KM 331 PROSES BENZETİM PROGRAMLARI
DERS NOTLARI [1-4]

Kaynaklar

1. Chemcad User Guide and Tutorial, Chemstations, Inc. Version 6.1.
2. Aspen Technology, Inc., Apsen HYSYS ® Version 7.
3. ChemCad Eğitim Notları , Chemstations, Inc- Houston,TX,USA.
4. A Guide for Getting Started in Aspen HYSYS
   Dinu Ajikutira, Sr. Director, Engineering Product Marketing, Aspen Technology, Inc.

Conversion Reaction

This chapter begins with a problem to develop a model that represents the partial oxidation reaction of methane to produce hydrogen. The partial oxidation method relies on the reaction of the methane with air in order to produce carbon oxides and hydrogen. The user will learn how to add the conversion reactions and reactions sets in HYSYS.

This reaction type does not require any thermodynamic knowledge. You must input the stoichiometry and the conversion of the basis reactant. The specified conversion cannot exceed 100%. The reaction will proceed until either the specified conversion has been reached or a limiting reagent has been exhausted.

Conversion reactions may not be grouped with any other form of reaction in a reaction set. However, they may be grouped with other conversion reactions and ranked to operate either sequentially or simultaneously. Lowest ranking occurs first (may start with either 0 or 1). Just as with single reactions, simultaneous reactions cannot total over 100% conversion of the same basis.

Conversion reactions cannot be used with Plug Flow Reactors or CSTRs. In general, they should only be used in Conversion Reactors.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Simulate conversion reactor and reactions in HYSYS
- Add the reactions and reaction sets
- Attach reaction sets to the fluid package

Prerequisites: Before beginning this chapter, the users need to know how to:

- Navigate the PFD
- Add Streams in the PFD or the Workbook
- Add and connect Unit Operations

Problem Statement

The interest in production of hydrogen from hydrocarbons has grown significantly in the last decade. Efficient production of hydrogen is an enabling technology, directly related to the fuel cell energy conversion device. The conversion of fuels to hydrogen can be carried out by the partial oxidation. The partial oxidation method relies on the reaction of the fuel for example methane with air in order to produce carbon oxides and hydrogen.

$$CH_4 + \tfrac{1}{2} O_2 \rightarrow CO + 2H_2$$

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

Develop a model that represents partial oxidation of methane to produce hydrogen.

Defining the Simulation Basis

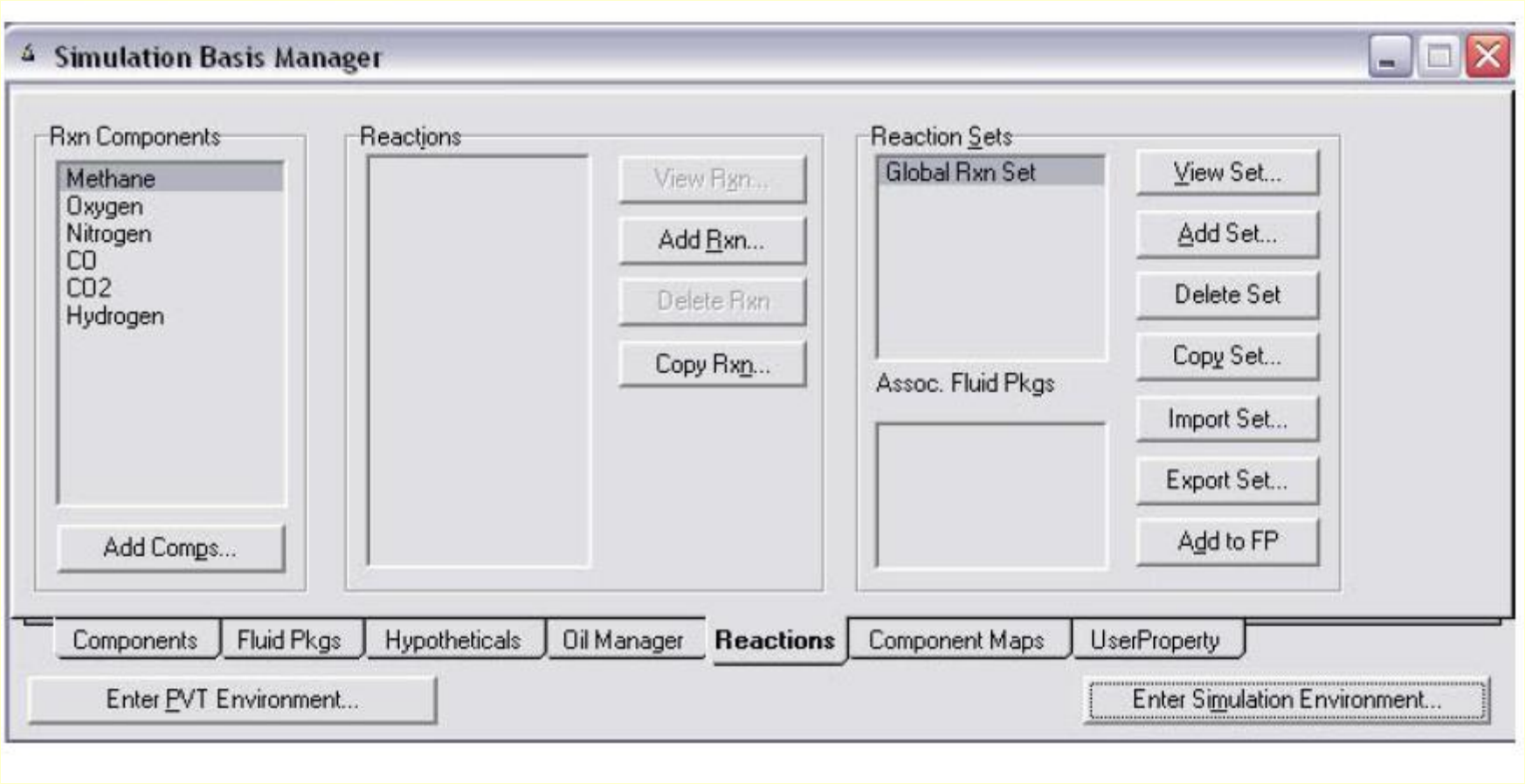
1. The first step in simulating a hydrogen production is choosing an appropriate fluid package. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	Peng-Robinson
Components	CH_4, O_2, N_2, CO, CO_2, H_2

