Stoichiometric Reactors: Aspen Plus 12.1

In this session you will learn how to install a stoichiometric (conversion) reactor in Aspen Plus 12.1

The reference for this section is the Aspen Plus 12.1 Unit Operation Models Chapter 5, Reactors.

Reactors

Model	Description	Purpose	Use For
RStoic	Stoichiometric reactor	Models stoichiometric reactor with specified reaction extent or conversion	Reactors where reaction kinetics are unknown or unimportant but stoichiometry and extent of reaction are known
RPlug	Plug flow reactor	Models plug flow reactor	One-, two-, or three-phase plug flow reactors with rate-controlled reactions in any phase based on known stoichiometry and kinetics
RGibbs	Equilibrium reactor with Gibbs energy Minimization	Performs chemical and phase equilibrium by Gibbs energy minimization	Reactors with phase equilibrium or simultaneous phase and chemical equilibrium. Calculating phase equilibrium for solid solutions and vapor-liquid- solid systems.

Use RStoic to model a reactor when:

- Reaction kinetics are unknown or unimportant and
- Stoichiometry and the molar extent or conversion is known for each reaction

RStoic can model reactions occurring simultaneously or sequentially. In addition, RStoic can perform product selectivity and heat of reaction calculations.

Specifying RStoic (From RStoic reference)

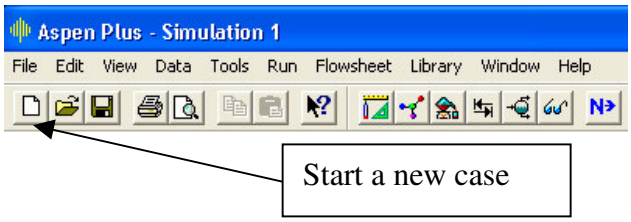
Use the Setup Specifications sheet to specify the reactor operating conditions and to select the phases to consider in flash calculations in the reactor.

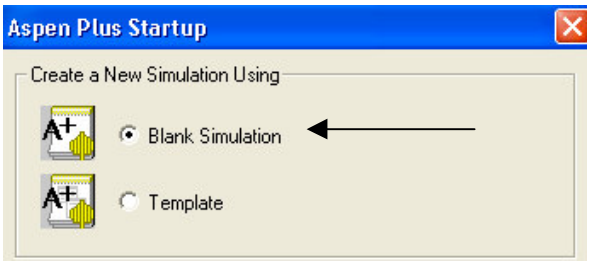
Use the Setup Reactions sheet to define the reactions occurring in the reactor. You must specify the stoichiometry for each reaction. In addition, you must specify either the molar extent or the fractional conversion for all reactions. Alternatively, you can use the Setup Combustion sheet to have RStoic generate combustion reactions.

Aspen Plus Stoichiometric Reactors – Tutorial on Styrene

Styrene is a monomer used in the production of many plastics. It has the fourth highest production rate behind the monomers of ethylene, vinyl chloride and propylene. Styrene is made from the dehydrogenation of ethylbenzene:

$$C_6H_5 - C_2H_5 \Leftrightarrow C_6H_5 - CH = CH_2 + H_2$$



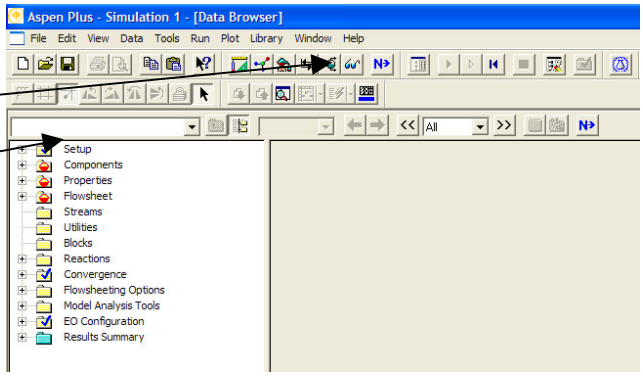


In this tutorial, you will install a stoichiometric reactor to be run both isothermally and adiabatically. The goal of the exercise will be to explore the effect of conversion of ethylbenzene on the heat duty of an isothermal reactor (at 250°C) in Case 1, and the effect of inlet temperature on the outlet temperature at conversion of 80% ethylbenzene in Case 2.

