



## Conversion Reaction Simulation

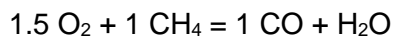




Example: ATR technologies play a crucial role in hydrogen, ammonia and methanol plants. In ATR reactors simply oxygen and natural gas, mainly methane react in a burner and as a result, produce heat required for catalytic zone in the reactor. The reaction is fast and all oxygen reacts with methane without 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 <sub>2</sub>	-	0.058
H <sub>2</sub>	-	0.3629
N <sub>2</sub>	-	0.0111
H <sub>2</sub> O	-	0.3528
O <sub>2</sub>	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**

Component	Type	Group
Oxygen	Pure Component	
Methane	Pure Component	
Nitrogen	Pure Component	
CO	Pure Component	
CO <sub>2</sub>	Pure Component	
Hydrogen	Pure Component	
H <sub>2</sub> O	Pure Component	

< Add Replace Remove

Simulation Name	Full Name / Synonym	Formula
Ethane	C2	C <sub>2</sub> H <sub>6</sub>
Propane	C3	C <sub>3</sub> H <sub>8</sub>
i-Butane	i-C4	C <sub>4</sub> H <sub>10</sub>
n-Butane	n-C4	C <sub>4</sub> H <sub>10</sub>
i-Pentane	i-C5	C <sub>5</sub> H <sub>12</sub>
n-Pentane	n-C5	C <sub>5</sub> H <sub>12</sub>
n-Hexane	C6	C <sub>6</sub> H <sub>14</sub>
n-Heptane	C7	C <sub>7</sub> H <sub>16</sub>
n-Octane	C8	C <sub>8</sub> H <sub>18</sub>
n-Nonane	C9	C <sub>9</sub> H <sub>20</sub>
n-Decane	C10	C <sub>10</sub> H <sub>22</sub>
n-C11	C11	C <sub>11</sub> H <sub>24</sub>

Status: OK

2. Select Peng-Robinson as the Fluid Package.

Fluid Package: Basis-1

Set Up Binary Coeffs StabTest Phase Order Tabular Notes

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

Property Package Selection: **Peng-Robinson**

Options:

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

Parameters:

Property Pkg: OK Edit Properties

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
------	------	---------------------------

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
------------------	------	------------	---------------------



4. Add a new reaction and select conversion.

Active Reactions	Type	Configured	Operations Attached
------------------	------	------------	---------------------

Add Reaction

New Reaction

Existing Reaction

Delete Reaction

Copy Reaction

Reactions

Reactant Source

☒ Hysys

☐ AspenProperties

Conversion

Equilibrium

Heterogeneous Catalytic

Kinetic

Simple Rate

Add Reaction



Set Info

Set Type:

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	
Rxn Phase	Oxygen
Co	VapourPhase
C1	100.0
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:

Active Reactions	Type	Configured	Operations Attached
<b>Rxn-1</b>	Conversion	✓	

Add 'Set-1'

*Basis-1* *NC: 7* *PP: Peng-Robinson*



7. Enter Simulation Environment and streams like below:

Material Stream: Oxygen

Worksheet Attachments Dynamics

**Worksheet**

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

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**

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

	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**

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

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

OK

Delete Define from Stream... View Assay

Material Stream: Reformed Gas

Worksheet Attachments Dynamics

**Worksheet**

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

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

Total 1.00000

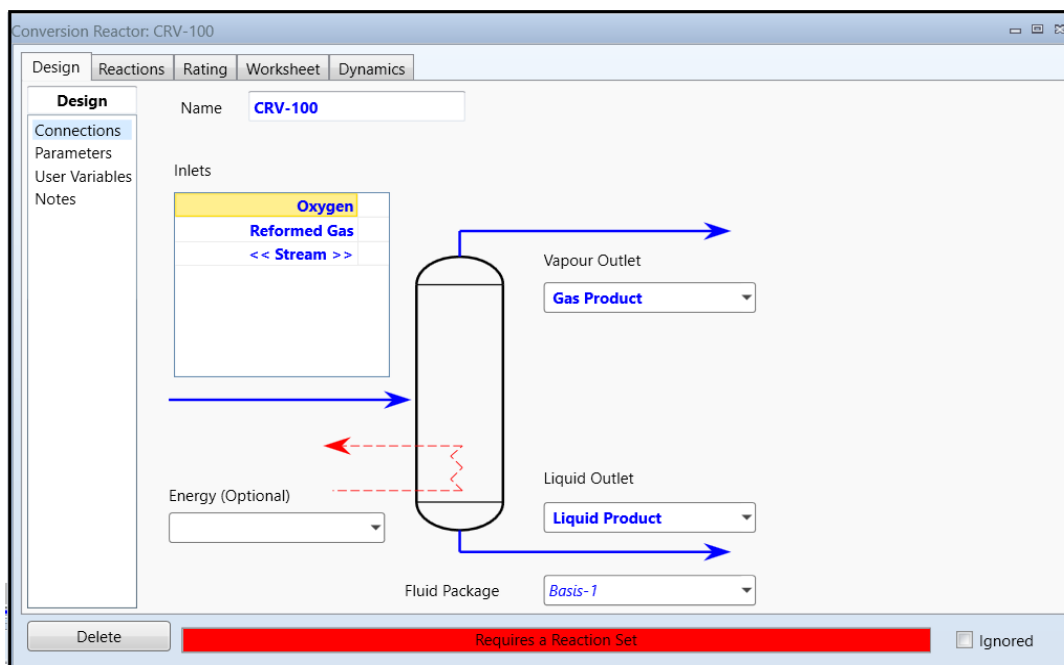
Edit... View Properties... Basis...

