpy
- Molar Flow
- pHValue
- Pressure
- Product Nozzle Elevation
- Std Ideal Liq Vol Flow
- Std Liq Vol Flow Spec
- Stock Tank Density
- Temperature
- Vapour Fraction

Description: Molar Flow

Disconnect Select

Select Source Object

Flowsheet: Case (Main)

Object:

- 3
- 4
- 5
- 23
- E-100
- ERV-100
- FeederBlock_Methane
- FeederBlock_Steam
- L
- Methane
- MIX-100
- ProductBlock_L
- ProductBlock_V
- Steam
- V

Object Filter:

- All
- Streams
- UnitOps
- Logicals
- ColumnOps
- Custom

Custom...

Disconnect

OK



Finally in Parameter tab, the multiplier is changed from 1 to 2.5.

SET-1

Connections Parameters User Variables Notes

Parameters

Multiplier **2.5000**

Offset [kgmole/h] 0.00000 kgmole/h

$Y = (2.5) * X + (0) \text{ [kgmole/h]}$

Y = Material Stream (Steam) : Molar Flow

X = Material Stream (Methane) : Molar Flow

OK

Delete

☐ Ignored

7. Now we add a mixer to mix them. Methane and Steam as inlets are selected and The Mixed stream is defined as the outlet stream.

Mixer: MIX-100

Design Rating Worksheet Dynamics

Design

Name **MIX-100**

Inlets

Methane
Steam
<< Stream >>

Outlet

The Mixed

Fluid Package

Basis-1

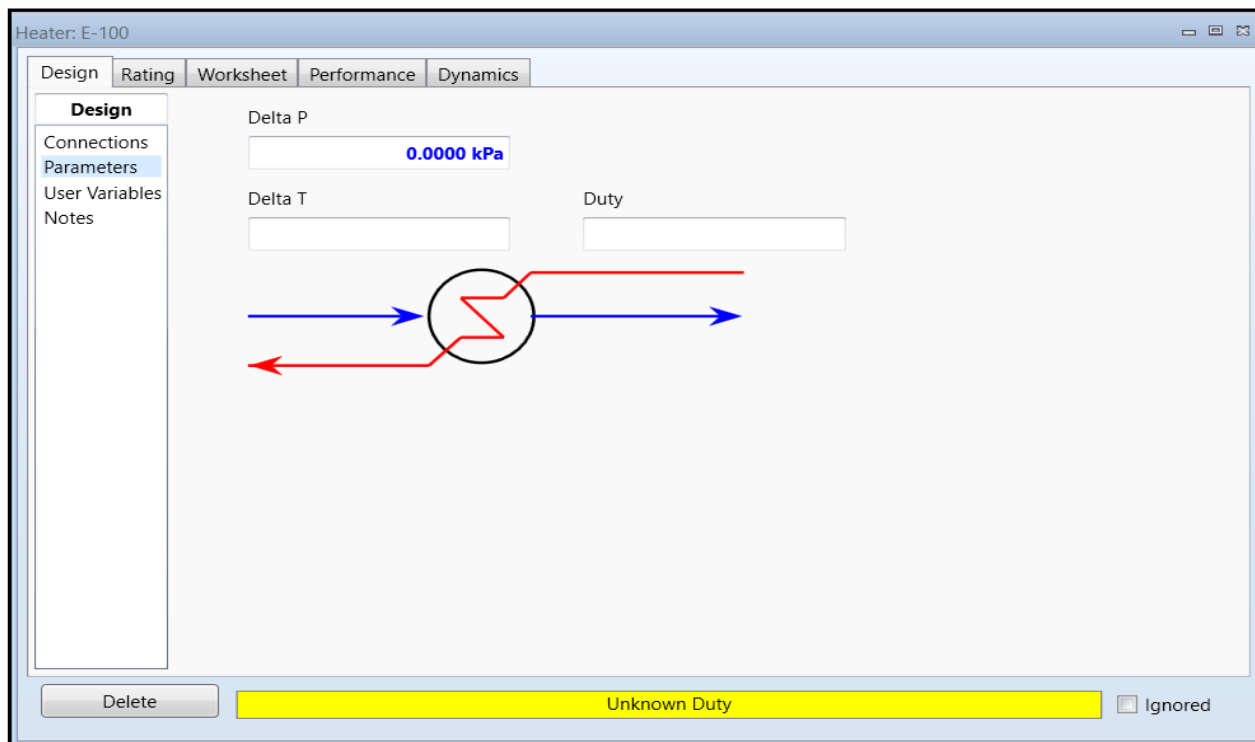
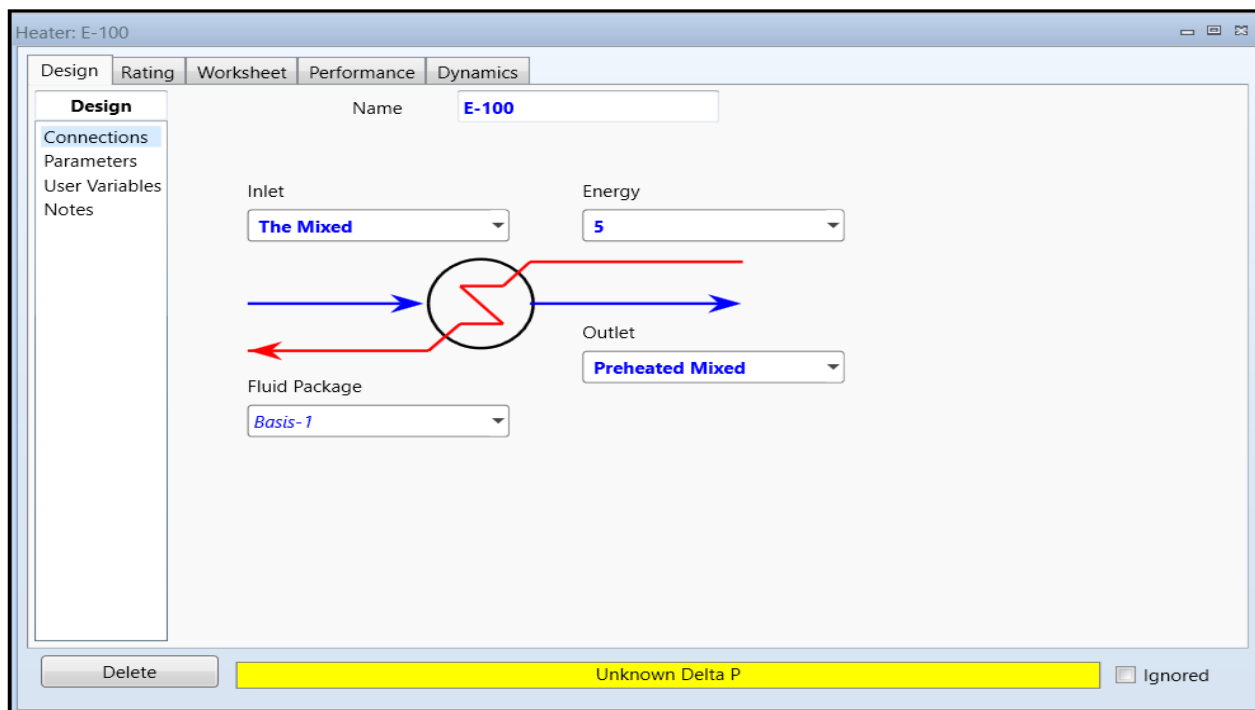
Delete

