Ammonia Synthesis with Aspen Plus® V8.0

Part 1 Open Loop Simulation of Ammonia Synthesis

1. Lesson Objectives

- Become comfortable and familiar with the Aspen Plus graphical user interface
  - Explore Aspen Plus flowsheet handling techniques
  - Understand the basic input required to run an Aspen Plus simulation
- Understand the various classes of reactor models available
  - Learn how to approximate the 'real' kinetic-based, heterogeneous reaction into an equilibrium reaction
  - Determine the appropriate reactor model type
- Determination of Physical Properties method for Ammonia Synthesis
- Apply acquired skill to build an open loop Ammonia Synthesis process simulation
  - Enter the minimum input required for an simplified Ammonia Synthesis model
  - Examine the open loop simulation results

2. Prerequisites

- Aspen Plus V8.0

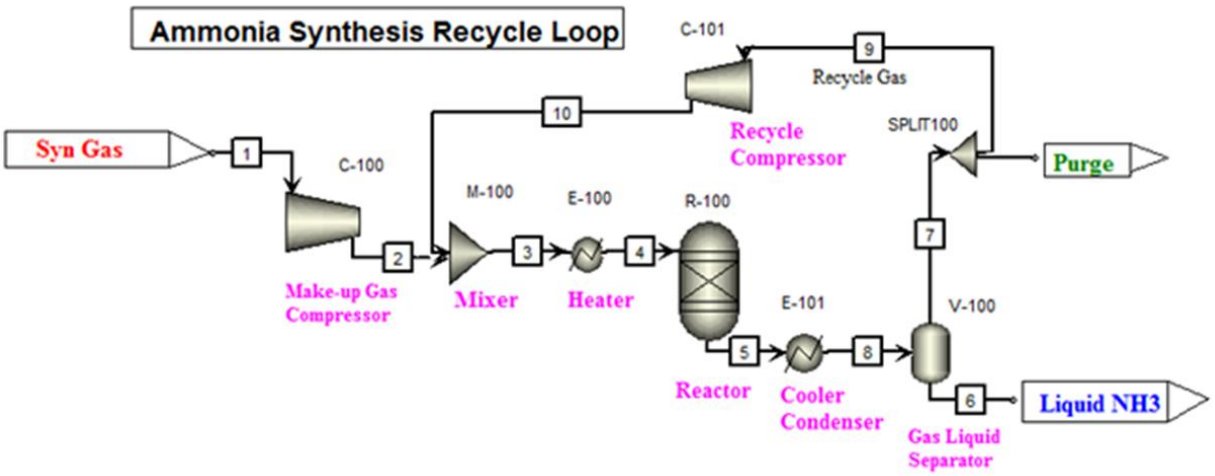
3. Background

Ammonia is one of the most highly produced chemicals in the world and is mostly used as fertilizers. In 1913 Fritz Haber and Carl Bosch developed a process for the manufacture of ammonia on an industrial scale (Haber-Bosch process). This process is known for extremely high pressures that are required to maintain a reasonable equilibrium constant. Today, this process produces 500 million tons of nitrogen fertilizer per year and is responsible for sustaining one-third of the Earth's population.

Ammonia is produced by reacting nitrogen from air with hydrogen. Hydrogen is usually obtained fro m steam reformation of methane, and nitrogen is obtained from deoxygenated air. The chemical reaction is shown below:

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

Our goal is to produce a simulation for the production of ammonia using Aspen Plus. We will create a very simplified version of this process in order to learn the basics of how to create a flowsheet in the Aspen Plus V7.3.2 user interface. A process flow diagram for this process is shown below.



Knowledge Base: Physical Properties for Ammonia Process

Equation-of-state models provide an accurate description of the thermodynamic properties of the high-temperature, high-pressure conditions encountered in ammonia plants. The Redlich-Kwong modification RKS-BM was chosen for this application.

RKS-BM

The RKS-BM property method uses the Redlich-Kwong-Soave (RKS) cubic equation of state with Boston-Mathias alpha function for all thermodynamic properties.

This property method is comparable to the PR-BM property method. It is recommended for gas-processing, refinery, and petrochemical applications. Example applications include gas plants, crude towers, and ethylene plants.

For accurate results in your VLE calculations, you must use binary parameters. The binary parameters available are automatically retrieved from the EOS-LIT databank.

Mixture Types

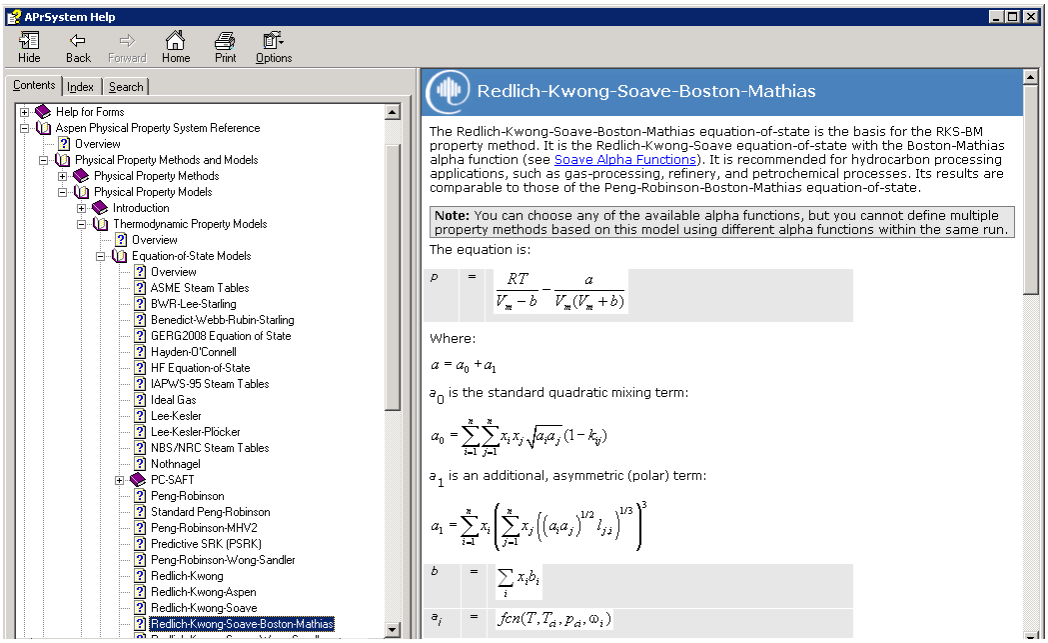
Use the RKS-BM property method for nonpolar or mildly polar mixtures. Examples are hydrocarbons and light gases, such as carbon dioxide, hydrogen sulfide, and hydrogen.

Range

You can expect reasonable results at all temperatures and pressures. The RKS-BM property method is consistent in the critical region. Results are least accurate in the region near the mixture critical point.

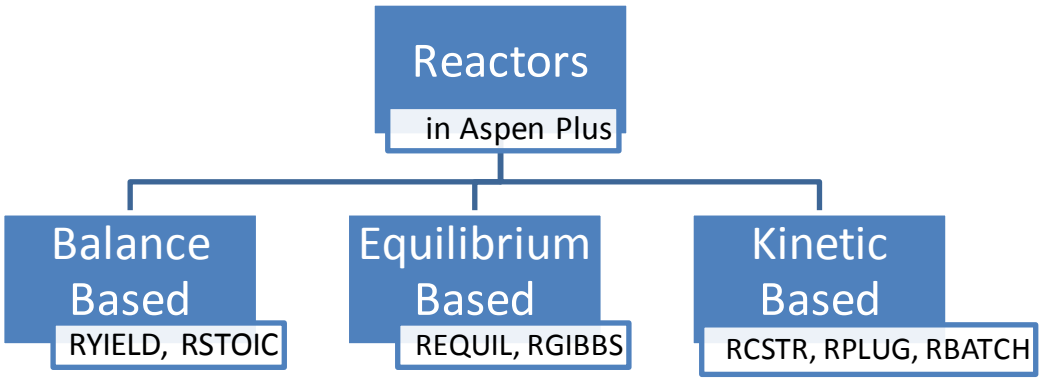
Refer to the tables labeled Parameters Required for the RKS-BM Property Method (below) and Parameters Required for Common Models for thermodynamic and transport property models, and their required parameters.

Find more information of Redlich-Kwong-Soave-Boston-Mathias (RKS-BM) method from Aspen Plus on-line help:



Knowledge Base: Reactor Model Types

Aspen Plus includes three types of reactor models. The type you choose depends on the level of rigor you want to use and the amount of information you have available:



(1) Balance Based (RYIELD, RSTOIC) - These reactors are for mass and energy balance purposes. You specify the conversion or yield and the reaction stoichiometry. In essence, you tell Aspen the expected result and it handles the details of the mass, energy, and species balances.

(2) Equilibrium Based (REQUIL, RGIBBS) - These reactor models are appropriate for fast reactions that reach equilibrium quickly (although there are ways to specify approach to equilibrium for non-ideal cases). RGIBBS is the most flexible model. It allows multiple phases (including multiple solid phases) and multiple species. This model uses Gibbs free energy minimization to predict results. It requires accurate thermodynamics since Gibbs energy is calculated from enthalpy and entropy.