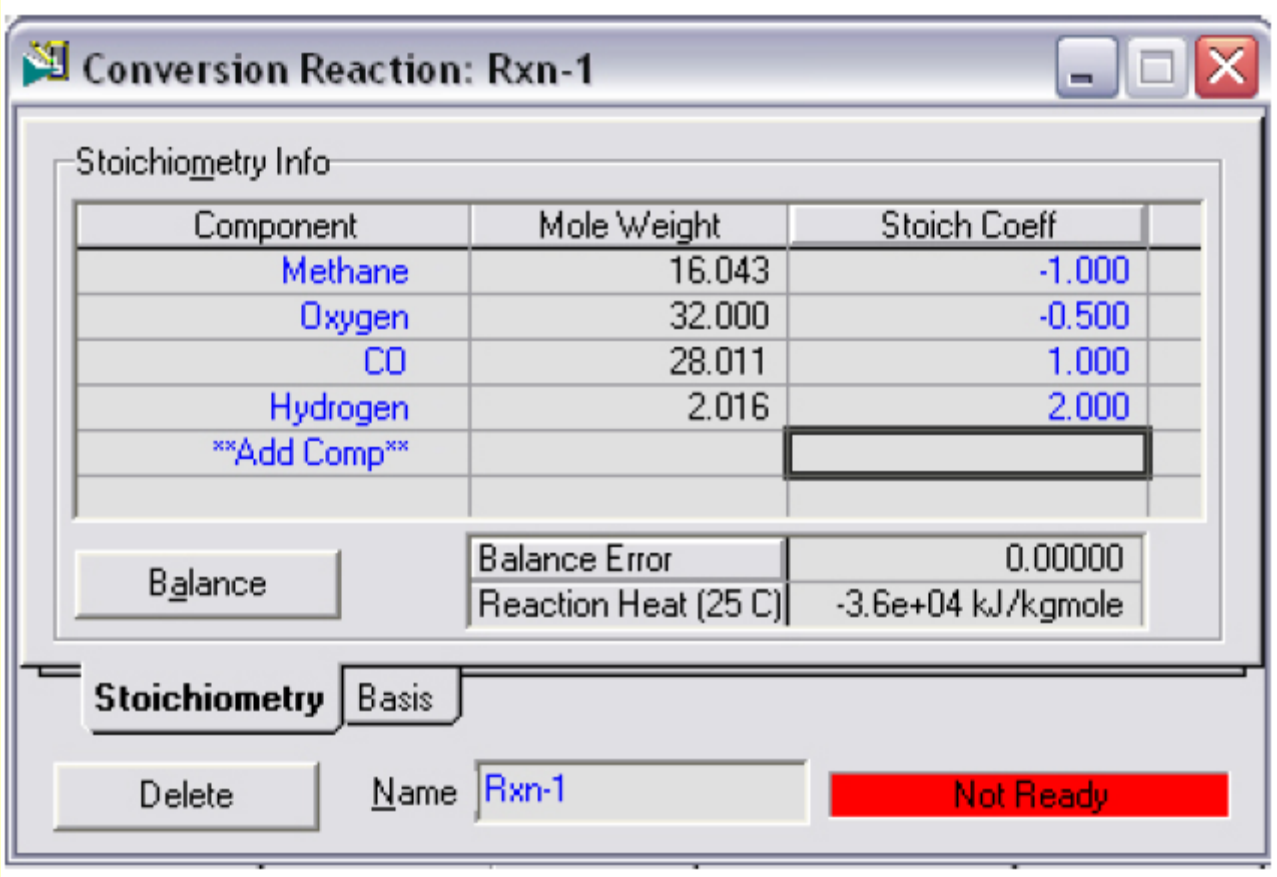
Adding the Reactions

Reactions in HYSYS are added in a manner very similar to the method used to add components to the simulation:

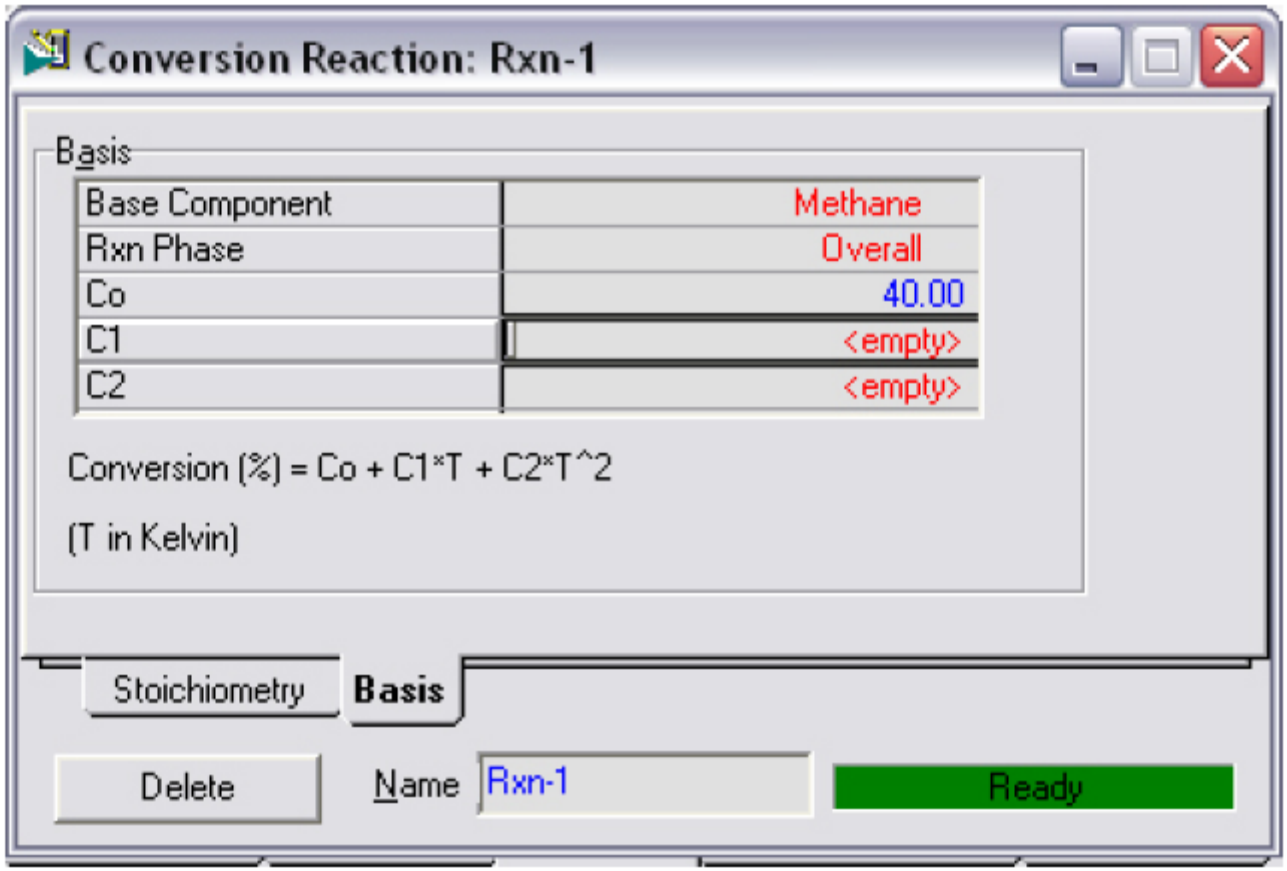
1. Click on the **Reactions** tab in the **Simulation Basis Manager** view. Note that all of the components are shown in the **Rxn Components** list.



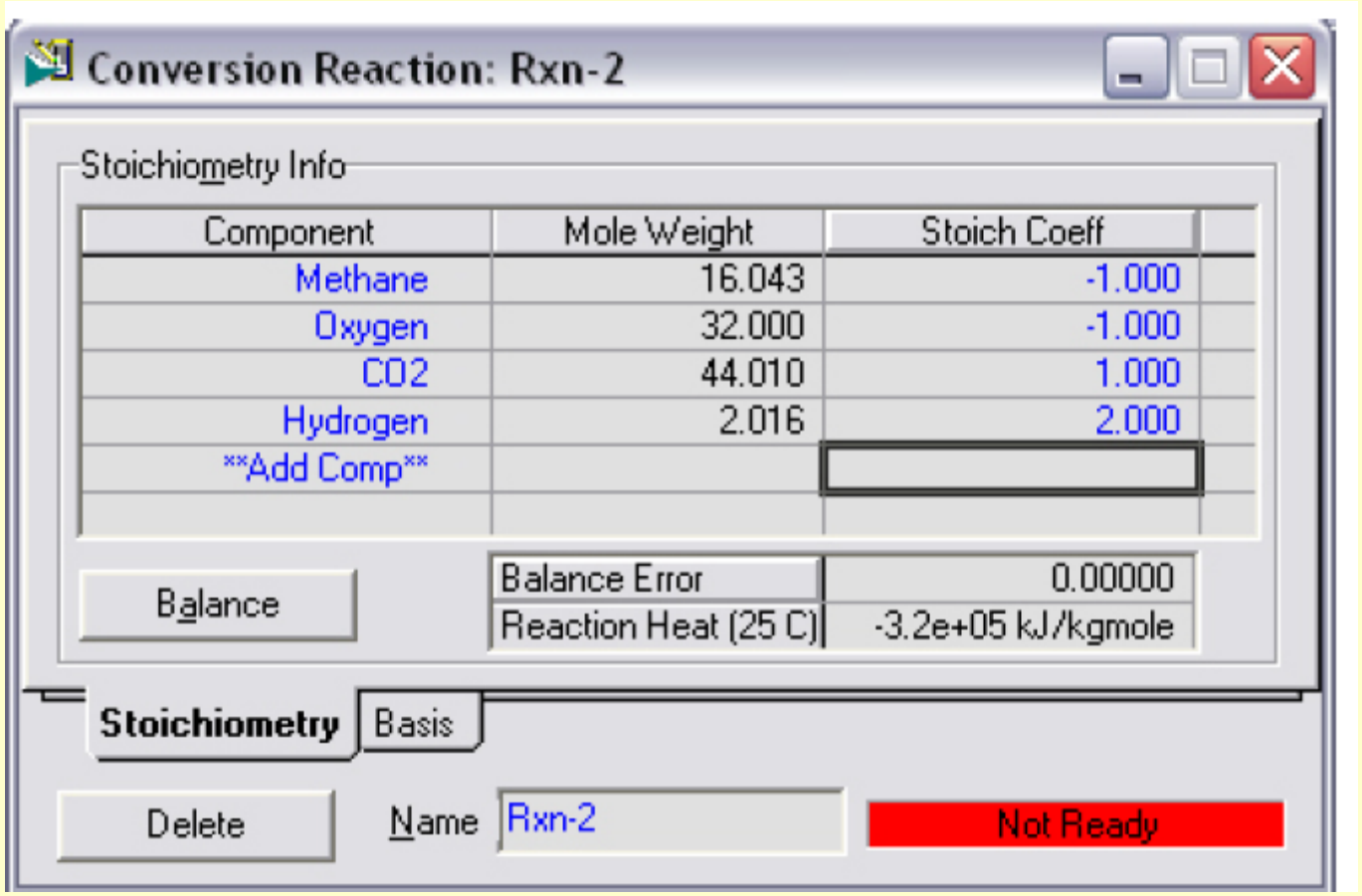
2. Click the **Add Rxn** button, and choose **Conversion** as the type from the displayed list. Enter the necessary information as shown:



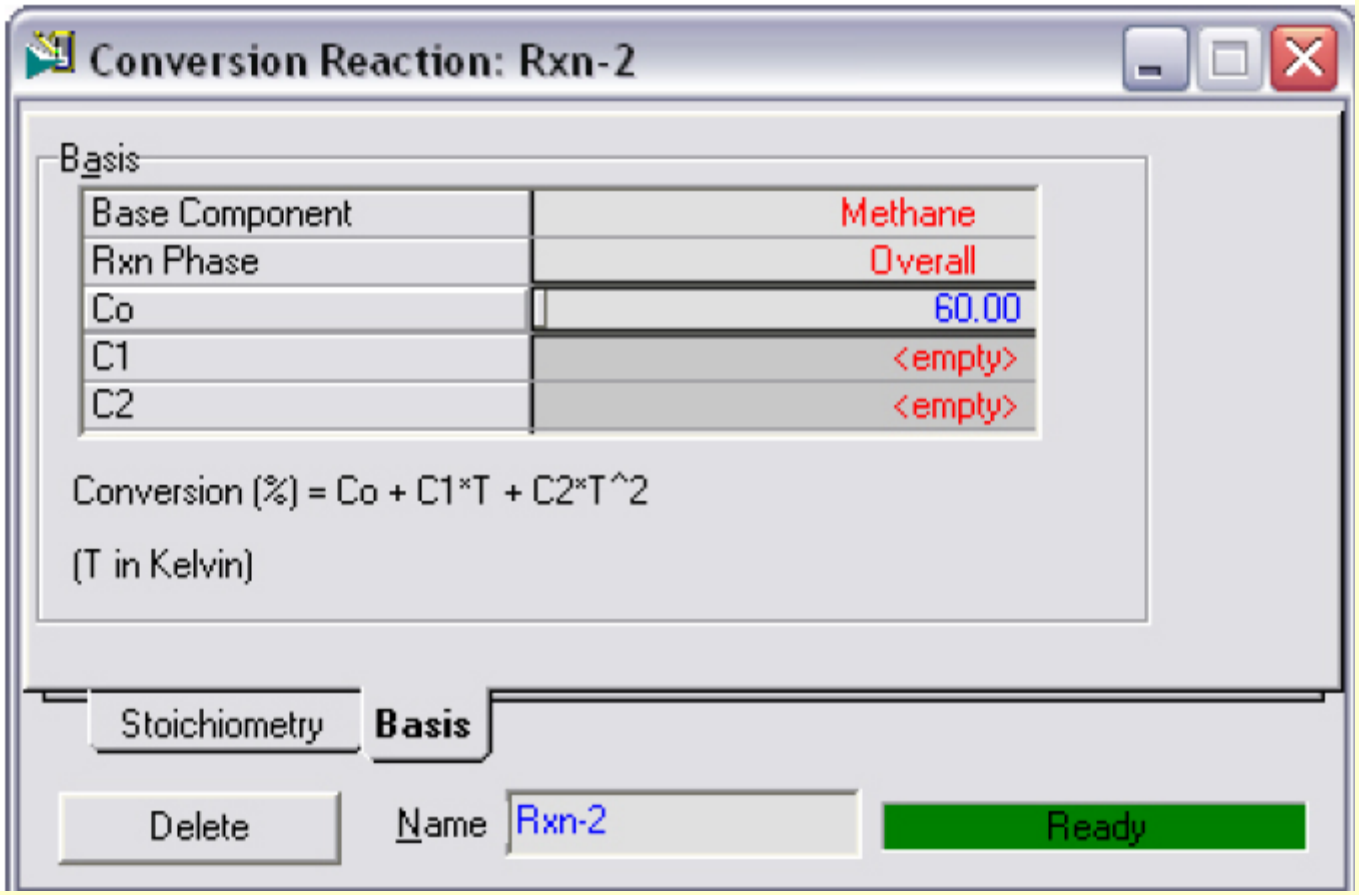
3. Move to the **Basis** tab and enter the information as shown:



4. For the second reaction, enter the information as shown:



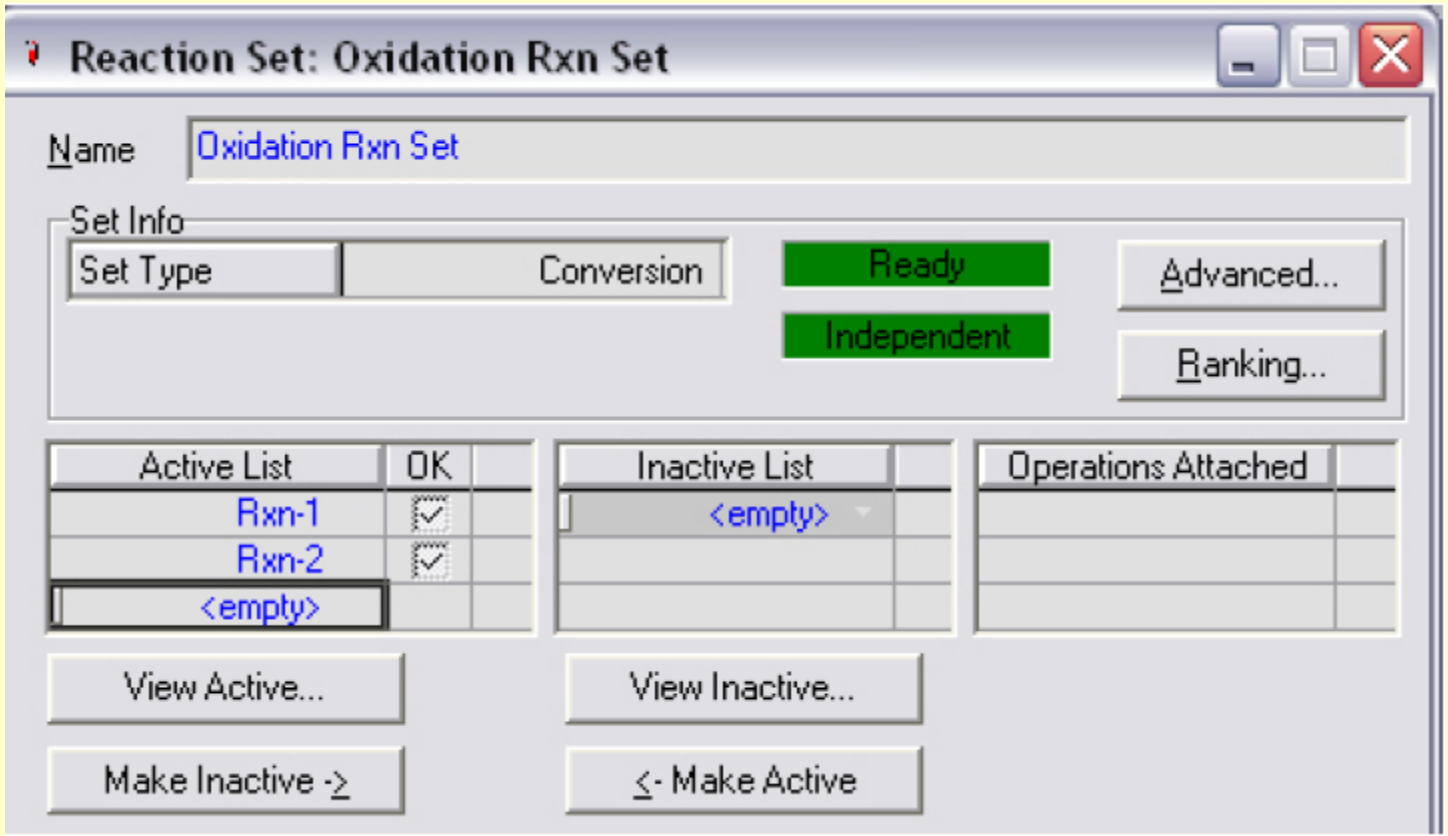
5. Move to the **Basis** tab and enter the information as shown:



Adding the Reaction Sets

Once all two reactions are entered and defined, you can create a reaction set for the conversion reactor.