OK

☐ Ignored



8. Add a heater to the flowsheet and heat The Mixed stream to 760C. Also, the pressure drop is zero. The outlet stream is called Preheat Mixed.





Heater: E-100

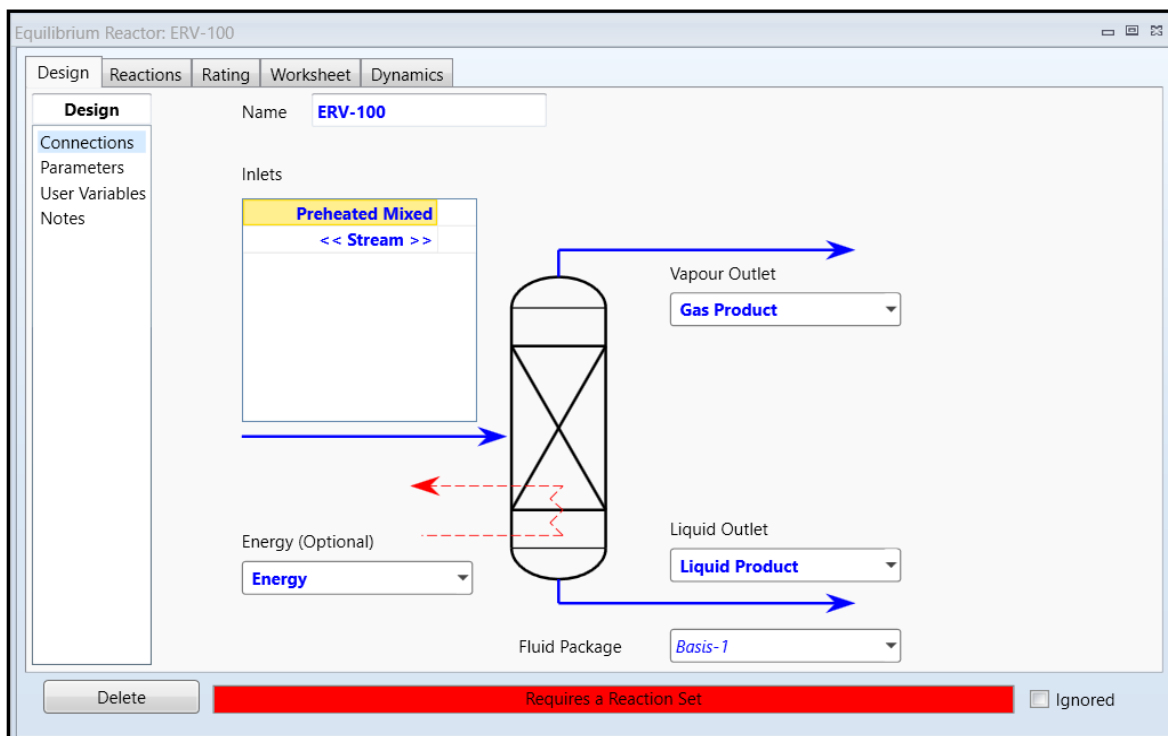
Design Rating Worksheet Performance Dynamics

Worksheet

Name	The Mixed	Preheated Mixed	5
Vapour	0.9865	1.0000	<empty>
Temperature [C]	140.4	760.0	<empty>
Pressure [kPa]	520.0	520.0	<empty>
Molar Flow [kgmole/h]	174.5	174.5	<empty>
Mass Flow [kg/h]	3046	3046	<empty>
Std Ideal Liq Vol Flow [m3/h]	4.922	4.922	<empty>
Molar Enthalpy [kJ/kgmole]	-1.908e+005	-1.629e+005	<empty>
Molar Entropy [kJ/kgmole-C]	177.8	218.5	<empty>
Heat Flow [kJ/h]	-3.330e+007	-2.843e+007	4.867e+006

Delete OK Ignored

9. Select Equilibrium Reactor from Model Palette/Reactors. Select Pre-heated Mixed as inlet and define Gas Product and Liquid Product as outlet streams.





10. As indicated in red indication, a reaction set is required. Under Reaction tab, select Set-1.

Equilibrium Reactor: ERV-100 - Set-1

Design Reactions Rating Worksheet Dynamics

Reactions

Equilibrium Reaction Details

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

☒ Stoichiometry ☐ Basis ☐ Keq ☐ Approach View Rxn...

