



Conversion Reaction Simulation

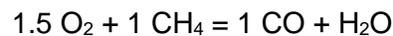




Example: ATR technologies play a crucial role in hydrogen, ammonia and methanol plants. In ATR reactors simply oxygen and natural gas, mainly methane react in a burner and as a result, produce heat required for catalytic zone in the reactor. The reaction is fast and all oxygen reacts with methane without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

Operating Conditions	Oxygen	Reformer Outlet
Flowrate	82700 kg/hr.	365500 kg/hr.
Temperature	230 C	738 C
Pressure	34barg	31.4barg
Composition		
Methane	-	0.17
CO	-	0.043
CO ₂	-	0.058
H ₂	-	0.3629
N ₂	-	0.0111
H ₂ O	-	0.3528
O ₂	1	-

Here is the reaction:





How to simulate:

1. Add all components like below to component list.

Source Databank: HYSYS

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

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

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 Peng-Robinson as the Fluid Package.

Fluid Package: Basis-1

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

Property Package Selection:

- 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
- Wilson
- Zudkevitch-Joffe

Options:

Enthalpy	Property Package EOS
Density	Costald
Modify Tc, Pc for H2, He	Modify Tc, Pc for H2, He
Viscosity Method	HYSYS Viscosity
Peng-Robinson Options	HYSYS
EOS Solution Methods	Cubic EOS Analytical Method
Phase Identification	Default
Surface Tension Method	HYSYS Method
Thermal Conductivity	API 12A3.2-1 Method

Status: **OK**

3. Under Properties/Reaction, add a set.



Properties < Reactions x +

All Items

- Component Lists
 - Component List - 1
- Fluid Packages
- Petroleum Assays
- Reactions
- Component Maps
- User Properties

Name	Type	Associated Fluid Packages
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Add Delete Set Copy Set Add to FP Detach from FP

Properties < Reaction Set: Set-1 x +

All Items

- Component Lists
- Fluid Packages
- Petroleum Assays
- Reactions
 - Set-1
- Component Maps
- User Properties

Set Info

Set Type: Unknown Not Ready

Add to FP
Detach from FP
Advanced...

Active Reactions	Type	Configured	Operations Attached
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4. Add a new reaction and select conversion.

Active Reactions	Type	Configured	Operations Attached
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Add Reaction ▾ Delete Reaction Copy Reaction

New Reaction
Existing Reaction

Reactions [-] [□] [×]

Reactant Source

Hysys
 AspenProperties

Conversion
Equilibrium
Heterogeneous Catalytic
Kinetic
Simple Rate

Add Reaction



Set Info

Set Type: Conversion

Not Ready

Independent

Add to FP

Detach from FP

Ranking...

Advanced...

Active Reactions	Type	Configured	Operations Attached
Rxn-1	Conversion	X	

Add Reaction

Delete Reaction

Copy Reaction

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

Conversion Reaction: Rxn-1

Stoichiometry Info

Component	Mole Weight	Stoich Coeff
Oxygen	32.000	-1.500
Methane	16.043	-1.000
CO	28.011	1.000
H2O	18.015	2.000
Add Comp		

Balance

Balance Error: 0.00000

Reaction Heat (25 C): -3.5e+05 kJ/kgmole

Basis

Base Component	Oxygen
Rxn Phase	VapourPhase
Co	100.0
C1	<empty>
C2	<empty>

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

(T in Kelvin)

Ready



6. Finally add it to FP.

Reaction Set: Set-1

Set Info

Set Type: Conversion

Ready

Independent

Add to FP

Detach from FP

Ranking...

Advanced...

Active Reactions	Type	Configured	Operations Attached
Rxn-1	Conversion	✓	

Add Reaction

Delete Reaction

Copy Reaction

Add 'Set-1'

Basis-1	NC: 7	PP: Peng-Robinson
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Add Set to Fluid Package