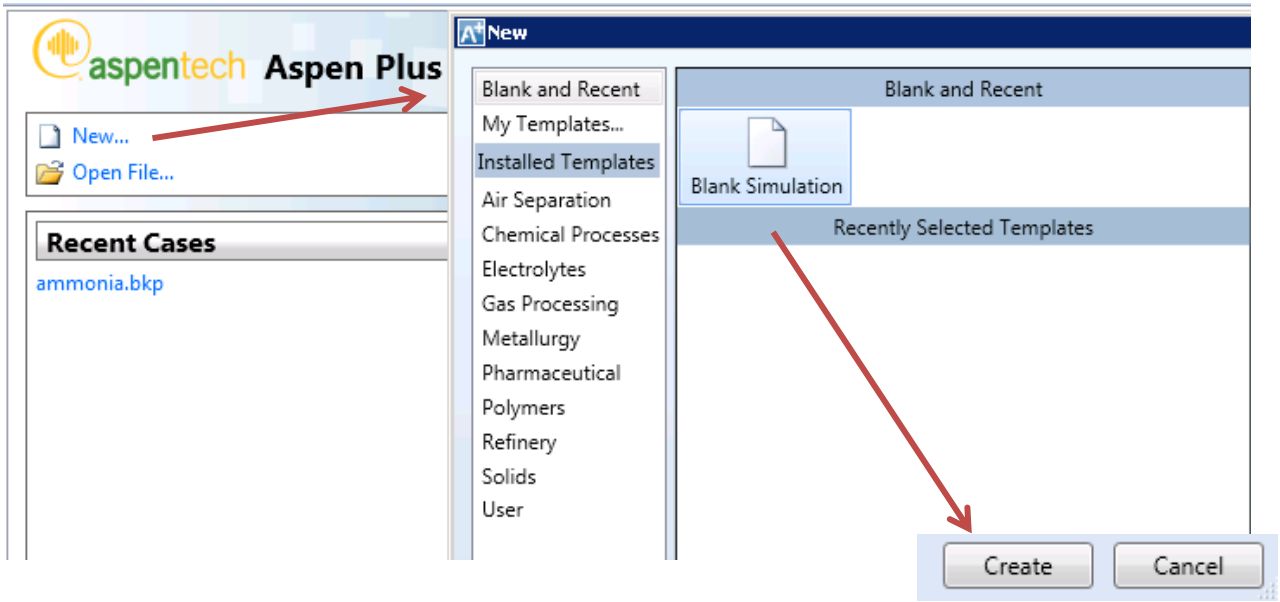
(3) Kinetic-Based, aka. Rate-Based (RCSTR, RPLUG, RBATCH) - These reactor models are appropriate when you know the reaction kinetics. You describe kinetics using one of the built-in reaction models (power law, LHHW, etc.) or your own user-defined kinetic subroutine. RBATCH and RCSTR are able to represent reactors with solid-phase catalysts. RPLUG can represent tubular or multi-tube plug flow reactors. RCSTR represents any well mixed stirred tank (or fluid bed) reactors. RBATCH is for batch reactors. These reactor models are more predictive, but they require more information to describe reaction rates.

The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.

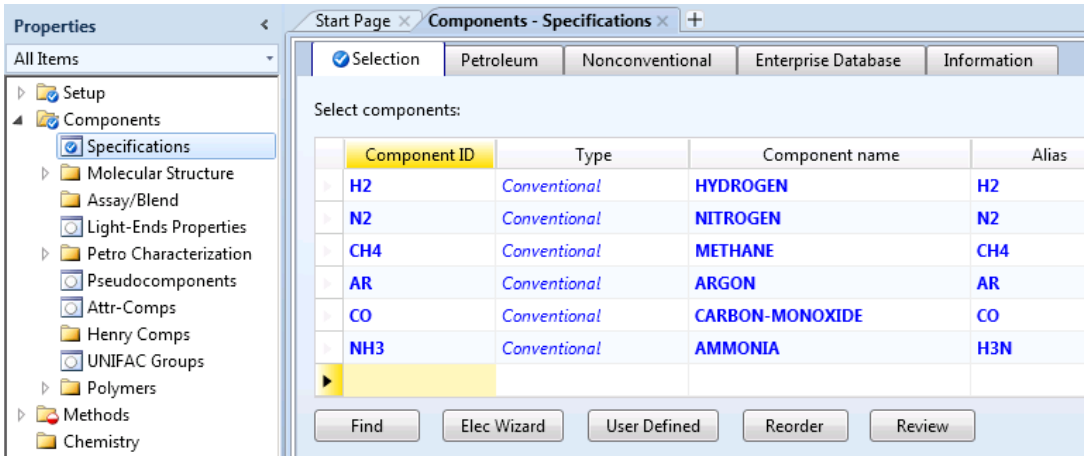
4. Aspen Plus Solution

Build a Process Simulation for Ammonia Synthesis

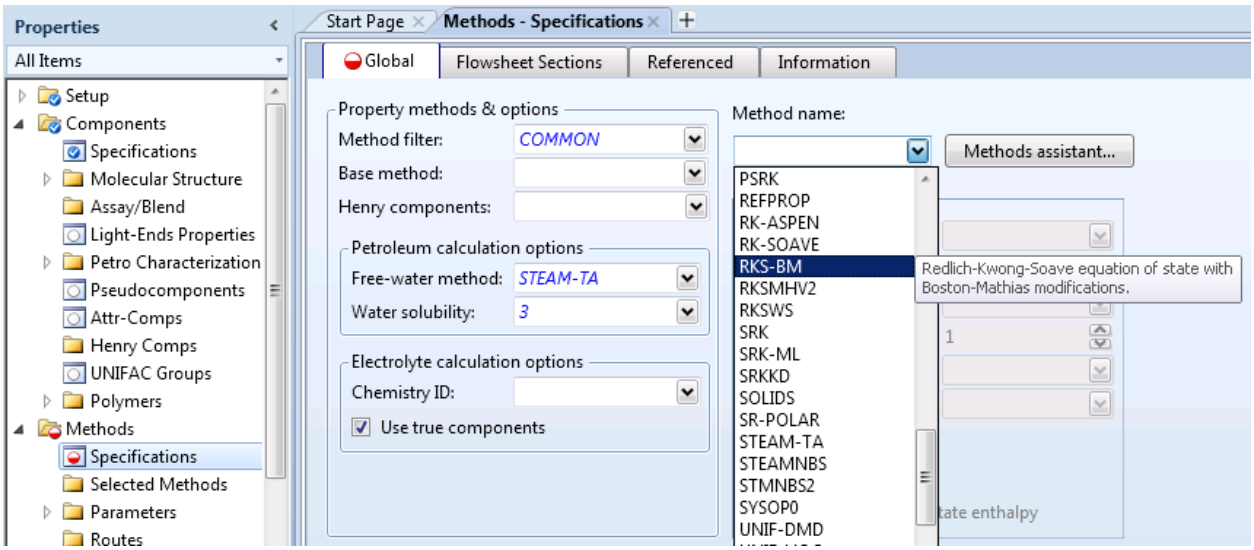
4.01. Start **Aspen Plus V8.0.** Select **New** on the **Start Page**, select **Blank and Recent** | **Blank Simulation**, press the **Create** button. We choose blank for this process because templates have default property methods, unit sets, and databanks selected. When using a specific method, such as RKS-BM, it is best to choose blank to ensure that the correct property method is selected.

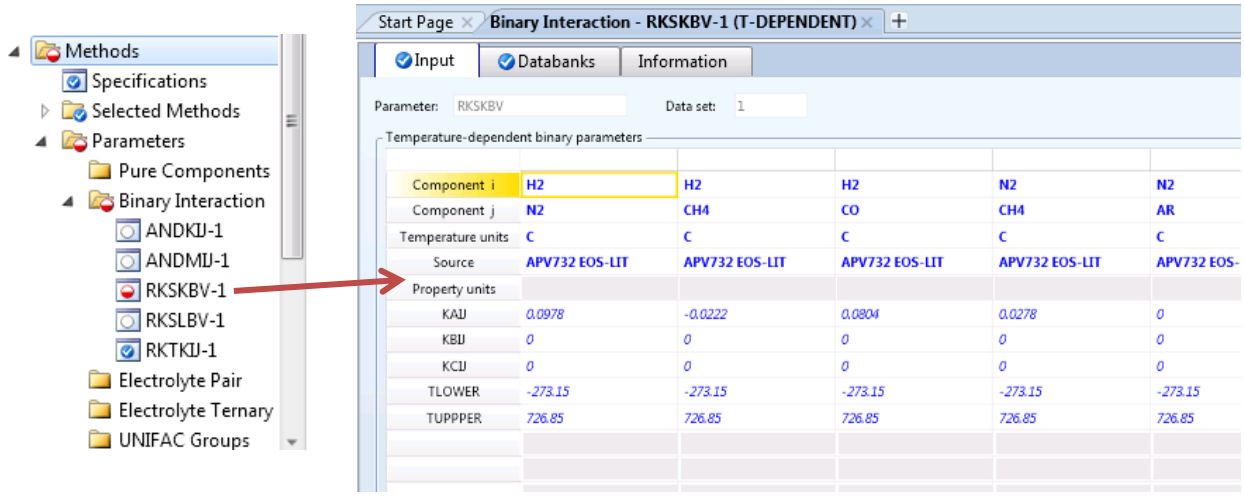


4.02. In **Properties** view, go to **Components | Specifications**, select components: **H2**, **N2**, **CH4**, **AR**, **CO**, and **NH3**.