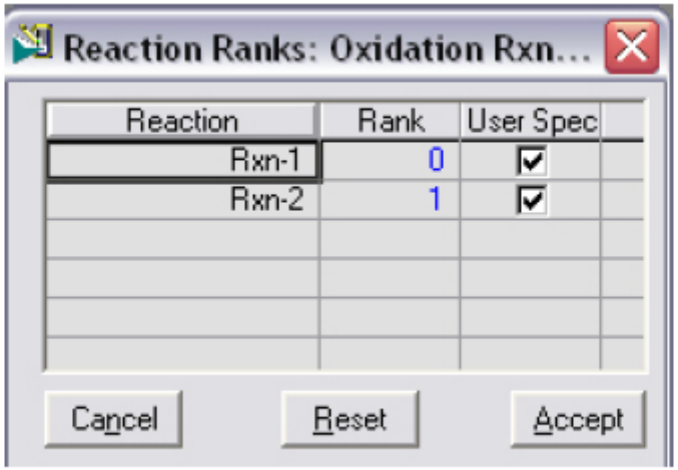
1. Still on the **Reactions** tab, click the **Add Set** button. Call the reaction set **Oxidation Rxn Set**, and add **Rxn-1** and **Rxn-2**. Reactions are added by highlighting the **<empty>** field in the **Active List** group, and selecting the desired reaction from the drop down list. The view should look like this after you are finished:



Making Sequential Reactions

Conversion reactions can be grouped with other conversion reactions and ranked to operate either sequentially or simultaneously. Lowest ranking occurs first (may start with either 0 or 1).

1. To make the reactions operate sequentially, in the **Oxidation Rxn Set**, click the **Ranking…** and enter the information as shown:



Attaching Reaction Set to the Fluid Package

After the reaction set has been created, it must be added to the current fluid package in order for HYSYS to use them.

1. Highlight the desired Reaction Set and press **Add to FP**.
2. Select the only available Fluid Package and press the **Add Set to Fluid Package** button.
3. If desired, you can save the Fluid Package with the attached reaction sets. This will allow you to reopen this FP in any number of HYSYS simulations.

Once the reaction set is added to the Fluid Package, you can enter the Simulation Environment and begin construction of the simulation.

Adding a Feed Stream

Add a new **Material** stream with the following values.

In this cell…	Enter…
Name	Methane
Temperature	25°C
Pressure	2 bar
Molar Flow	100 kgmole/h
Component Mole Fraction	
C_1	1.000

Add another new **Material** stream with the following values.

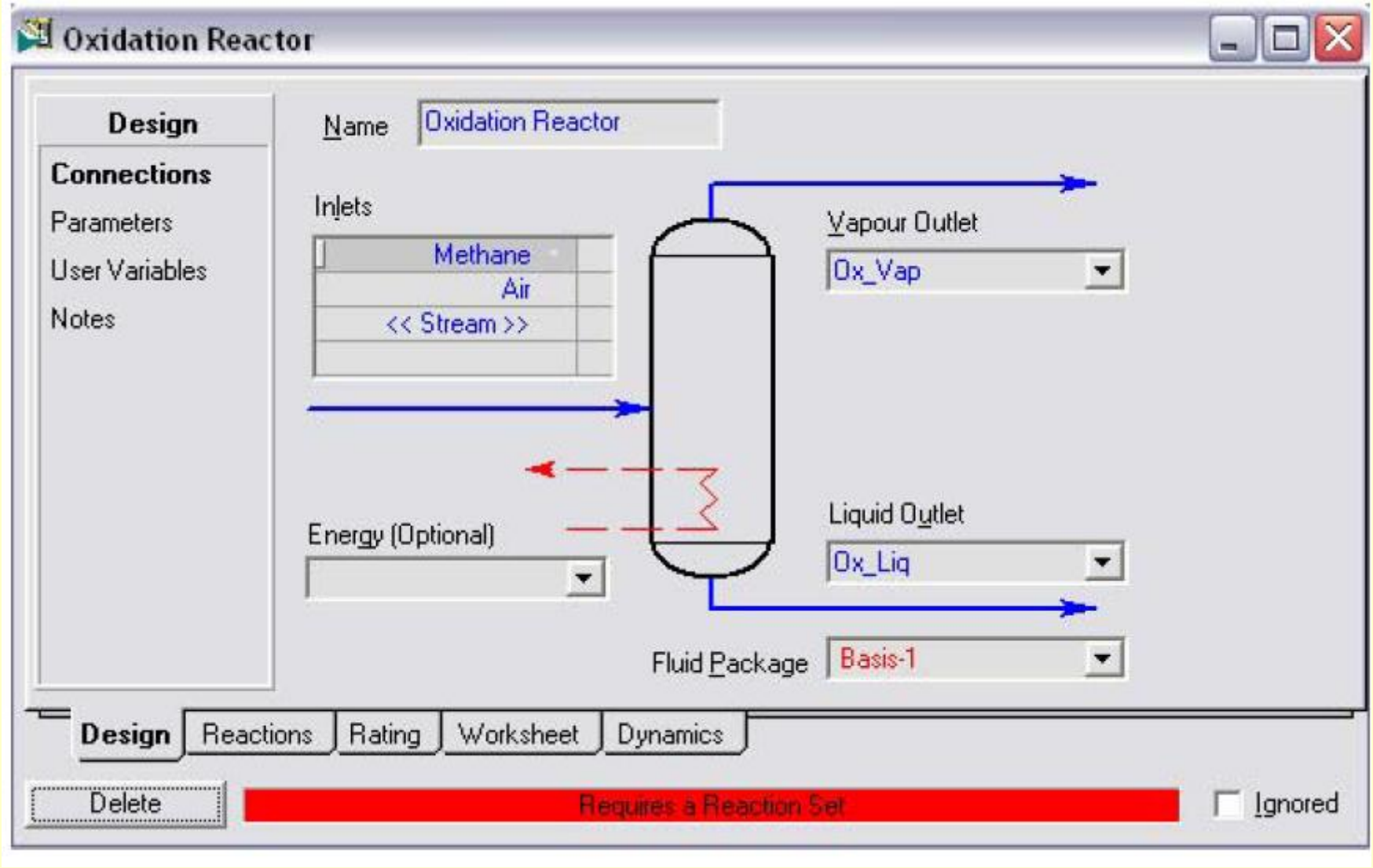
In this cell…	Enter…
Name	Air
Temperature	25°C
Pressure	2 bar
Molar Flow	260 kgmole/h
Component Mole Fraction	
N_2	0.790
O_2	0.210