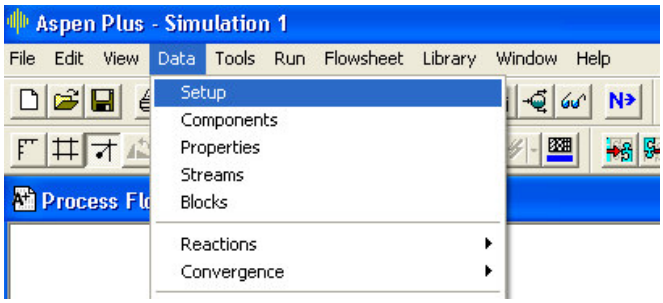
Procedure to Install a Stoichiometric Reaction Set:

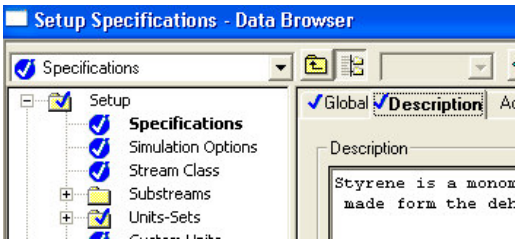
1. Start Aspen Plus 12.1
   Open a new case by clicking on the blank white page or use the commands *File New* or by choosing the blank simulation option. Alternatively, you may choose the template option. The most appropriate template for most applications is *Specialty Chemicals in Metric Units*.

2. Choose *Data* from the main menu and click *Setup,* or use *Data Browser* from the eyeglass icon, and select Setup.

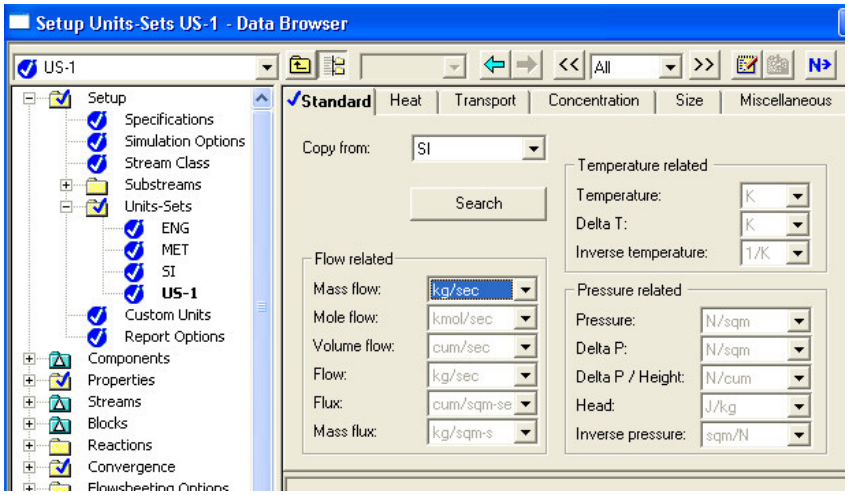


   - Select *Specifications*, and you may enter a title in the *Title* field, and a brief description of the process by choosing the *Description* tab. You should also specify input and output units for your simulation



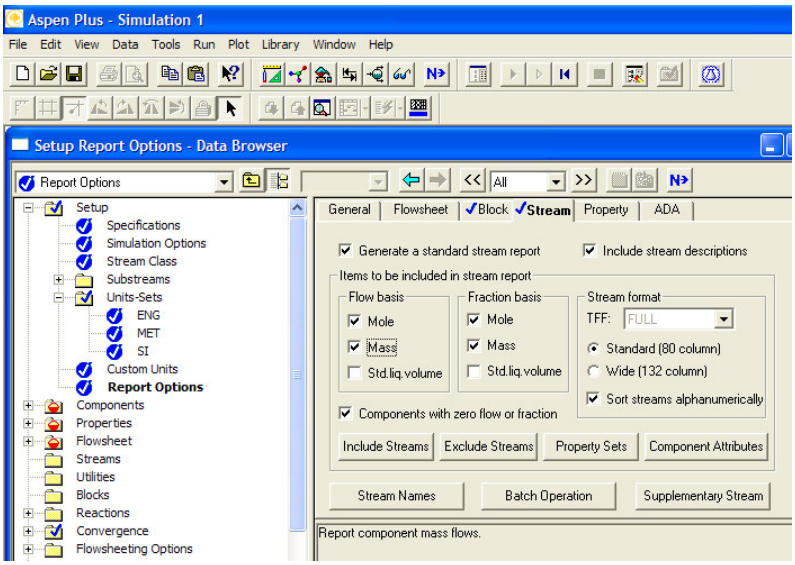


3. You may choose your own Units Set by choosing *Setup / Unit sets* and then choose *New*. Name the new unit set and then click ok. You have an option to set the new unit set as the *Global unit set*. If you have started your simulation using a template, a unit set will be assumed.