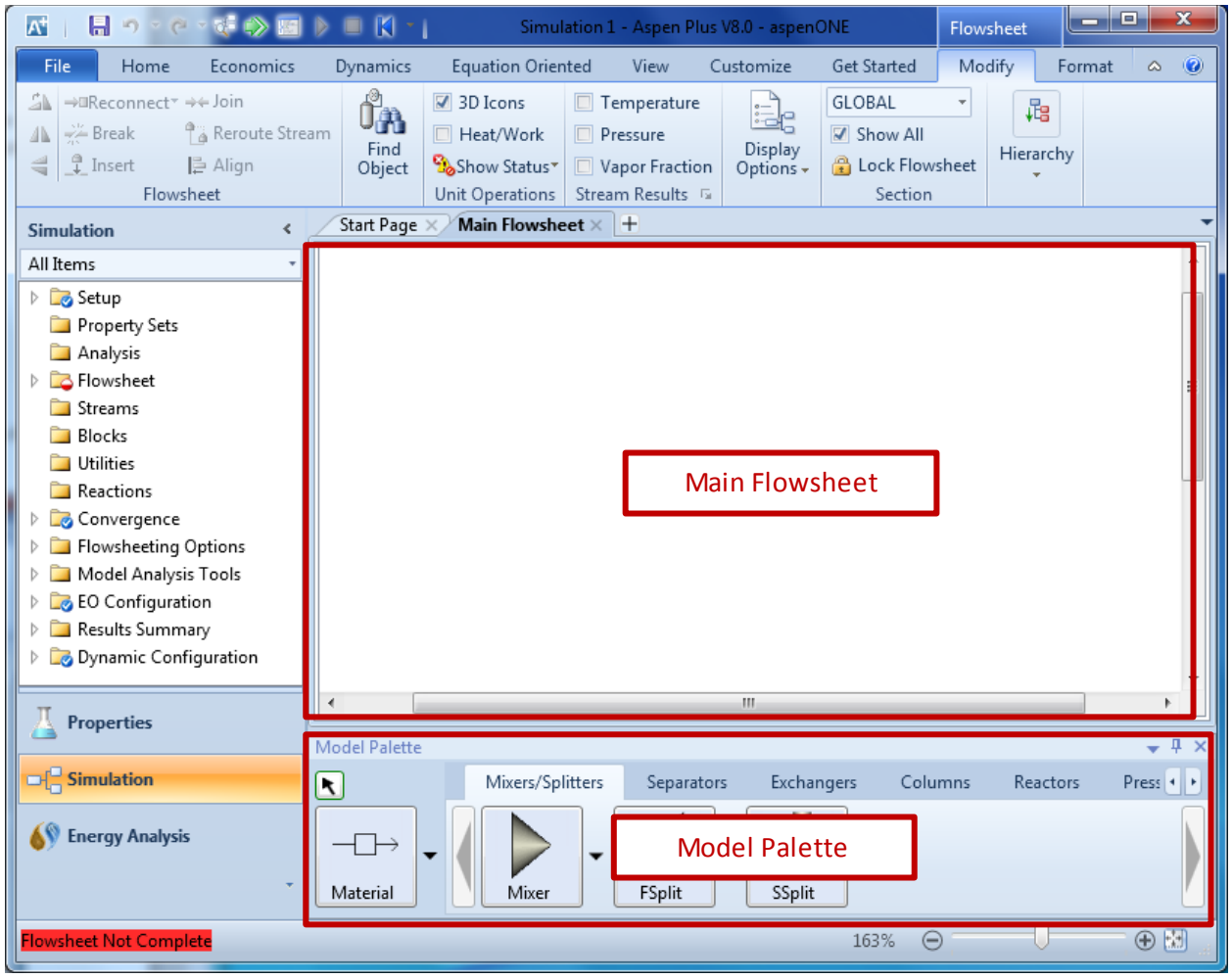
4.03. Go to **Methods | Specifications**. In the drop-down **Method name** combo box, find **RKS-BM** and select it. After that, click on **Methods | Parameters | Binary Interaction | RKSBV-1**, it will retrieve the binary interaction parameters to complete RKS-BM for use in the simulation. If these parameters do not populate, make sure that the databank **EOS-LIT** is selected in the **Databanks** tab under **RKSBV-1**.





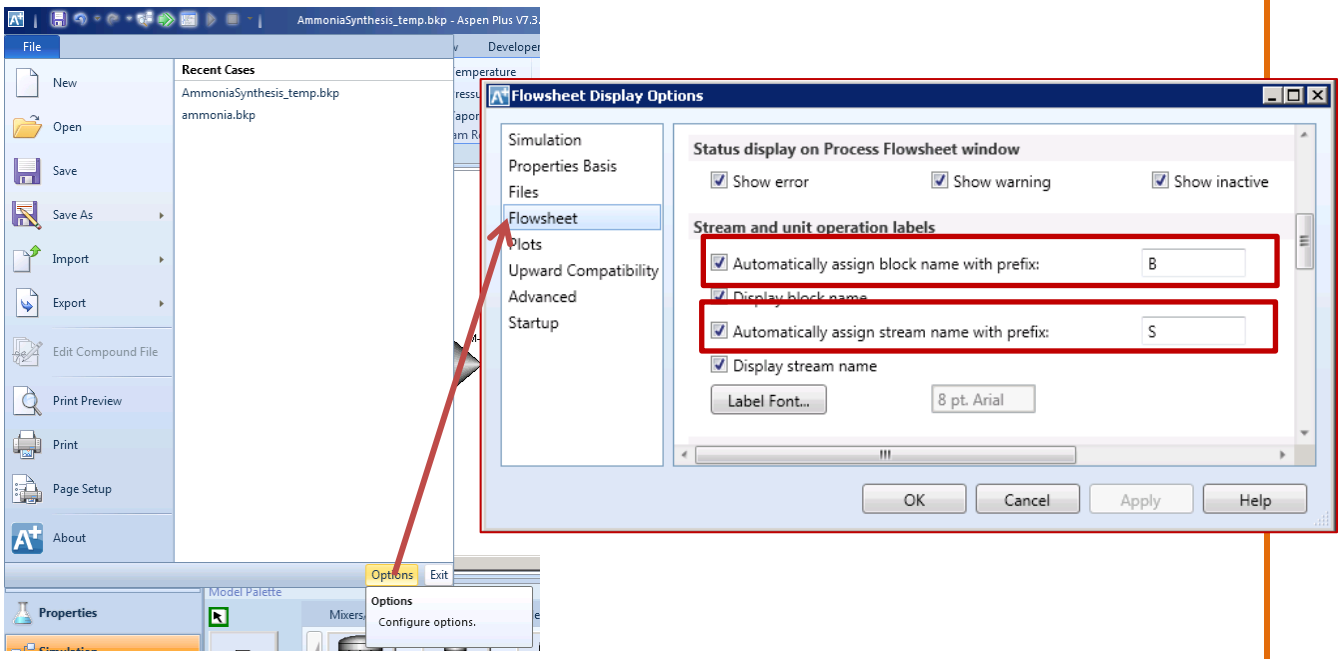
4.04. Go to the simulation environment. For that, click on the **Simulation** button in the bottom left of the screen. Then find the **Main Flowsheet** tab. The **Main Flowsheet** is the main simulation flowsheet where you will create a simulation.

4.05. In the **Simulation** view, you can find **Main Flowsheet** as well as **Model Palette (F10)** where you can find all the Aspen Plus models and streams.

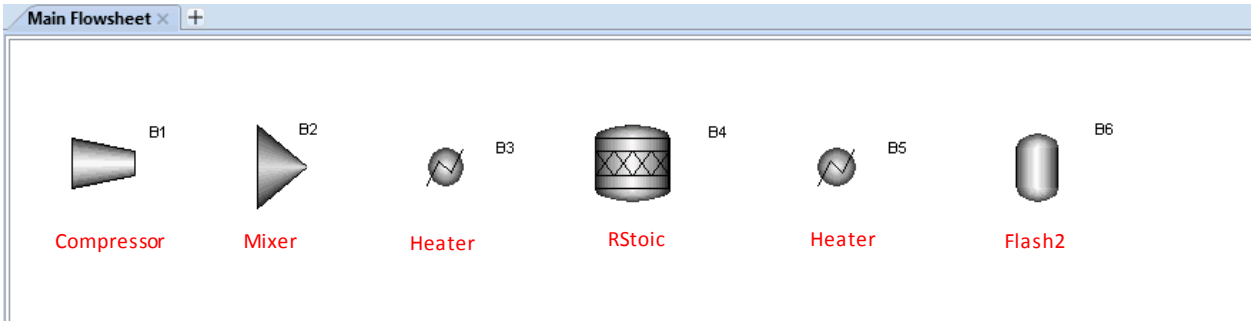


(FAQ) Useful Option To Know: Automatically Assign Block/Stream Name with Prefix

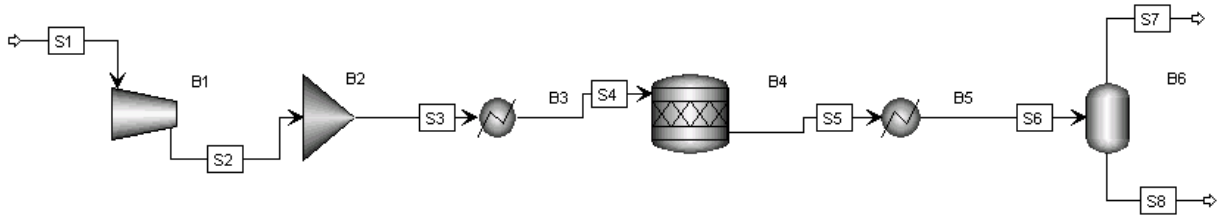
Description: Have blocks/streams automatically assigned a name beginning with the specified character string. For example, if B is entered for block's prefix, the blocks will be named B1, B2, B3, etc. By default, B is used for block's prefix and S is used for stream's prefix. When this option is off, Aspen Plus will prompt you to enter an ID each time a block or a stream is created. To enable and disable this option, go to File menu, find the Option button (as shown below), you could find two checkboxes to set these options on and off.