Stoichiometry Info

Component	Mole Wt.	Stoich Coeff
Methane	16.043	-1.000
H2O	18.015	-1.000
CO	28.011	1.000
Hydrogen	2.016	3.000
Add Comp		

Balance Error 0.00000

Reaction Heat (25 C) 2.1e+05 kJ/kgmole

Delete Unknown Duty Ignored

11. Under Worksheet, set the Gas Product stream outlet temperature to 760C.

Equilibrium Reactor: ERV-100 - Set-1

Design Reactions Rating Worksheet Dynamics

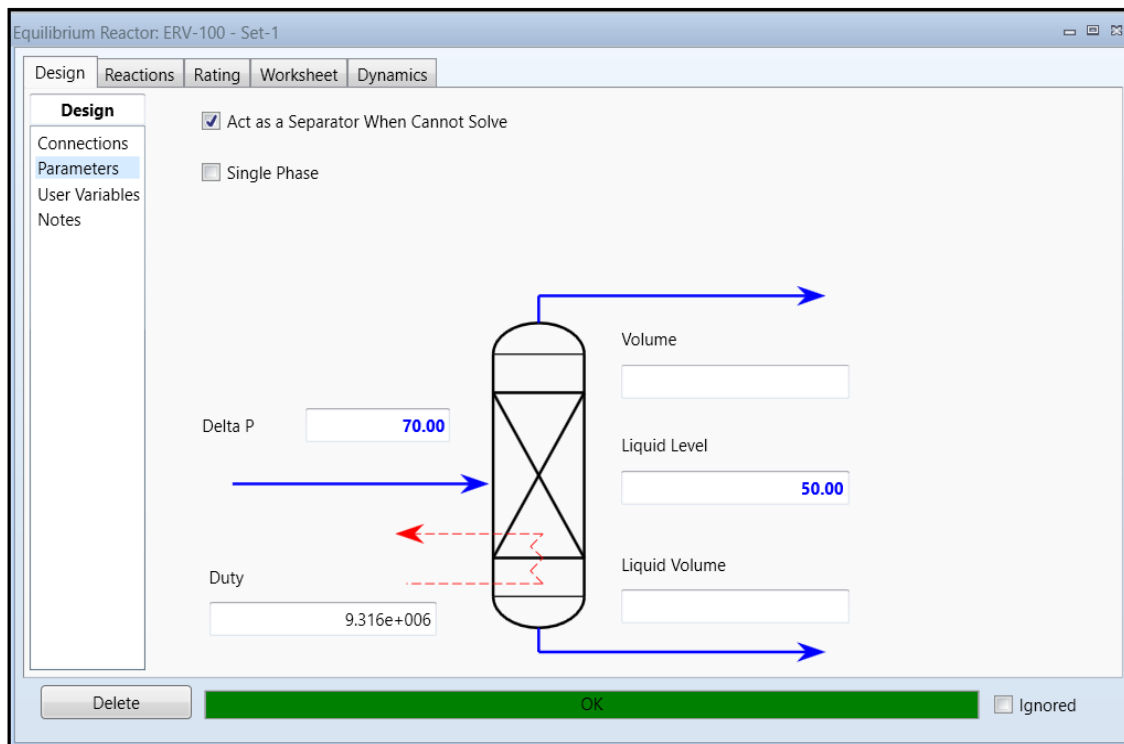
Worksheet

Name	Preheated Mixed	Liquid Product	Gas Product	Energy
Vapour	1.0000	0.0000	1.0000	<empty>
Temperature [C]	760.0	760.0	760.0	<empty>
Pressure [kPa]	520.0	520.0	520.0	<empty>
Molar Flow [kgmole/h]	174.5	0.0000	259.5	<empty>
Mass Flow [kg/h]	3046	0.0000	3046	<empty>
Std Ideal Liq Vol Flow [m3/h]	4.922	0.0000	7.490	<empty>
Molar Enthalpy [kJ/kgmole]	-1.629e+005	-7.468e+004	-7.468e+004	<empty>
Molar Entropy [kJ/kgmole-C]	218.5	181.6	181.6	<empty>
Heat Flow [kJ/h]	-2.843e+007	-0.0000	-1.938e+007	9.050e+006

Delete OK Ignored



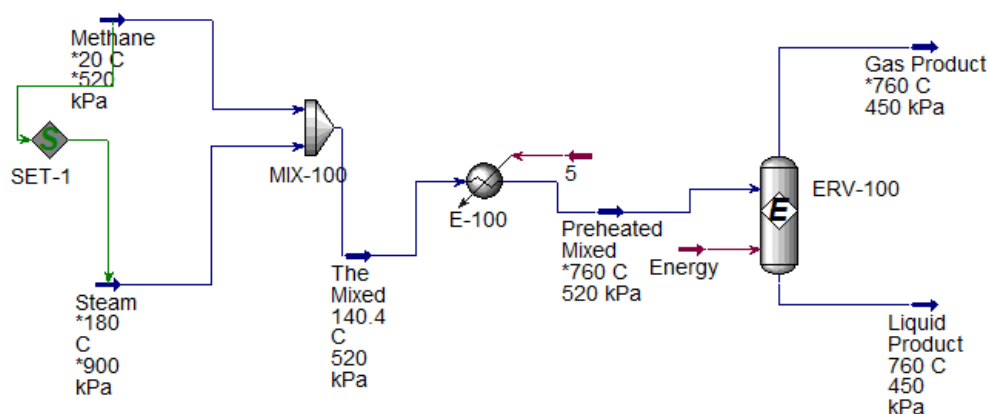
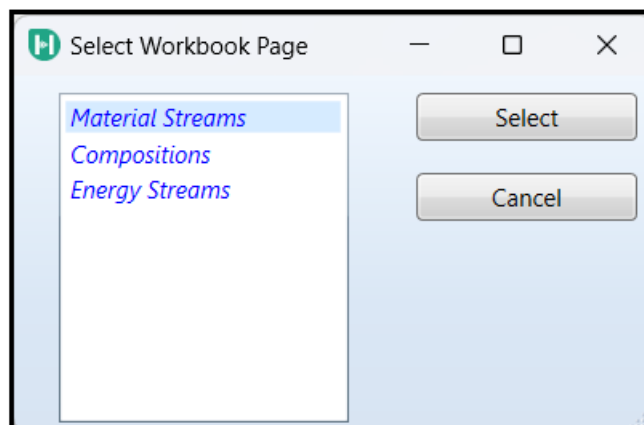
12. Now under Design/Parameter, change the pressure drop to 70 kPa.