Adding the Conversion Reactor

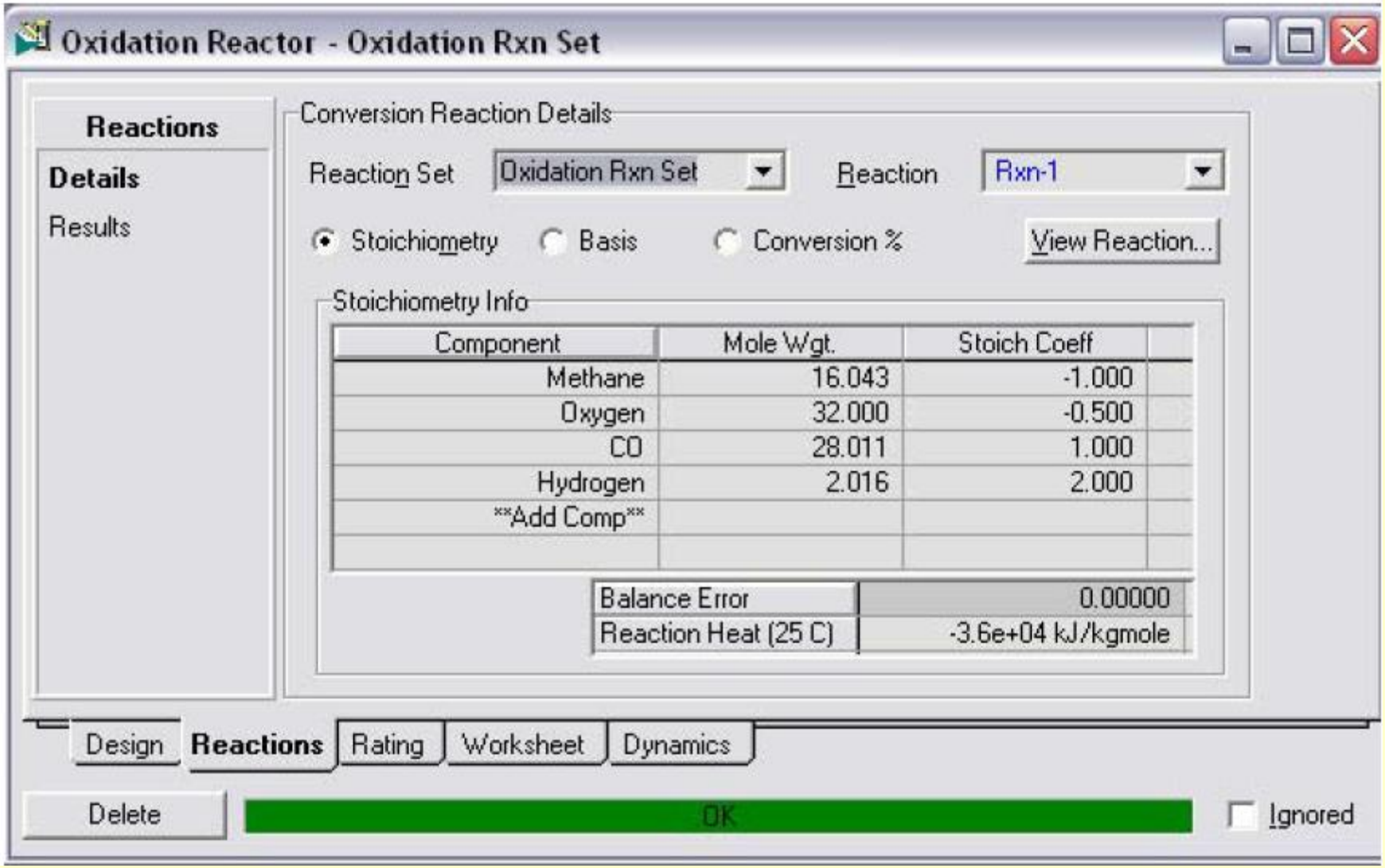
1. From the Object Palette, click **General Reactors.** Another palette appears with four reactor types: Gibbs, Equilibrium, Conversion and Yield. Select the **Conversion Reactor**, and enter it into the PFD.

Conversion Reactor icon

2. Name this reactor **Oxidation Reactor** and attach **Methane** and **Air** as feeds. Name the vapor outlet **Ox_Vap** and even though the liquid product from this reactor will be zero, we still must name the stream. Name the liquid product stream as **Ox_Liq**.


Oxidation Reactor
Design
Connections
Parameters
User Variables
Notes
Name
Oxidation Reactor
Inlets
Methane
Air
<< Stream >>
Vapour Outlet
Ox_Vap
Liquid Outlet
Ox_Liq
Energy (Optional)
Fluid Package
Basis-1
Design
Reactions
Rating
Worksheet
Dynamics
Delete
Requires a Reaction Set
Ignored

3. On the **Details** page of the **Reactions** tab, select **Oxidation Rxn Set** as the reaction set. This will automatically connect the proper reactions to this reactor.