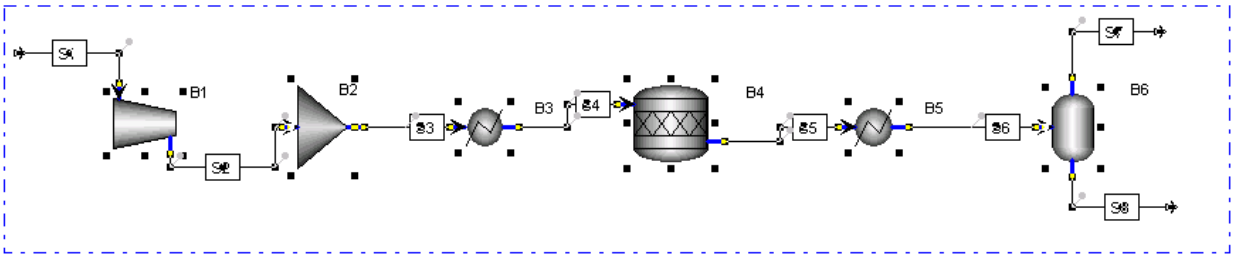
4.06. Find the following models from the **Model Palette**, and drop them onto the flowsheet.

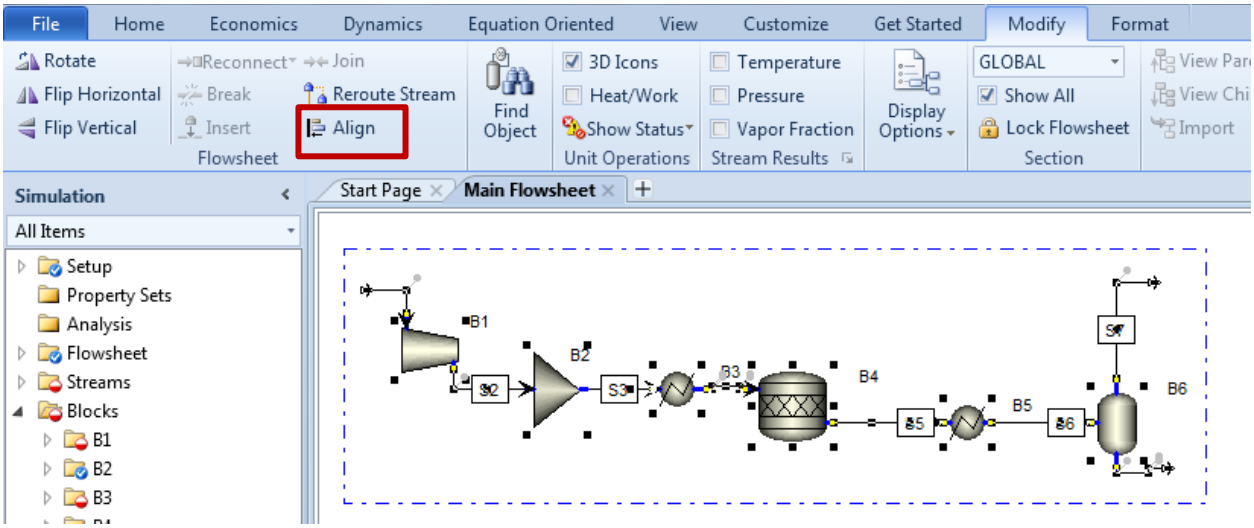


4.07. Find **Material Stream** from the **Model Palette**, and use it to connect model blocks.

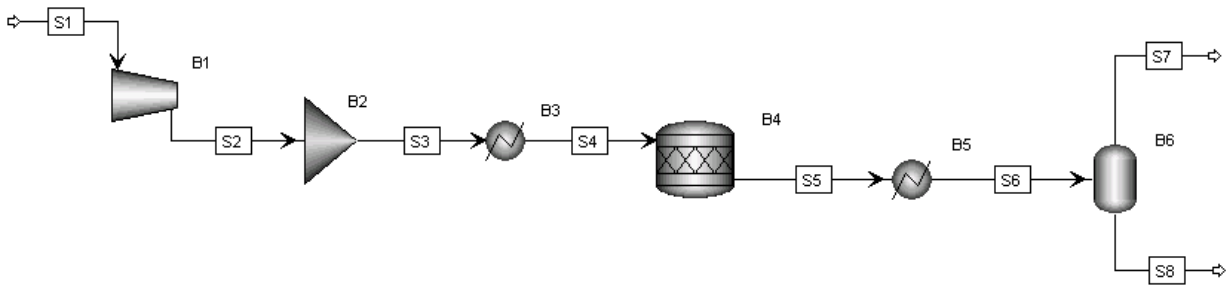


4.08. Select all blocks and streams; and find **Align (Ctrl + B)** to align all blocks automatically. You can also right click a stream and select **Align**, or select a section of the flowsheet and right click to select **Align**. You could try **Reroute Stream (Ctrl + J)** to reroute streams. These tools will help you to manage flowsheets and keep them organized and easy to read.

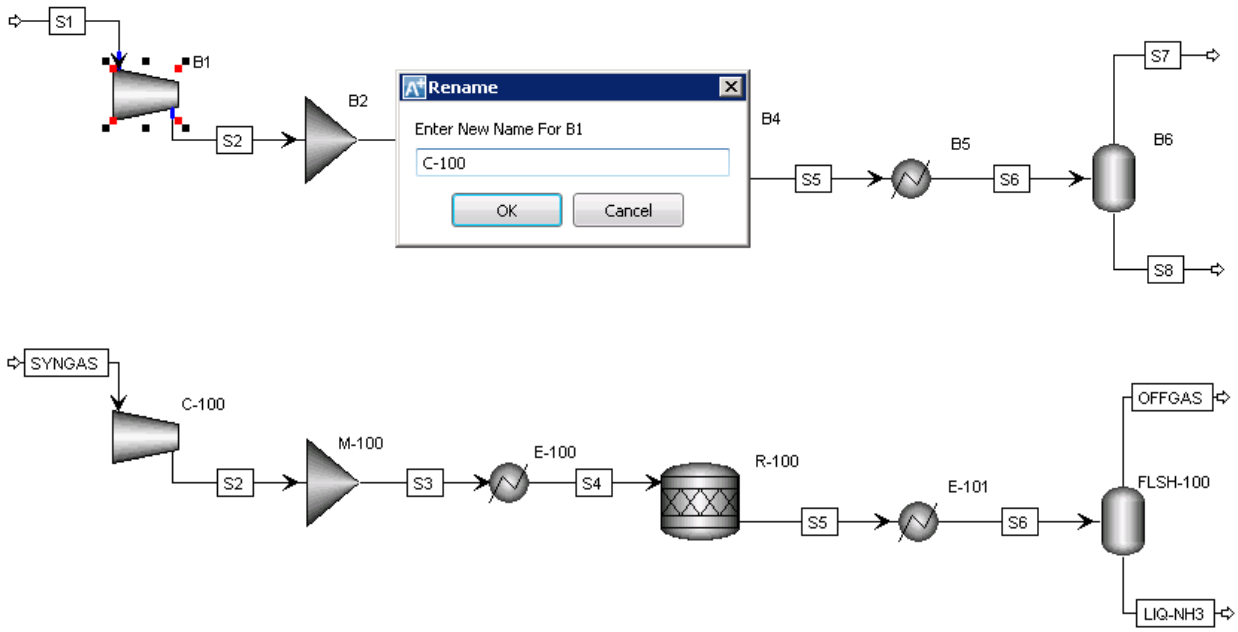




4.09. Make your simulation flowsheet as neat as possible. It is a very good habit that will really help you in the future when you need to deal with very complex simulations, which can include hundreds of model blocks on a single flowsheet.

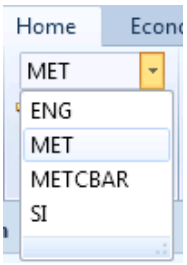


4.10. Also it is good to provide a meaningful name for each model block. For instance, use C-xxx for compressor, M-xxx for mixer, E-xxx for heat exchanger or heater, etc. Press **Ctrl + M** to rename a block. Also rename feed and product streams as shown below.