13. Based on the result, 55.8% of Gas Product is made of hydrogen and 2.3% of methane has not reacted.

	Preheated Mixed	Liquid Product	Gas Product
Methane	0.2857	0.0237	0.0237
CO	0.0000	0.1083	0.1083
CO2	0.0000	0.0584	0.0584
H2O	0.7143	0.2510	0.2510
Hydrogen	0.0000	0.5586	0.5586

We are done with simulation but before ending the simulation, let's go to Flowsheet and select Workbook and Material Stream. Also activate temperature and pressure.

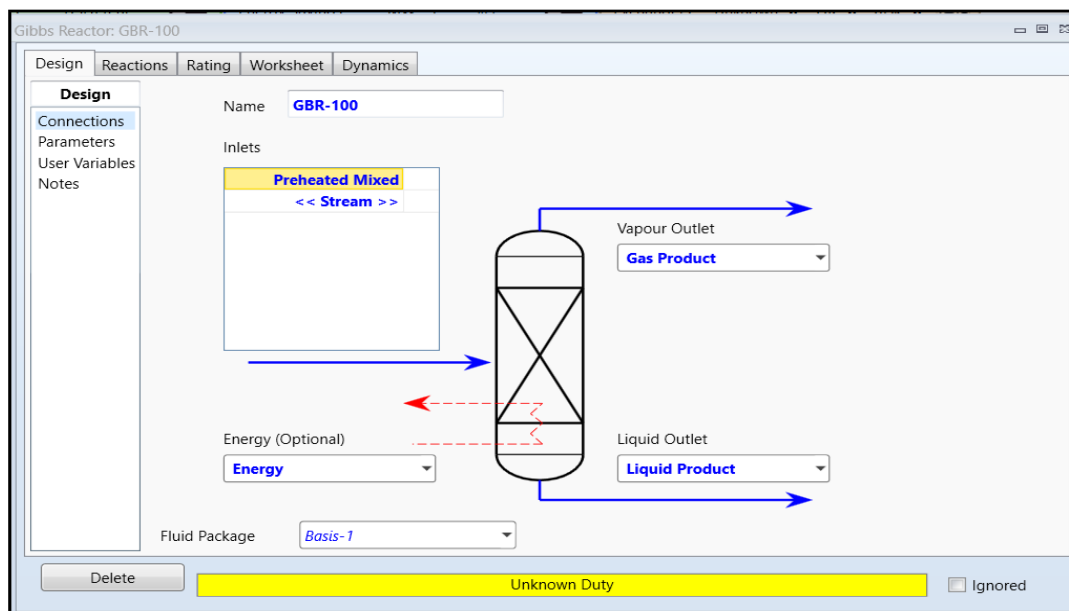


Material Streams							
		Methane	Steam	The Mixed	Preheated Mixed	Gas Product	Liquid Product
Vapour Fraction		1.0000	1.0000	0.9865	1.0000	1.0000	0.0000
Temperature	C	20.00	180.0	140.4	760.0	760.0	760.0
Pressure	kPa	520.0	900.0	520.0	520.0	450.0	450.0
Molar Flow	kgmole/h	49.87	124.7	174.5	174.5	261.8	0.0000
Mass Flow	kg/h	800.0	2246	3046	3046	3046	0.0000
Liquid Volume Flow	m3/h	2.672	2.250	4.922	4.922	7.549	0.0000
Heat Flow	kJ/h	-3.749e+006	-2.955e+007	-3.330e+007	-2.843e+007	-1.911e+007	-0.0000



Example 2: Regarding the first example, use Gibbs Reactor to convert methane to hydrogen. Compare this example result with previous example result.

1. Select Gibbs Reactor from Model Palette/Reactors. Connect Preheat Mixed stream as the inlet to the reactor, define Gas Product as the outlet and Liquid Product as the second outlet, and Energy as the heat provided to the reactor.