To setup custom unit sets

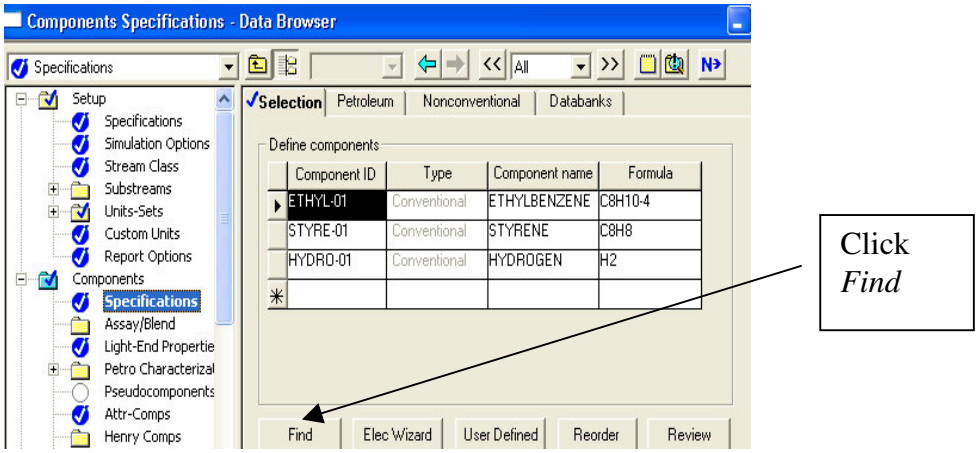
4. Before proceeding, move to *Report Options* where you can specify the information provided to your final report. Under the *Stream* tab, select both mole and mass in the flow basis field as well as the fraction basis field. Close the *Setup* section.

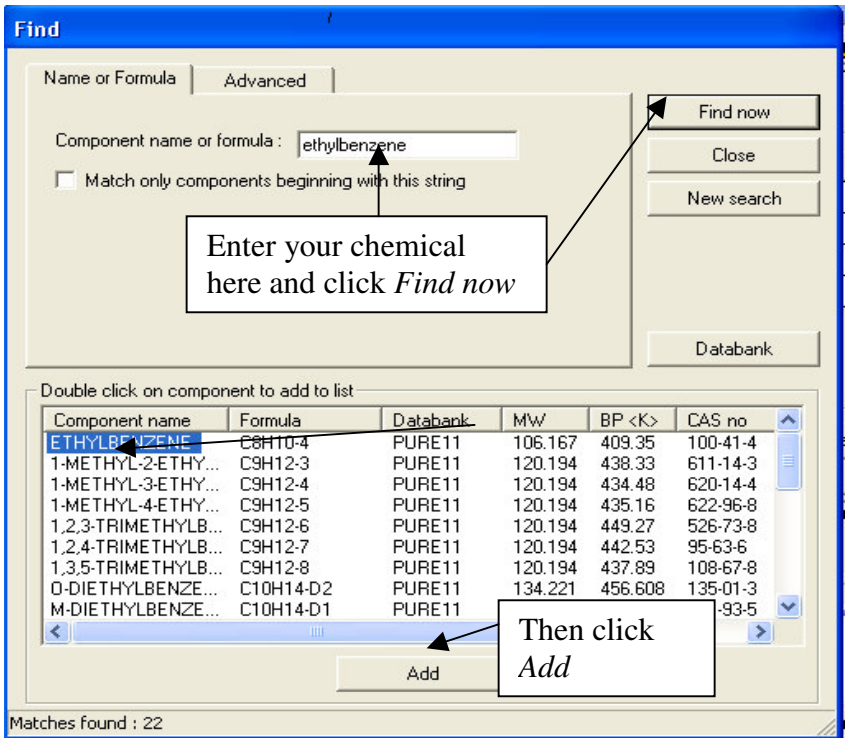


Click  . It takes you to next Input step.