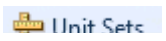


(FAQ) How to Change Unit of Measure

Description: A units set is a collection of unit specifications for each dimensional quantity used in Aspen Plus. Aspen Plus provides these basic units sets: International system units (SI), English engineering units (ENG), and Metric engineering units (MET). You can change the global unit set in the ribbon. Use the units selector on the Home tab to select a unit set:



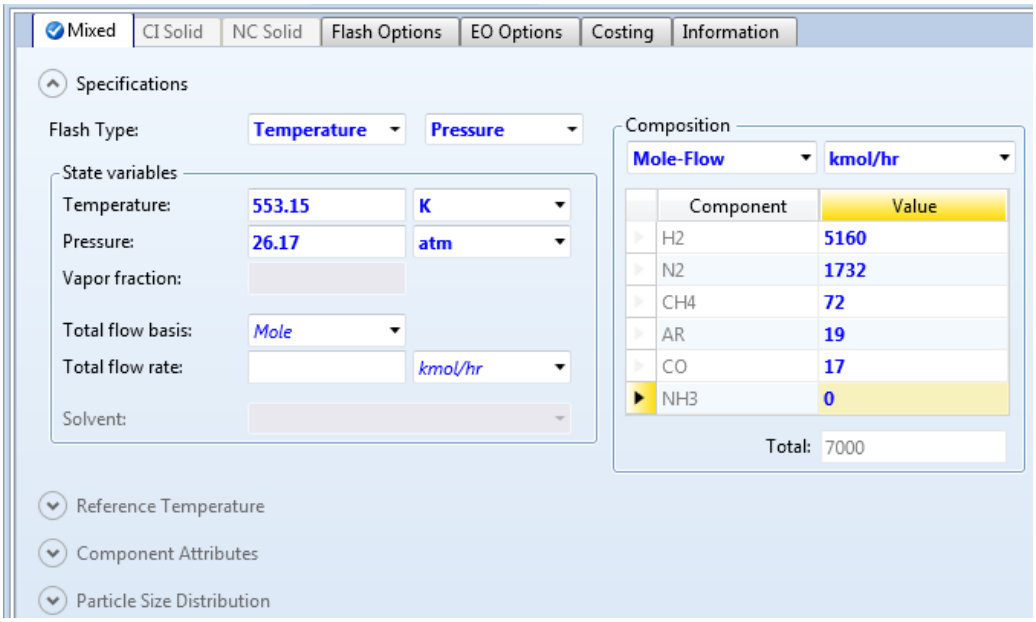
Tip: In the Home tab ribbon, find Unit Sets button to create your own unit sets.



This unit set specification applies to all forms. When you change these units, Aspen Plus changes the units on all forms to the ones from the specified units set, and converts the values.

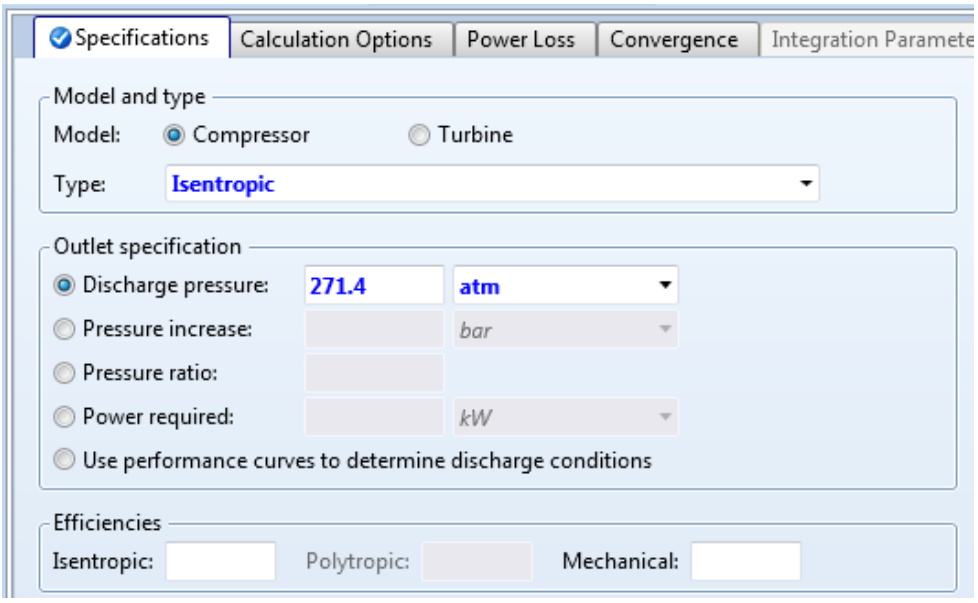
4.11. Specify feed stream (**SYNGAS**). Double click on the stream labeled **SYNGAS** on the main flowsheet or navigate to **Streams | SYNGAS | Input**.

- **T = 553.15 K, P = 26.17 atm**
- **Component Mole-Flow:** H2 = 5160 kmol/hr, N2 = 1732 kmol/hr, CH4 = 72 kmol/hr, AR = 19 kmol/hr, CO = 17 kmol/hr



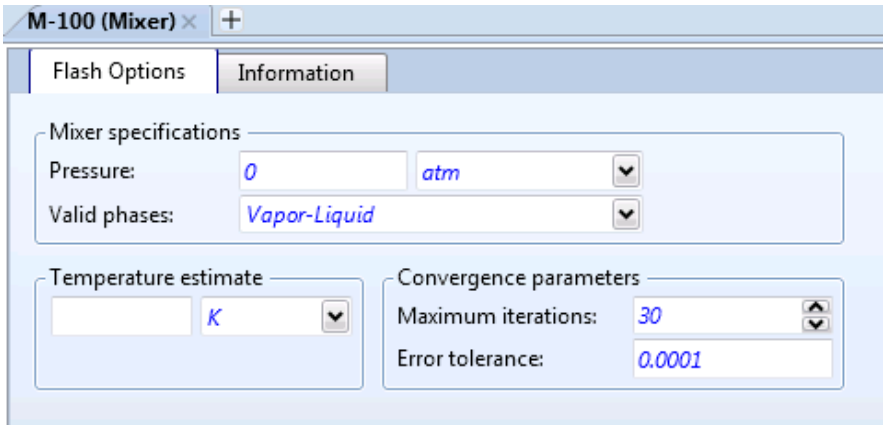
4.12. Configure/Specify Compressor (**C-100**). Double click the compressor block (**C-100**) or navigate to **Blocks | C-100 | Setup.**

- **Isentropic Compressor**
- **Discharge pressure = 271.4 atm**



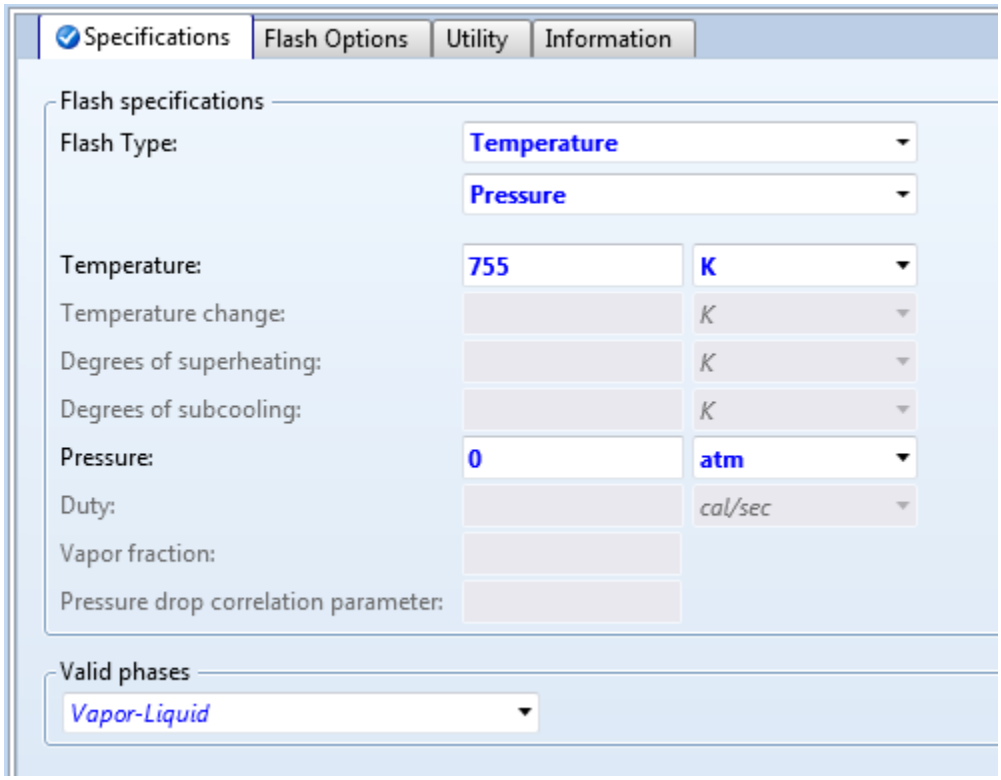
4.13. Configure/Specify Mixer (**M-100**). Double click on the mixer block (**M-100**) or navigate to **Blocks | M-100 | Input**.

- Verify that the input sheet contains a **0** in the **Pressure** spec. Note that in the Pressure field, if you enter a number greater than 0, this will be the discharge or operating pressure. If you enter a number less than or equal to zero, this will be the pressure drop through the unit.