2. Under Worksheet tab, change the Gas Product temperature to 760C.

Gibbs Reactor: GBR-100

Design Reactions Rating Worksheet Dynamics

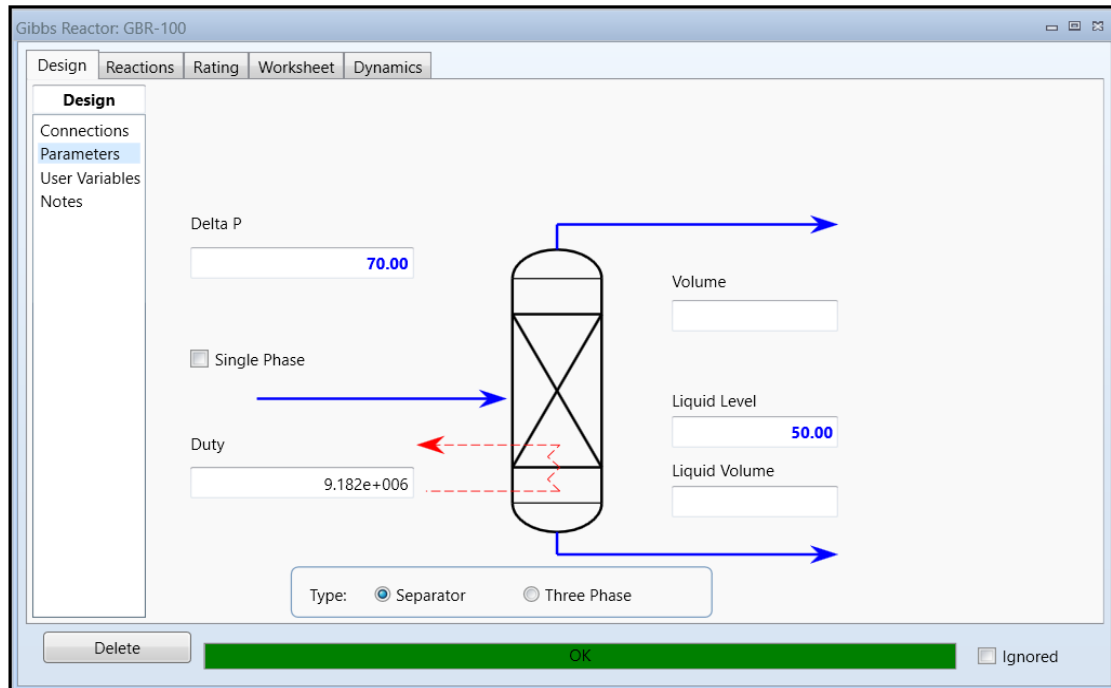
Worksheet

Name	Preheated Mixed	Liquid Product	Gas Product	Energy
Vapour	1.0000	0.0000	1.0000	<empty>
Temperature [C]	760.0	760.0	760.0	<empty>
Pressure [kPa]	520.0	520.0	520.0	<empty>
Molar Flow [kgmole/h]	174.5	0.0000	258.3	<empty>
Mass Flow [kg/h]	3046	0.0000	3046	<empty>
Std Ideal Liq Vol Flow [m3/h]	4.922	0.0000	7.473	<empty>
Molar Enthalpy [kJ/kgmole]	-1.629e+005	-7.557e+004	-7.557e+004	<empty>
Molar Entropy [kJ/kgmole-C]	218.5	181.9	181.9	<empty>
Heat Flow [kJ/h]	-2.843e+007	-0.0000	-1.952e+007	8.906e+006

Delete OK Ignored



3. Finally change the pressure drop to 70 kPa



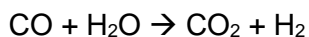
4. Here is the result:

	Preheated Mixed	Liquid Product	Gas Product
Methane	0.2857	0.0259	0.0259
CO	0.0000	0.1051	0.1051
CO2	0.0000	0.0602	0.0602
H2O	0.7143	0.2525	0.2525
Hydrogen	0.0000	0.5563	0.5563

5. Comparison



Example 3: Regarding the first example result, CO mole fraction in the stream is approximately 10%. In this example we will show how to convert all CO to hydrogen via water-gas-shift reaction in a Plug Flow Reactor or PFR.



The reaction takes place around 430C. Run the software for two scenarios; in first scenario, the length and diameter of reactor are 15m and 3m respectively while in second scenario, the length and diameter of the reactor are 12m and 2.4m.

Note: It is not possible to use equilibrium reaction for PFR. Only kinetic reactions are used inside such reactors.

1.Open the first example file and define new set in which new reaction is added and the information like below is provided:

Kinetic Reaction: Rxn-3

Stoichiometry and Rate Info

Component	Mole Wt.	Stoich Coeff	Fwd Order	Rev Order
CO	28.011	-1.000	1.00	0.00
H2O	18.015	-1.000	1.00	0.00
CO2	44.010	1.000	0.00	1.00
Hydrogen	2.016	1.000	0.00	1.00
Add Comp				

Balance

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

Basis

Basis: Molar Concn
Base Component: CO
Rxn Phase: Overall
Min. Temperature: -273.1 C
Max Temperature: 3000 C

Basis Units: kgmole/m3
Rate Units: kgmole/m3-s

Forward Reaction

A: 5.9000e+008
E: 1.1630e+005
b: <empty>

Reverse Reaction

A': 8.7000e+008
E': 1.5700e+005
b': <empty>

Equation Help

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

Ready

2.Enter Simulation Environment and set-up the simple heater and reduce the temperature to 430C.



Cooler: E-101

Design Rating Worksheet Performance Dynamics

Design

Name **E-101**

Connections
Parameters
User Variables
Notes

Inlet **Gas Product** Energy **Coolant**

Outlet **PFR Inlet**

Fluid Package **Basis-1**

Delete **Unknown Delta P** Ignored

Cooler: E-101

Design Rating Worksheet Performance Dynamics

Design

Connections
Parameters
User Variables
Notes

Delta P **24.00 kPa**

Delta T Duty

Delete **Unknown Duty** Ignored



Cooler: E-101

Design Rating Worksheet Performance Dynamics

Worksheet

Conditions Properties Composition PF Specs

Name	Gas Product	PFR Inlet	Coolant
Vapour	1.0000	1.0000	<empty>
Temperature [C]	760.0	430.0	<empty>
Pressure [kPa]	450.0	426.0	<empty>
Molar Flow [kgmole/h]	261.8	261.8	<empty>
Mass Flow [kg/h]	3046	3046	<empty>
Std Ideal Liq Vol Flow [m3/h]	7.549	7.549	<empty>
Molar Enthalpy [kJ/kgmole]	-7.299e+004	-8.451e+004	<empty>
Molar Entropy [kJ/kgmole-C]	181.9	169.0	<empty>
Heat Flow [kJ/h]	-1.911e+007	-2.213e+007	3.014e+006