7. Enter Simulation Environment and streams like below:

Material Stream: Oxygen

Worksheet Attachments Dynamics

Worksheet

Stream Name	Oxygen	Vapour Phase
Vapour / Phase Fraction	1.0000	1.0000
Temperature [C]	230.0	230.0
Pressure [kPa]	3501	3501
Molar Flow [kgmole/h]	2656	2656
Mass Flow [kg/h]	8.500e+004	8.500e+004
Std Ideal Liq Vol Flow [m3/h]	74.71	74.71
Molar Enthalpy [kJ/kgmole]	6087	6087
Molar Entropy [kJ/kgmole-C]	131.1	131.1
Heat Flow [kJ/h]	1.617e+007	1.617e+007
Liq Vol Flow @Std Cond [m3/h]	6.274e+004	6.274e+004
Fluid Package	Basis-1	
Utility Type		

OK

Delete Define from Stream... View Assay ← →

Material Stream: Oxygen

Worksheet Attachments Dynamics

Worksheet

	Mole Fractions	Vapour Phase
Oxygen	1.0000	1.0000
Methane	0.0000	0.0000
Nitrogen	0.0000	0.0000
CO	0.0000	0.0000
CO2	0.0000	0.0000
Hydrogen	0.0000	0.0000
H2O	0.0000	0.0000

Total 1.00000

Edit... View Properties... Basis...

OK

Delete Define from Stream... View Assay ← →



Material Stream: Reformed Gas

Worksheet Attachments Dynamics

Worksheet

Stream Name	Reformed Gas	Vapour Phase
Vapour / Phase Fraction	1.0000	1.0000
Temperature [C]	738.0	738.0
Pressure [kPa]	3241	3241
Molar Flow [kgmole/h]	2.623e+004	2.623e+004
Mass Flow [kg/h]	3.655e+005	3.655e+005
Std Ideal Liq Vol Flow [m3/h]	814.4	814.4
Molar Enthalpy [kJ/kgmole]	-9.916e+004	-9.916e+004
Molar Entropy [kJ/kgmole-C]	183.3	183.3
Heat Flow [kJ/h]	-2.601e+009	-2.601e+009
Liq Vol Flow @Std Cond [m3/h]	6.178e+005	6.178e+005
Fluid Package	Basis-1	
Utility Type		

OK

Delete Define from Stream... View Assay ← →

Material Stream: Reformed Gas

Worksheet Attachments Dynamics

Worksheet

	Mole Fractions	Vapour Phase
Oxygen	0.0000	0.0000
Methane	0.1714	0.1714
Nitrogen	0.0111	0.0111
CO	0.0433	0.0433
CO2	0.0585	0.0585
Hydrogen	0.3629	0.3629
H2O	0.3528	0.3528

Total 1.00000

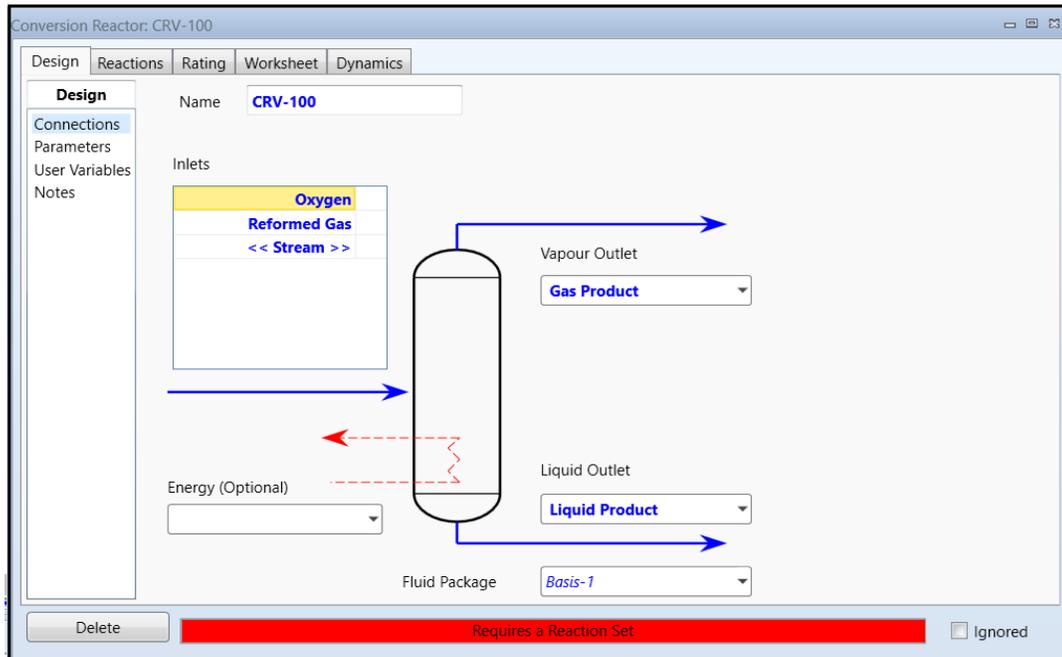
Edit... View Properties... Basis...