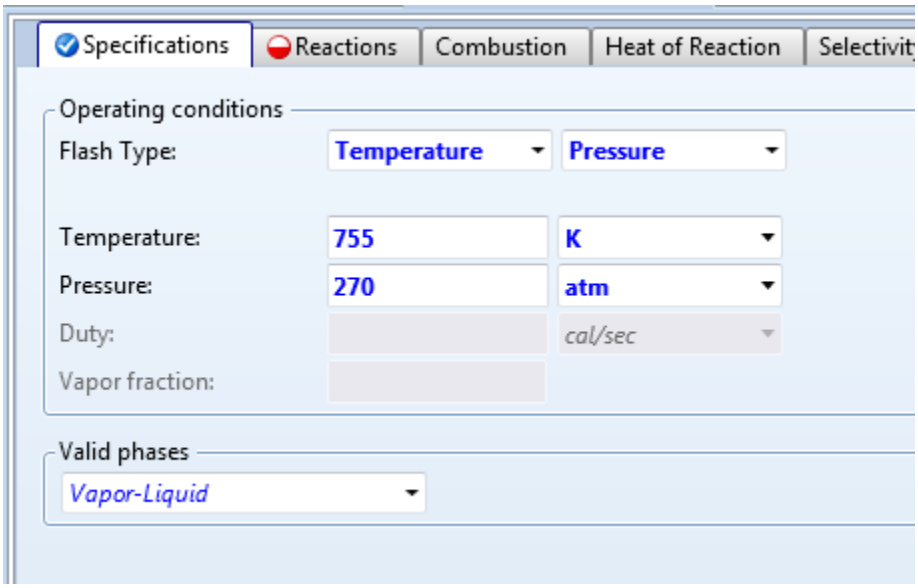
4.14. Configure/Specify Heater (**E-100**). Double click on the heater block (**E-100**) or navigate to **Blocks | E-100 | Input**.

- **Temperature = 755 K** (Outlet temperature)
- Heater with zero pressure drop – enter **0** in the **Pressure** spec



4.15. Configure/Specify Reactor (**R-100**). Double click the reactor (R-100) or navigate to **Blocks | R-100 | Setup**.

- Reaction temperature and pressure: **755 K**, **270 atm**

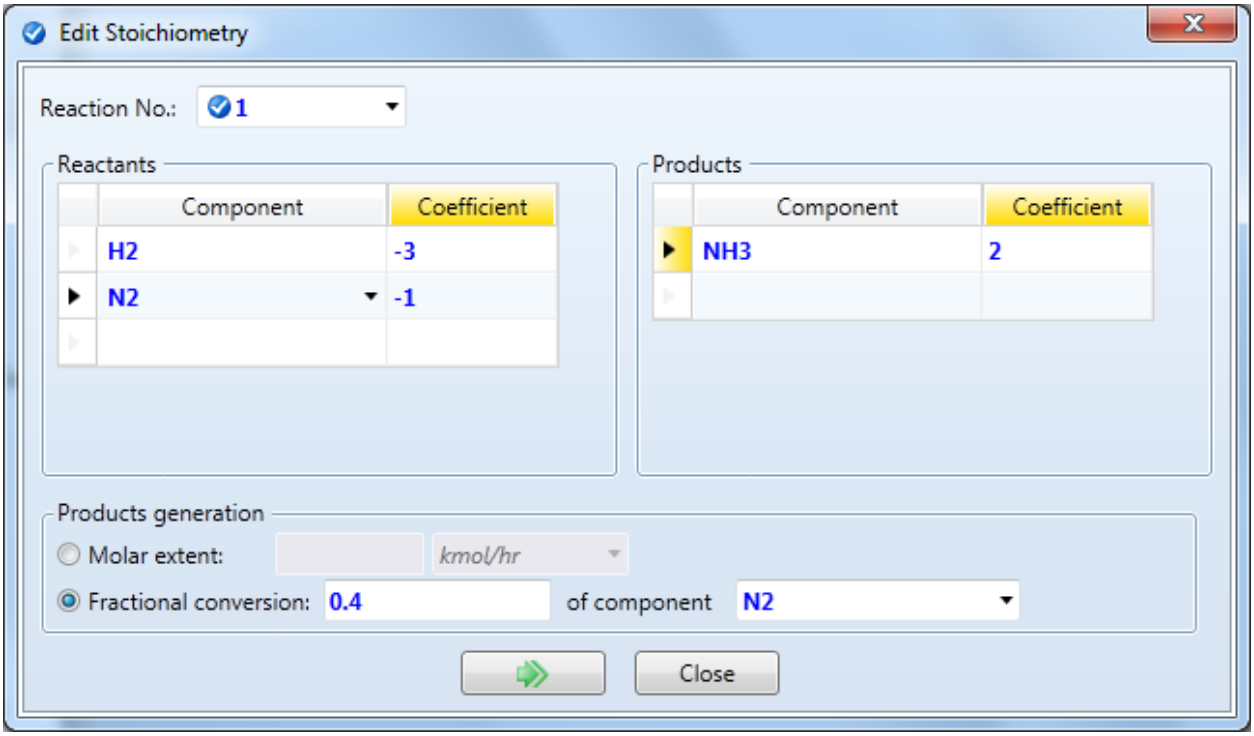


4.16. Go to the **Reactions** tab and click **New** to specify the reaction.

- Reaction **Stoichiometric Coefficients**: N2=-1, H2 = -3, NH3 = +2

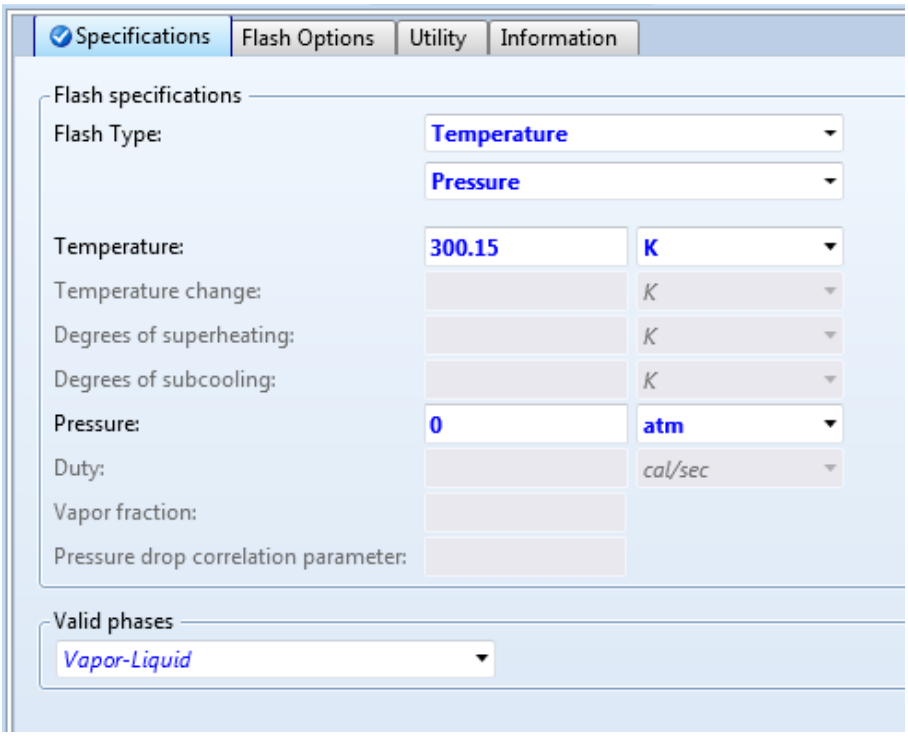
$$N_2 + 3H_2 = 2NH_3$$

- Specify Product Regeneration: **Fractional conversion** = **40%** of the reactant **N2**



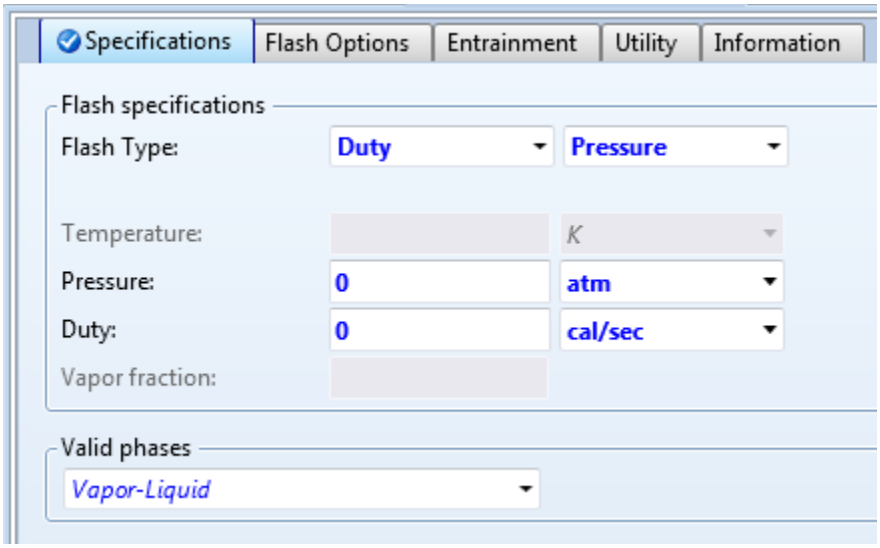
4.17. Configure/Specify Heater (**E-101**). Double click on the heater (**E-101**) or navigate to **Blocks | E-101 | Input**.