OK

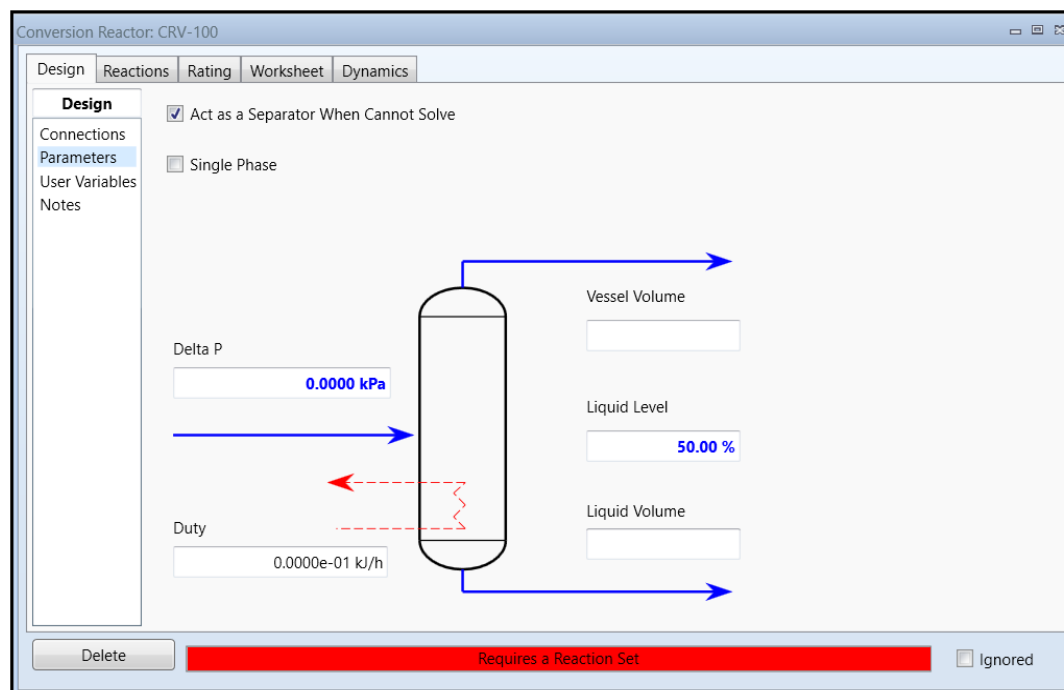
Delete Define from Stream... View Assay



8. Now it is time to set-up the conversion reactor. Select conversion reactor from Model 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 % [View Reaction...](#)

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
<b>**Add Comp**</b>		

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

Delete OK Ignored

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

Material Stream: Gas Product

Worksheet Attachments Dynamics

**Worksheet**

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

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		

OK

Delete Define from Stream... View Assay



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

Conversion Reactor: CRV-100 - Set-1

Design	Reactions	Rating	Worksheet	Dynamics
<b>Worksheet</b>				
Conditions				
Properties				
Composition				
PF Specs				
	Oxygen	1.0000	0.0000	0.0000
	Methane	0.0000	0.1714	0.0915
	Nitrogen	0.0000	0.0111	0.0098
	CO	0.0000	0.0433	0.0977
	CO2	0.0000	0.0585	0.0515
	Hydrogen	0.0000	0.3629	0.3197
	H2O	0.0000	0.3528	0.4298