OK

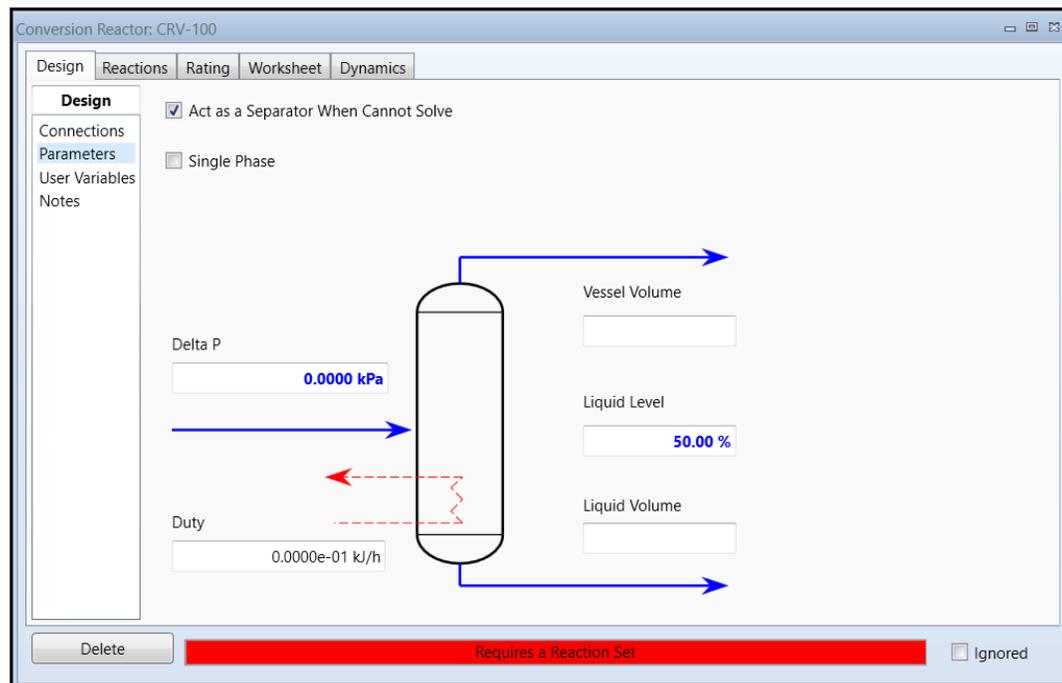
Delete Define from Stream... View Assay ← →



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



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





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

Conversion Reactor: CRV-100 - Set-1

Design Reactions Rating Worksheet Dynamics

Reactions

Details
Results

Conversion Reaction Details

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

Stoichiometry Basis Conversion %

Stoichiometry Info

Component	Mole Wgt.	Stoich Coeff
Oxygen	32.000	-1.500
Methane	16.043	-1.000
CO	28.011	1.000
H2O	18.015	2.000
Add Comp		

Balance Error: 0.00000
Reaction Heat (25 C): -3.5e+05 kJ/kgmole

Ignored

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

Material Stream: Gas Product

Worksheet Attachments Dynamics

Worksheet

Stream Name	Gas Product	Vapour Phase
Vapour / Phase Fraction	1.0000	1.0000
Temperature [C]	1403	1403
Pressure [kPa]	3241	3241
Molar Flow [kgmole/h]	2.977e+004	2.977e+004
Mass Flow [kg/h]	4.505e+005	4.505e+005
Std Ideal Liq Vol Flow [m3/h]	845.5	845.5
Molar Enthalpy [kJ/kgmole]	-8.682e+004	-8.682e+004
Molar Entropy [kJ/kgmole-C]	204.4	204.4
Heat Flow [kJ/h]	-2.585e+009	-2.585e+009
Liq Vol Flow @Std Cond [m3/h]	1039	1039
Fluid Package	Basis-1	
Utility Type		



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

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