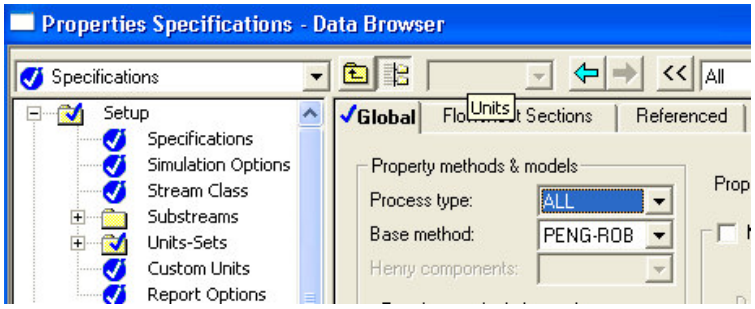
5. Choose *Components* option in the data browser window to start adding chemical components, and select *Specifications*. The *Databanks* tab shows the preferred databanks from which Aspen will draw physical and thermodynamic properties. For most cases, we will use the default selection.

6. Next elect the chemicals for a your reaction systems, using the *Selection* tab. Use the *Find* button to search for components for this problem, styrene, ethylbenzene, and hydrogen. Select your component from the list, and then *Add* it. When finished, close the *Components* section.

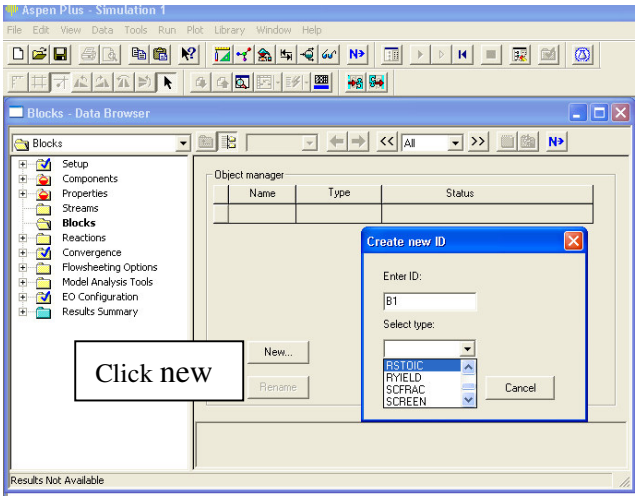


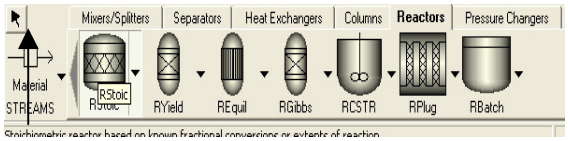


7. Next, select as base method for system properties, by selecting *Properties, Specifications*. Since these compounds are hydrocarbons, use the Peng-Robinson thermodynamic package by selecting PENG-ROB under the *Base method* tab. (*Additional information on Aspen Plus thermodynamics packages can be found in aspen Plus User guide. Chapter 28:Property sets).* Close the *Properties* section and the *Data Browser*.



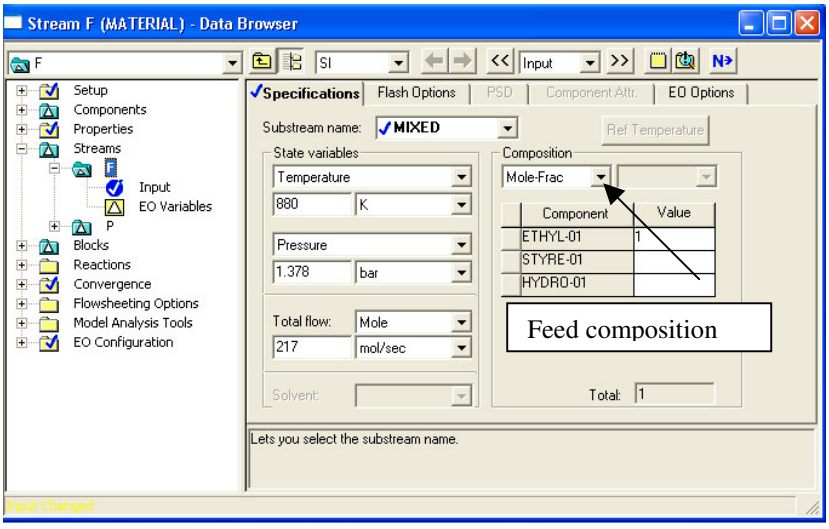
8. You are now ready to setup your flowsheet. Install the stoichiometric (conversion) reactor using the RStoic reactor block, either through the
   - 8.1 *Data, Blocks, New*
   - 8.2 Or from the *Model Library*, click on *Reactors* and then choose *RStoic*. Click on the *RStoic* icon, then release left mouse button. Move cursor to pfd screen and then press left mouse button only once. Double click on the reactor to open and specify details. Rename the reactor using a descriptive name by right clicking and selecting *Rename Block*.