Delete OK Ignored

3. Select a PFR from Model Palette/Reactor, select PFR Inlet as the inlet, and define PFR Outlet as the outlet stream.

Plug Flow Reactor: PFR-100

Design Reactions Rating Worksheet Performance Dynamics

Design

Connections Parameters Heat Transfer User Variables Notes

Name: PFR-100

Inlets

PFR Inlet
<empty>

Outlet: PFR Outlet

Energy (Optional):

Fluid Package: Basis-1

Delete Requires a Reaction Set Ignored



4. The red indication states that a reaction set is required. Under Reaction tab, select Set-2.

Plug Flow Reactor: PFR-100 - Set-2

Design Reactions Rating Worksheet Performance Dynamics

Reactions

Overall
Details
Results

Reaction Info

Reaction Set: **Set-2**

Initialize segment reactions from:

☒ Current ☐ Previous ☐ Re-init

Integration Information

Number of Segments	20
Minimum Step Fraction	1.0e-06
Minimum Step Length	<empty>

Catalyst Data

Void Fraction is specified as 1.000
(no catalyst information is needed)

Delete

Unknown Dimensions

Ignored

5. Under Rating/Sizing, specify length and diameter for first scenario.

Plug Flow Reactor: PFR-100 - Set-2

Design Reactions Rating Worksheet Performance Dynamics

Rating

Sizing
Nozzles

Tube Dimensions

Total Volume	106.0 m3
Length	15.00 m
Diameter	3.000 m
Number of Tubes	1
Wall Thickness	5.000e-003 m

Tube Packing

Void Fraction	1.000
Void Volume	106.0 m3

Delete

Unknown Delta P

Ignored



6. Based on yellow indication, the pressure drop should be specified. To do so, Under Design/Parameter, specify 10 kPa as the pressure drop.

Plug Flow Reactor: PFR-100 - Set-2

Design Reactions Rating Worksheet Performance Dynamics

Design

Connections
Parameters
Heat Transfer
User Variables
Notes

Pressure Drop Parameters

Delta P

☒ User Specified ☐ Ergun Equation

☐ Single Phase

Duty Parameters

Duty

☐ Formula ☒ Direct Q Value

Delete OK Ignored

7. Results:

Plug Flow Reactor: PFR-100 - Set-2

Design Reactions Rating Worksheet Performance Dynamics

Worksheet

Name	PFR Inlet	PFR Outlet
Vapour	1.0000	1.0000
Temperature [C]	430.0	545.3
Pressure [kPa]	426.0	416.0
Molar Flow [kgmole/h]	261.8	261.8
Mass Flow [kg/h]	3046	3046
Std Ideal Liq Vol Flow [m3/h]	7.549	8.353
Molar Enthalpy [kJ/kgmole]	-8.451e+004	-8.451e+004
Molar Entropy [kJ/kgmole-C]	169.0	169.4
Heat Flow [kJ/h]	-2.213e+007	-2.213e+007

Delete OK Ignored



Plug Flow Reactor: PFR-100 - Set-2

Design Reactions Rating Worksheet Performance Dynamics

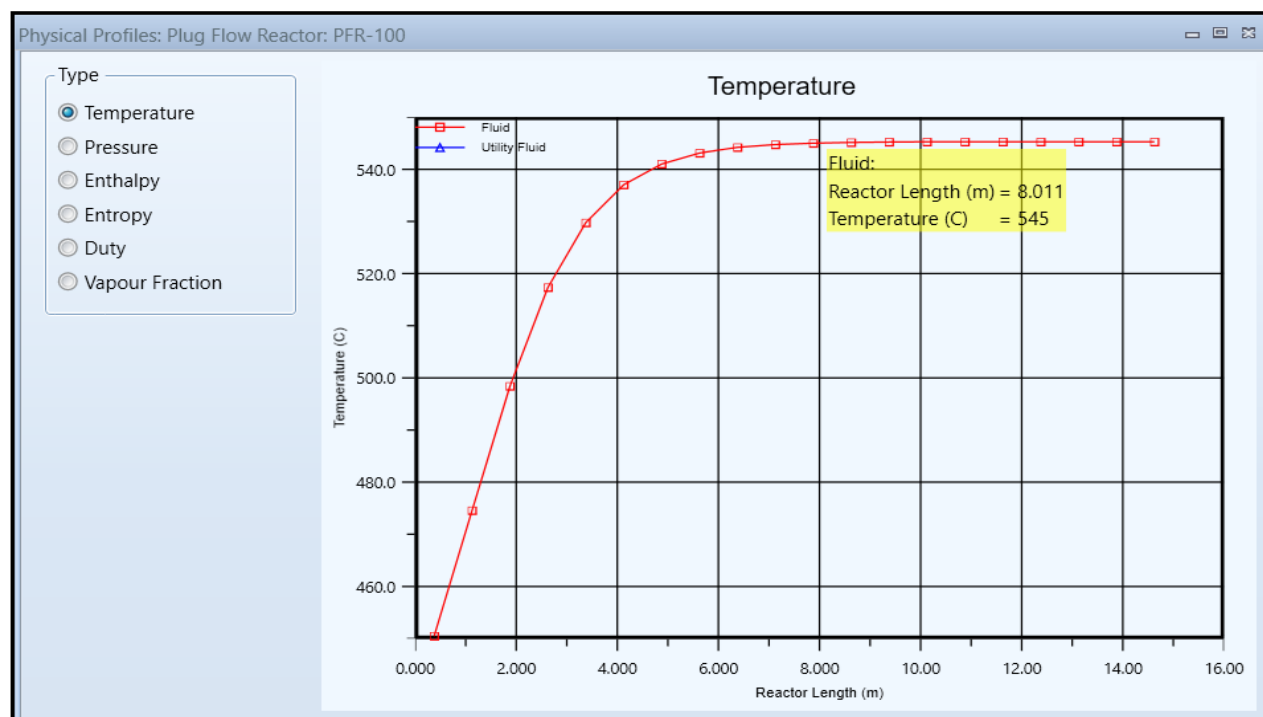
Worksheet

Conditions
Properties
Composition
PF Specs

	PFR Inlet	PFR Outlet
Methane	0.0237	0.0237
CO	0.1083	0.0028
CO2	0.0584	0.1639
H2O	0.2510	0.1455
Hydrogen	0.5586	0.6641