- Actually, this is a 'cooler', cooling to **300.15 K**
- No pressure drop – enter **0** for the **Pressure** spec



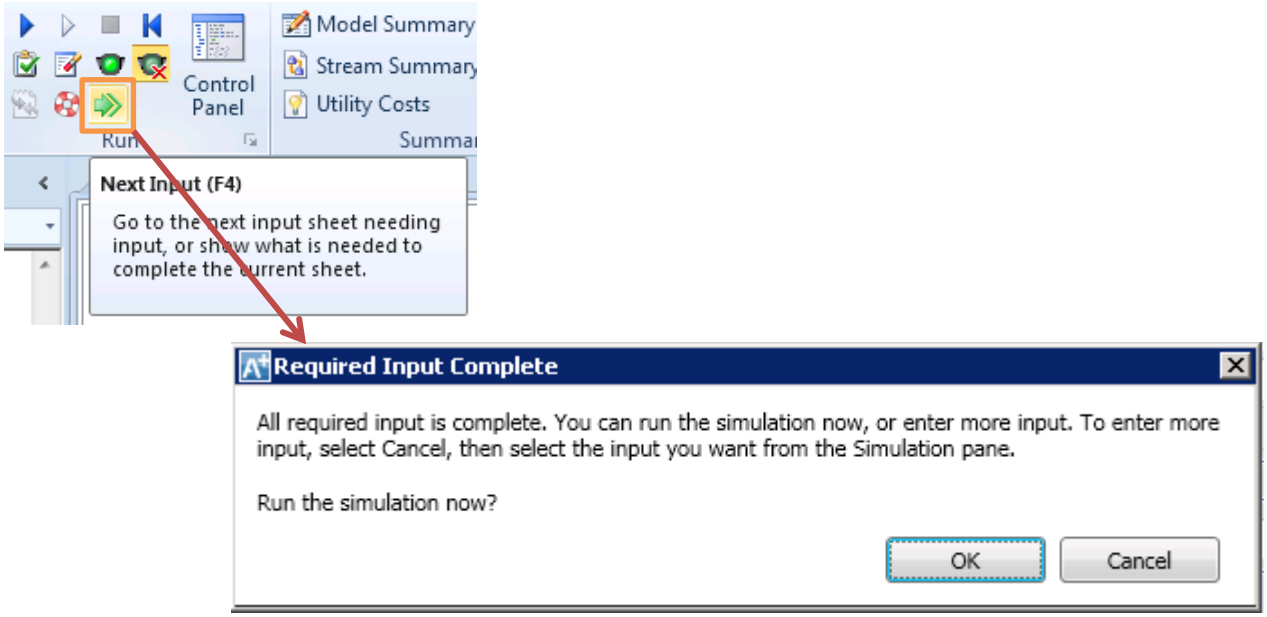
4.18. Configure/Specify Flash Drum (**FLSH-100**). Double click the flash drum (**FLSH-100**) or navigate to **Blocks | FLSH-100 | Input**.

- No additional heat; **Heat Duty = 0**
- No pressure drop – enter **0** for the **Pressure** spec

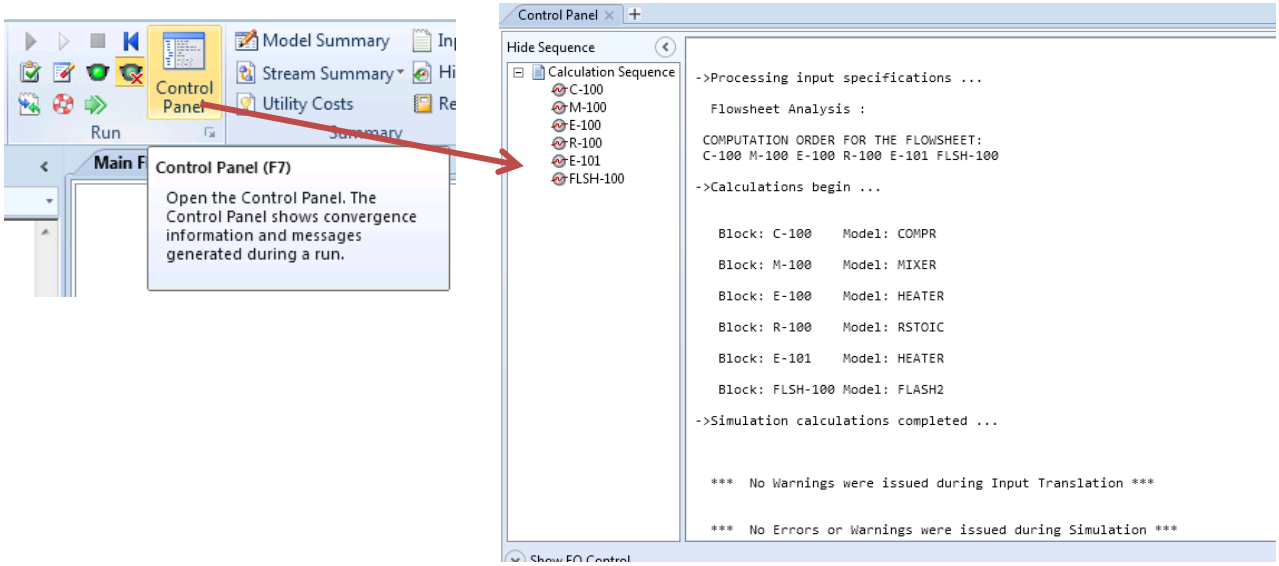


4.19. Check if the simulation is all set to run:

- Your simulation should be all set to run. To check if you have missed any data to enter, press **Next Input (F4)** button in the **Home** ribbon:

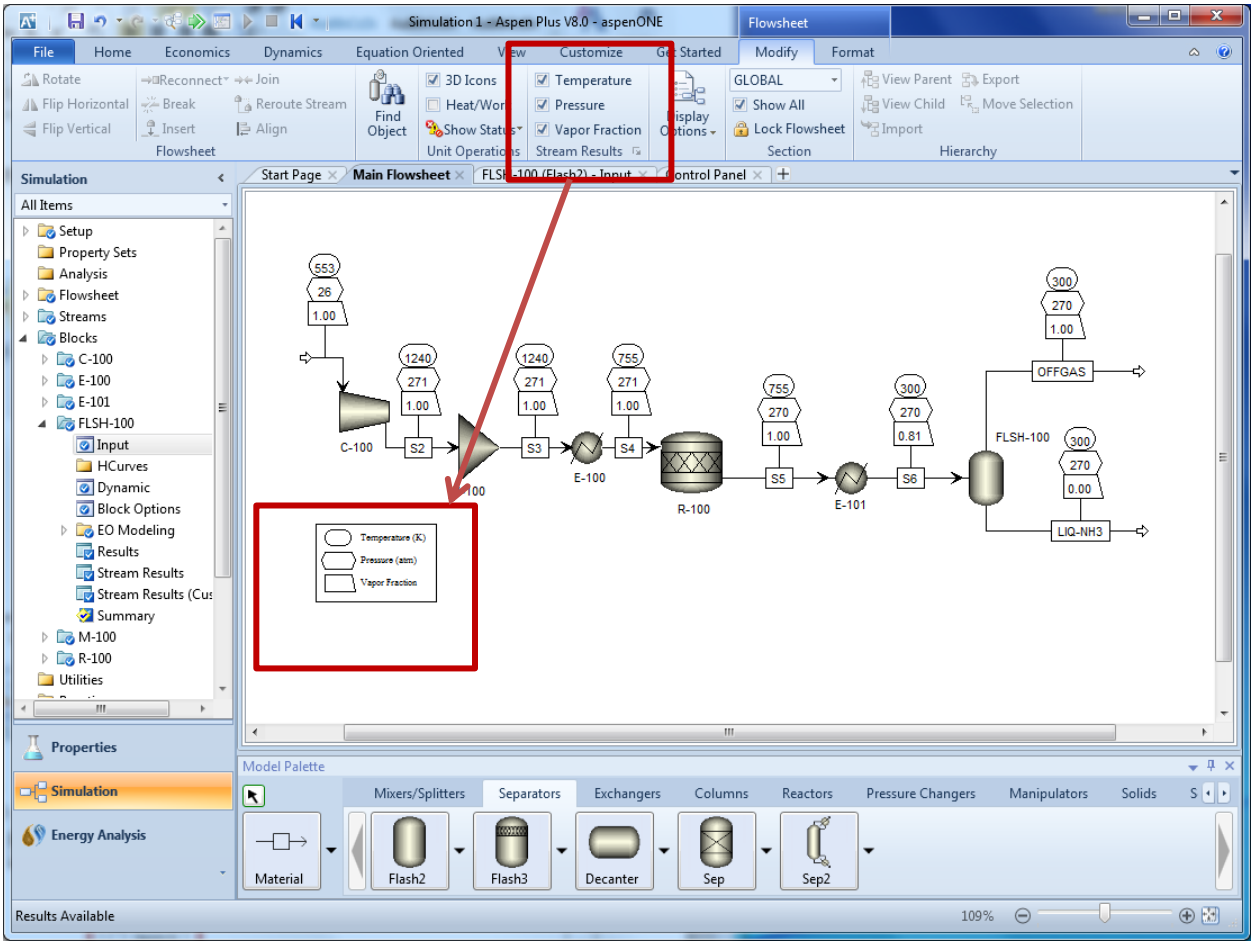


4.20. Click **OK** to run the simulation. Open **Control Panel (F7)** to check if the simulation calculations completed with or without any errors or warning.