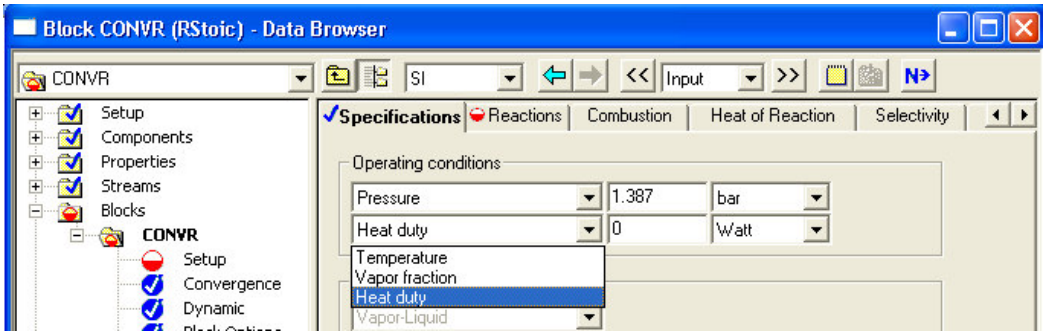
After adding the reactor, click the small arrow on the left bottom corner of the Aspen Plus Process Flowsheet Window.

9. To add feed and effluent streams, use the *Model Library* to select the *Material STREAMS* tab and click once. This will allow you to place multiple streams as needed. Move the cursor, now a crosshair, onto the process flowsheet. Click once, drag the cursor to connect the first stream to the feed port of your vessel (shown in red) and click again. You have just created stream 1. Add outlet stream to the reactor in a similar way. To modify your stream connections, select the small arrow, right click on the stream in question as select *Reconnect Source* or *Reconnect Destination.*
10. Specify the feed stream (Double click on the stream or right click on it and then choose input) having a composition of pure ethylbenzene at 217gmol/s, 880 K, 1.378 bar. Specify the feed composition as a mole fraction. Close the *Streams* tab.

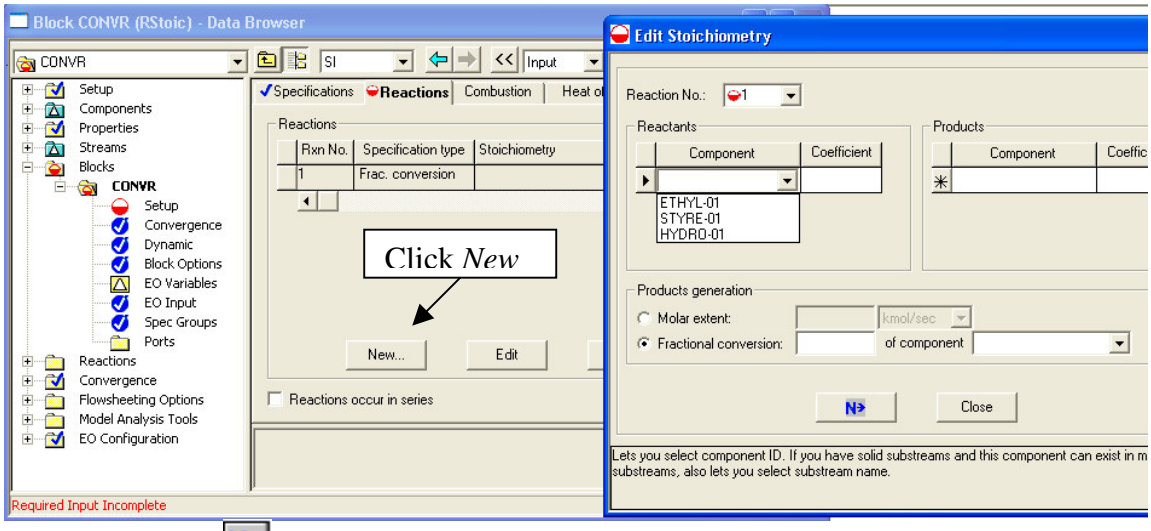


11. To input the reactor specifications, double click on the reactor block. The reactor *Data Browser* opens. You can input values for pressure, temperature, heat duty, vapor fraction (You need to input values for only two variables –Use the drop down list). For an isothermal reactor specify the outlet temperature and for the adiabatic

reactor specify the heat duty as zero. For this first case, enter pressure and temperature. Click  or the *Reactions* tab.