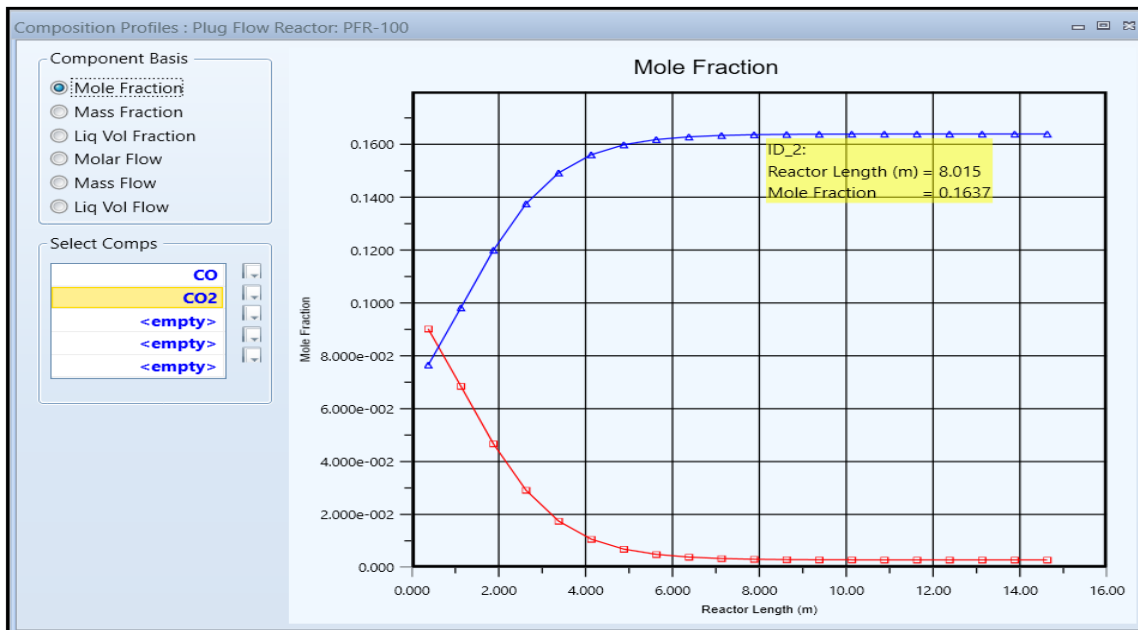
Delete OK Ignored

8. Under Performance select Plot.





9. Under Performance, click on composition and then plot it. Select CO and CO₂.



It is clear that after 8m of the length, temperature and compositions are unchanged. It means the reactor is oversized.

10. For the second scenario, under Rating/Sizing, change the length to 12m and diameter to 2.4m.

Parameter	Value
Total Volume	54.29 m3
Length	12.00 m
Diameter	2.400 m
Number of Tubes	1
Wall Thickness	5.000e-003 m