4. Go to the **Worksheet** tab. On the **Composition** page, analyze the composition in the **Ox_Vap** stream.

What is the molar flow of the following components?

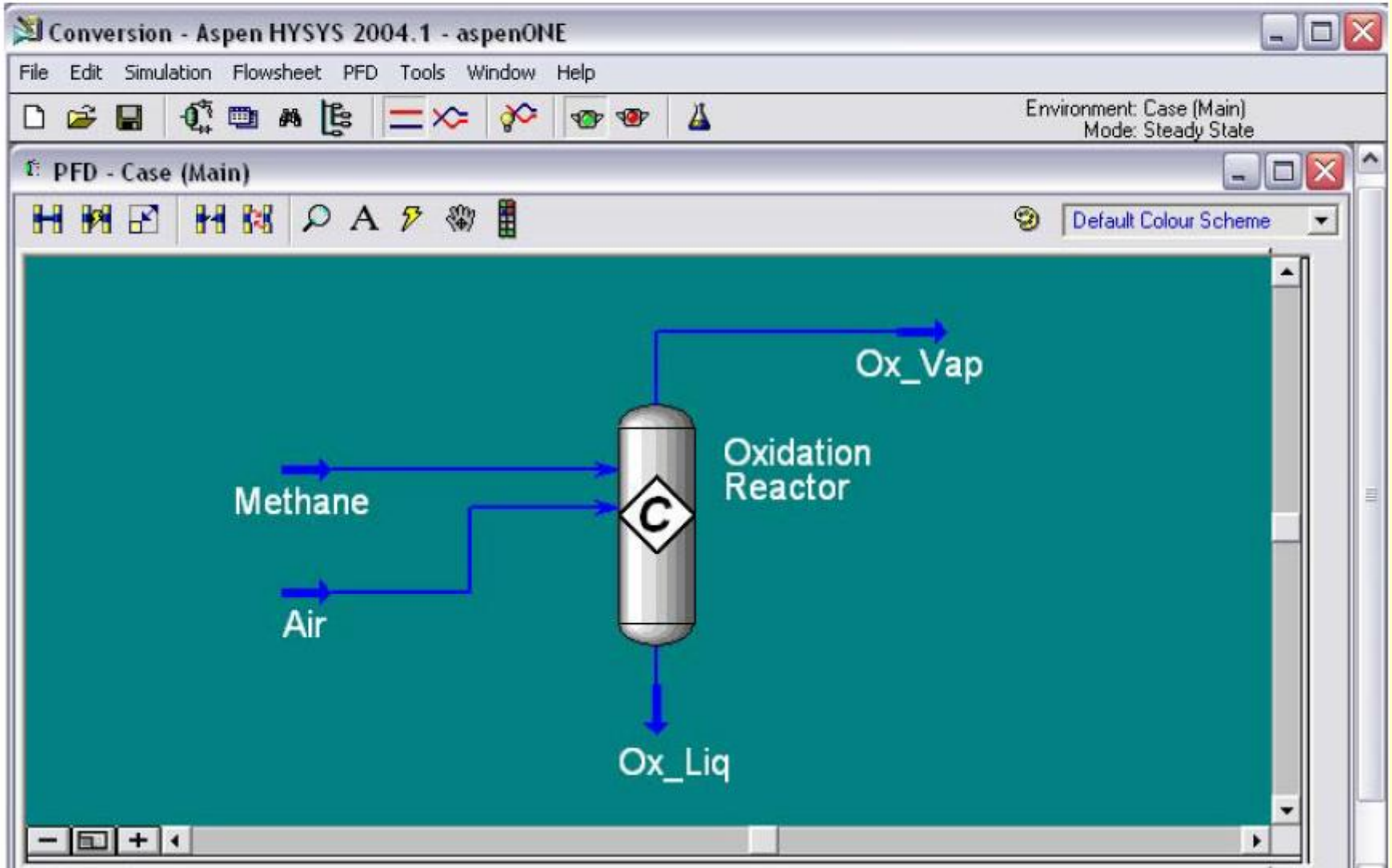
Methane: _____ Nitrogen: _____

Oxygen: _____ CO: _____

CO2: _____ Hydrogen: _____

Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Conversion** then press the OK button.



RESULTS

Workbook - Case (Main)

Name	Metan	O2	vapor	lliquid
Vapour Fraction	1.0000	1.0000	1.0000	0.0000
Temperature [C]	25.00	25.00	844.3	844.3
Pressure [bar]	2.000	2.000	2.000	2.000
Molar Flow [kgmole/h]	100.0	260.0	454.6	0.0000
Mass Flow [kg/h]	1604	7501	9105	0.0000
Liquid Volume Flow [USGPM]	23.59	38.18	70.66	0.0000
Heat Flow [kW]	-2082	-1.165	-2083	0.0000

Workbook - Case (Main)

Name	Metan	O2	vapor	lliquid
Comp Mole Frac (Methane)	1.0000	0.0000	0.0559	0.0559
Comp Mole Frac (Oxygen)	0.0000	0.2100	0.0000	0.0000
Comp Mole Frac (Nitrogen)	0.0000	0.7900	0.4518	0.4518
Comp Mole Frac (CO)	0.0000	0.0000	0.0880	0.0880
Comp Mole Frac (CO2)	0.0000	0.0000	0.0761	0.0761
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.3282	0.3282

Material Streams | **Compositions** | Energy Streams | Unit Ops