12. Click *New*, choose the reactants and products using the drop down list, input the stochiometric coefficients and also specify the fractional conversion (0.8) and then click  .



Then click  in the Data Browser window. A dialog box opens saying "All required input is complete'. Run the simulation by clicking ok.

13. To view the results right click on the reactor block and choose *Results*.
14. Save this simulation twice, as case 1 and case 2. Then proceed to the next steps for each case.

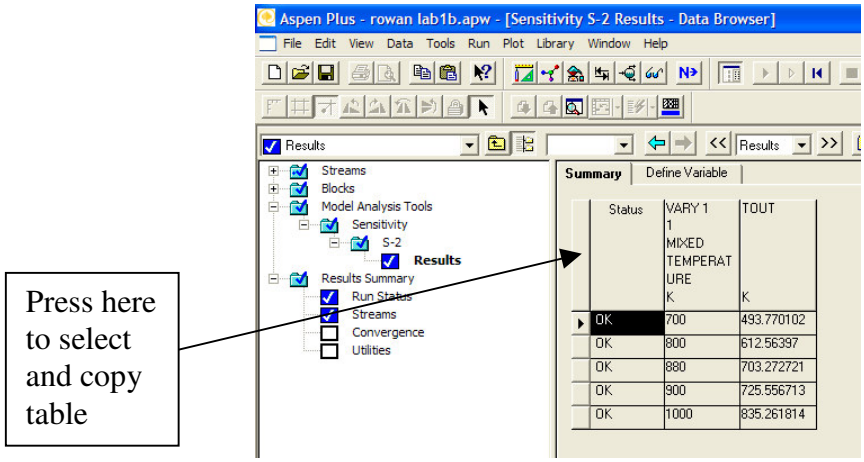
Next, let's explore the sensitivity of results to your input variables. We will examine the following:

Case 1) The effect of conversion of ethylbenzene on the heat duty of an isothermal reactor at a constant temperature of 250º C

Case 2) The effect of inlet temperature on outlet temperature for an adiabatic reactor at a conversion of 80%

15. Select the data browser, Model Analysis Tools, and Sensitivity. (Illustrated first for Case 1).
    a) Click New to create a new Sensitivity Block.
    b) Define the variables of interest, select New, create names for your variables, such as 'CONV' and 'DUTY'. A Variable Definition screen will pop-up. Select a Category (choose Blocks), Type (Block-Var). Identify the applicable block or stream, and then select variable. Choose CONV and NET-DUTY for conversion and Duty variables.
    c) Next, determine the manipulated variable (CONV & specified applicable reaction number (1) under ID1) using the VARY tab, and provide a range for variation.
    d) Finally, specify output varible for tabulation (the manipulated variable will be automatically tabulated). Tabulate the Heat Duty.
16. You will repeat this procedure for Case 2 using the 2nd previously saved simulation file.
    a) Define variables for inlet and outlet stream temperatures. The variable category in this case is Streams, and Variable Type is Stream-Var. To select variables, choose TEMP for inlet and outlet streams.
    b) Under VARY tab set up manipulated variable, in this case inlet T.
    c) Select variable to be tabulated – here as Outlet T.

17. At the end of each simulation run using the Sensitivity Analysis, create plots of the effect you explored in each case. To do so, view results under, Model Analysis, Sensitivity, and your sensitivity block, where you'll see a table of results. To copy this table to a spreadsheet, click on the upper left hand corner, then past into a spreadsheet. Create your graph from here.



18. To create a report file, for printing, select the File menu & Export. Under the Export screen choose Report Files (*.rep) as your file type and save.
19. At the end of this exercise submit a printout of the following:
    Make the following plots from your Conversion reactor simulation:
    a) The effect of conversion of ethylbenzene on the heat duty of an isothermal reactor at a constant temperature of 250º C

b) The effect of inlet temperature on outlet temperature for an adiabatic reactor at a conversion of 80%
c) Printout the report file for both simulations of ASPEN Plus