Parameter	Value
Void Fraction	1.000
Void Volume	54.29 m3



11.Results

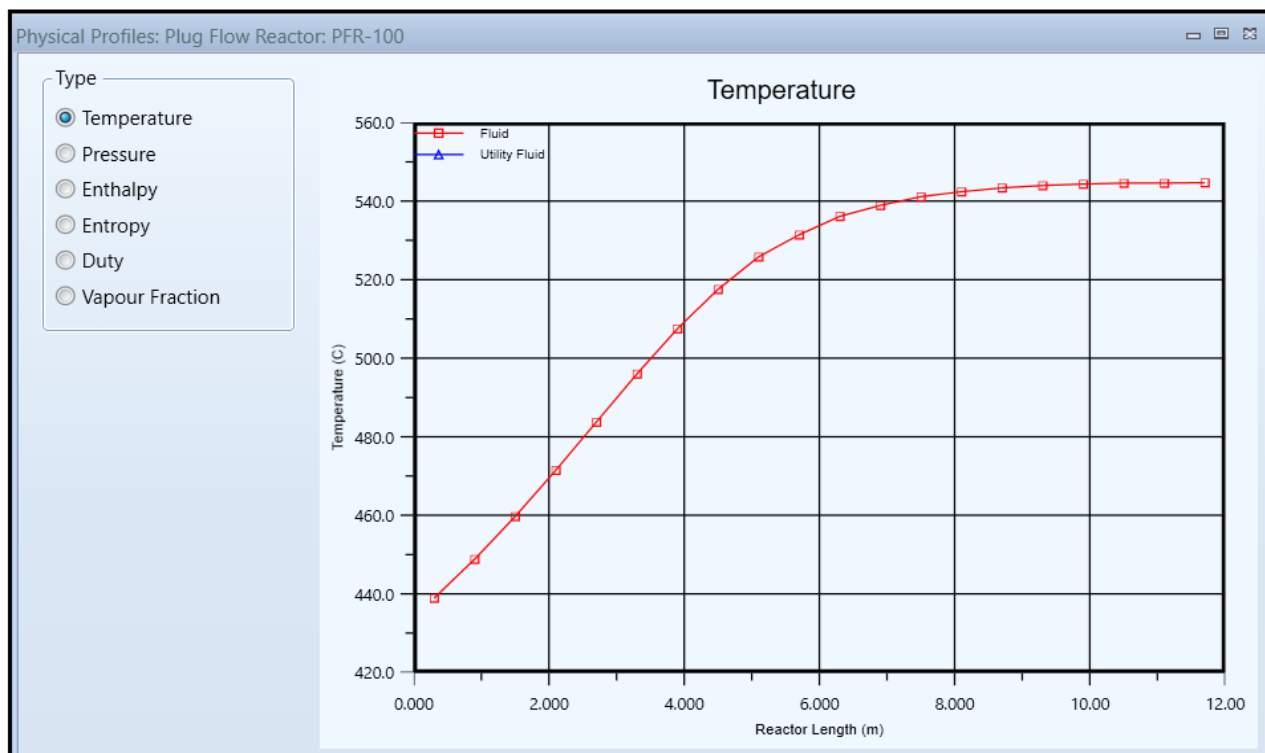
Plug Flow Reactor: PFR-100 - Set-2

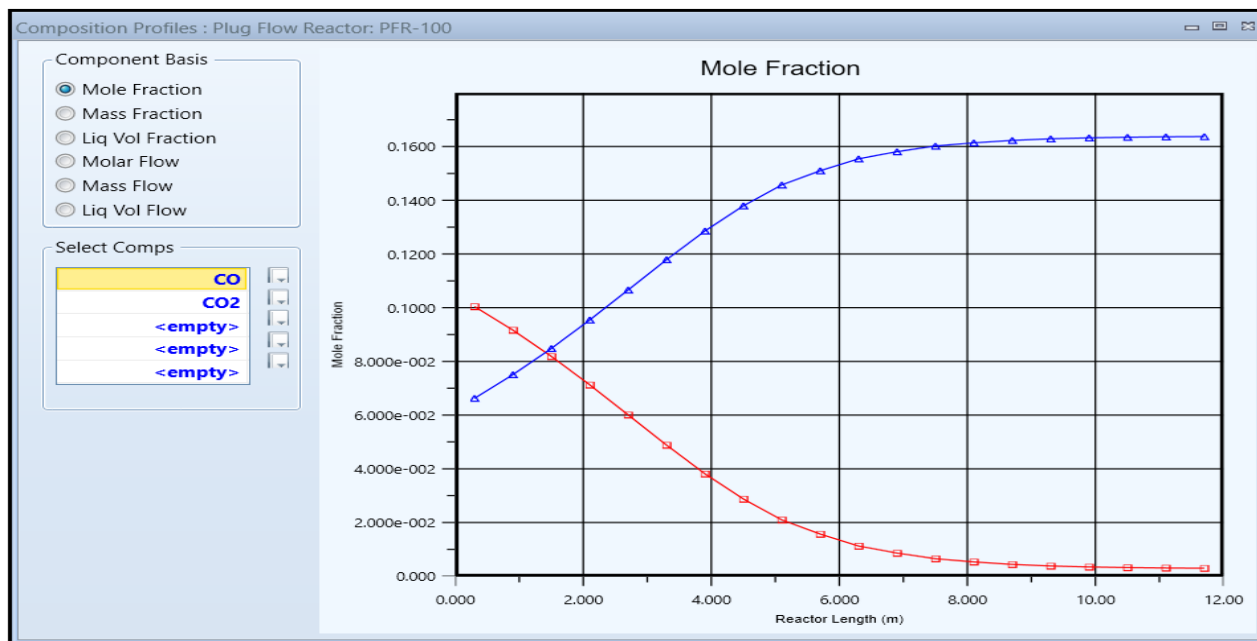
Design Reactions Rating Worksheet Performance Dynamics

Worksheet

	PFR Inlet	PFR Outlet
Methane	0.0237	0.0237
CO	0.1083	0.0030
CO2	0.0584	0.1638
H2O	0.2510	0.1456
Hydrogen	0.5586	0.6639

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Based on the plots, it seems that the PFR in second scenario is better sized.

12.If we want to include catalysts in our simulation, under Rating/Sizing, void fraction could be changed. By default, the value is 1 but in reality, it is between 0.6-0.8. The void fraction is a function of reactor and catalyst design.

Plug Flow Reactor: PFR-100 - Set-2

Design Reactions Rating Worksheet Performance Dynamics

Rating

Sizing

Nozzles

Tube Dimensions

Total Volume	54.29 m3
Length	12.00 m
Diameter	2.400 m
Number of Tubes	1
Wall Thickness	5.000e-003 m

Tube Packing

Void Fraction	0.700
Void Volume	38.00 m3

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13. In previous steps, we dictate the pressure drop to the software. Now we can select Ergun Equation to calculate the pressure drop.

Plug Flow Reactor: PFR-100 - Set-2

Design Reactions Rating Worksheet Performance Dynamics

Design

Connections
Parameters
Heat Transfer
User Variables
Notes

Pressure Drop Parameters

Delta P 3.266

☐ User Specified ☒ Ergun Equation

☐ Single Phase

Duty Parameters

Duty 0.0000

☐ Formula ☒ Direct Q Value

Delete OK Ignored

14. Here is the final result:

Plug Flow Reactor: PFR-100 - Set-2

Design Reactions Rating Worksheet Performance Dynamics

Worksheet

Conditions
Properties
Composition
PF Specs

Name	PFR Inlet	PFR Outlet
Vapour	1.0000	1.0000
Temperature [C]	430.0	542.5
Pressure [kPa]	426.0	422.7
Molar Flow [kgmole/h]	261.8	261.8
Mass Flow [kg/h]	3046	3046
Std Ideal Liq Vol Flow [m3/h]	7.549	8.333
Molar Enthalpy [kJ/kgmole]	-8.451e+004	-8.451e+004
Molar Entropy [kJ/kgmole-C]	169.0	169.4
Heat Flow [kJ/h]	-2.213e+007	-2.213e+007

Delete OK Ignored



Plug Flow Reactor: PFR-100 - Set-2

Design Reactions Rating Worksheet Performance Dynamics

Worksheet

Conditions
Properties
Composition
PF Specs

	PFR Inlet	PFR Outlet
Methane	0.0237	0.0237
CO	0.1083	0.0054
CO2	0.0584	0.1614
H2O	0.2510	0.1480
Hydrogen	0.5586	0.6615

Delete OK Ignored