4.21. Review simulation results:

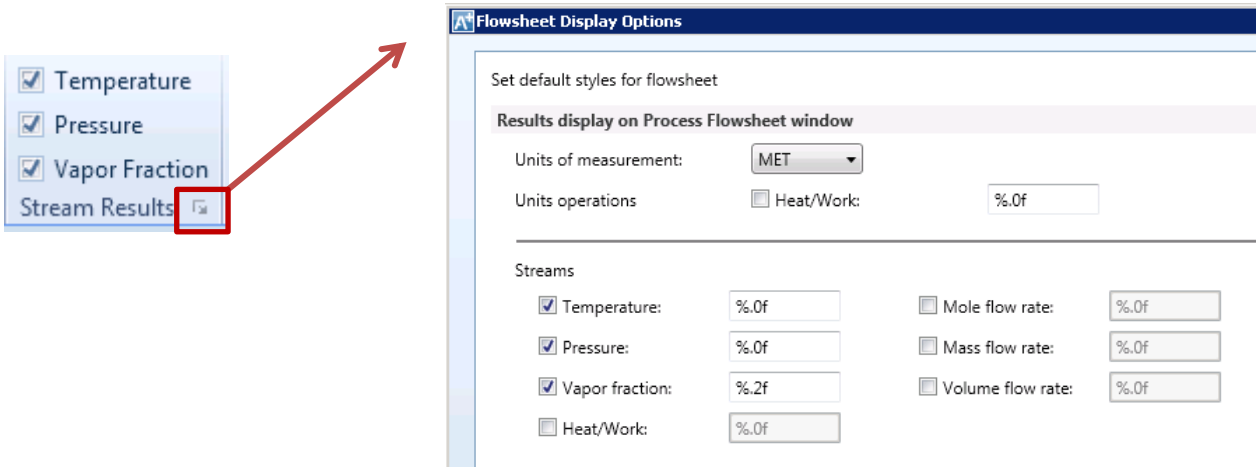
- Display Stream Results on Flowsheet



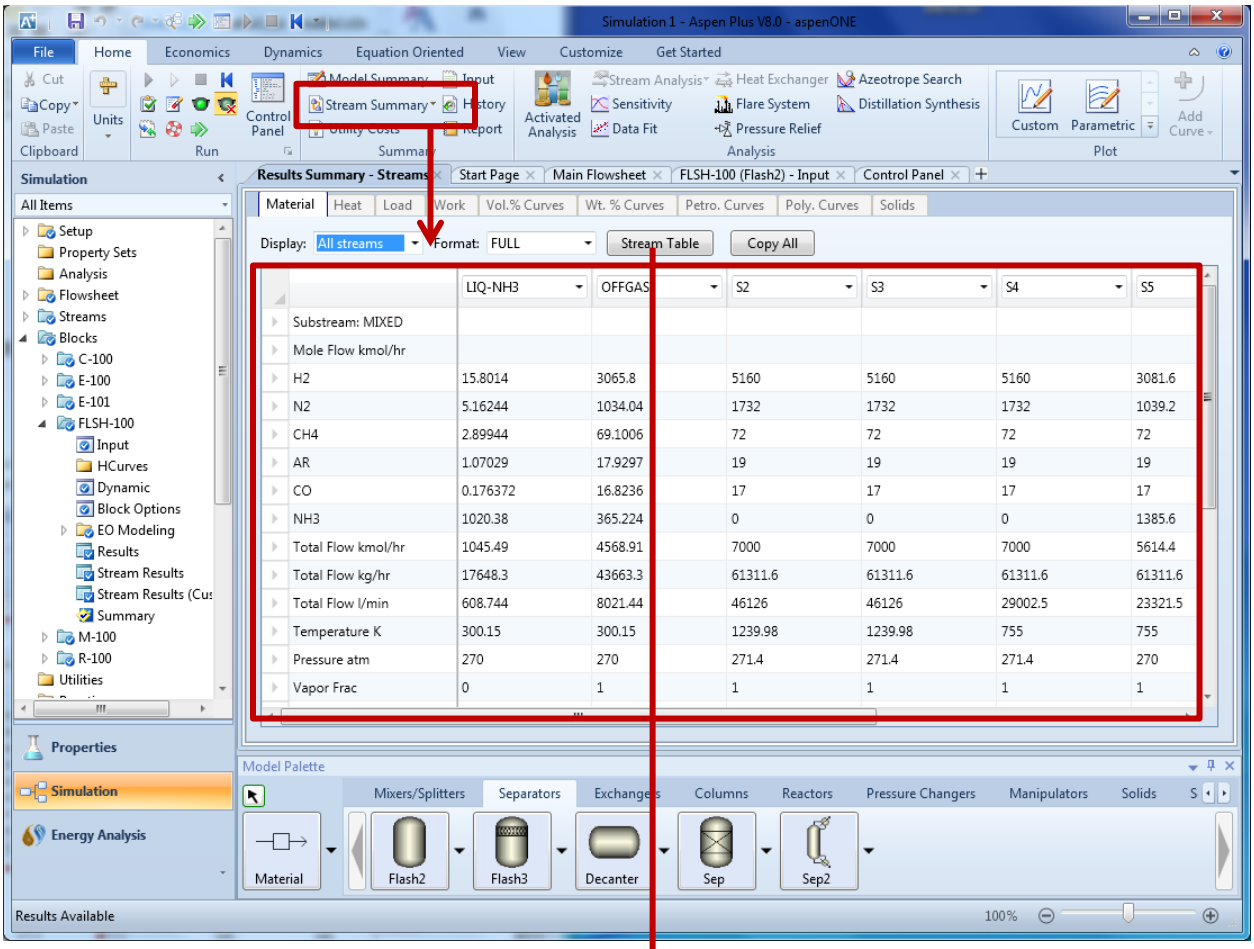
(FAQ) Flowsheet Display Option – Enabling More Stream Results Visible on Flowsheet

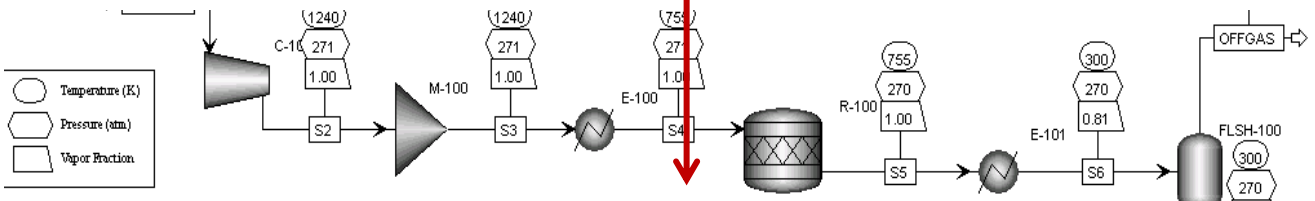
Description: In the Modify ribbon, you can access the 'Flowsheet Display Option' which allows you to change the following results to visible or invisible.

- Temperature, Pressure, Vapor Fraction
- Heat/Work
- Mole flow rate, Mass flow rate, Volume flow rate



4.22. Use **Stream Summary** to display all stream results in a single view: In the **Home** tab, find **Stream Summary** button in **Summary** group.





Heat and Material Balance Table									
Stream ID		LIQ-NH3	OFFGAS	S2	S3	S4	S5	S6	SYNGAS
Temperature	K	300.0	300.0	1240.0	1240.0	755.0	755.0	300.0	553.1
Pressure	atm	270.00	270.00	271.40	271.40	271.40	270.00	270.00	26.17
Vapor Frac		0.000	1.000	1.000	1.000	1.000	1.000	0.813	1.000
Mole Flow	kmol/hr	1047.101	4567.299	7000.000	7000.000	7000.000	5614.400	5614.400	7000.000
Mass Flow	kg/hr	17676.043	43635.513	61311.556	61311.556	61311.556	61311.556	61311.556	61311.556
Volume Flow	l/min	609.468	8015.722	46125.997	46125.997	29002.507	23321.537	8625.189	204640.320
Enthalpy	MMBtu/hr	-64.671	-23.035	187.074	187.074	86.341	14.587	-87.707	43.064
Mole Flow	kmol/hr								
H2		15.780	3065.820	5160.000	5160.000	5160.000	3081.600	3081.600	5160.000
N2		5.155	1034.045	1732.000	1732.000	1732.000	1039.200	1039.200	1732.000
CH4		2.902	69.098	72.000	72.000	72.000	72.000	72.000	72.000
AR		1.072	17.928	19.000	19.000	19.000	19.000	19.000	19.000
CO		0.176	16.824	17.000	17.000	17.000	17.000	17.000	17.000
NH3		1022.015	363.585				1385.600	1385.600	

4.23. After completing this simulation, you should save the file as a .bkp file. It is also good practice to save periodically as you create a simulation so you do not risk losing any work. The open loop simulation is now ready to add a recycle stream, which we will then call a closed loop simulation. See module **Design-002** for the closed loop design.

5. Copyright