

Stoichiometric Reactor Simulation

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In this session you will learn how to create a stoichiometric reactor model in Aspen Plus. The best source of documentation for most Aspen unit operations is to use the online help by selecting the F1 key while in a unit operation setup.

The following table provides a description of commonly used reactor model blocks. During the course of the semester we will explore the use of these reactors to model reaction chemistry.

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
REquil	Equilibrium reactor	REquil calculates simultaneous phase and chemical equilibrium. REquil allows restricted chemical equilibrium specifications for reactions that do not reach equilibrium.	Reactors with when reaction stoichiometry is known and some or all reactions are at equilibrium. REquil can model one- and two-phase reactors.

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

In this module we will use RStoic to model the production of styrene.

Aspen Plus Stoichiometric Reactors – Tutorial on Styrene

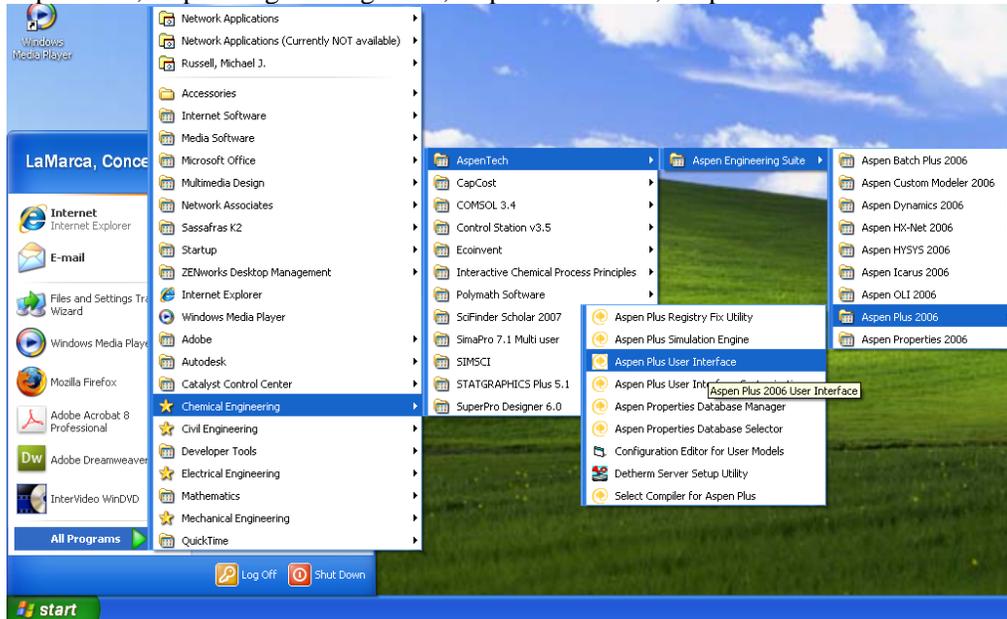
Styrene is a monomer used in the production of many plastics. It has the fourth highest production rate after the monomers of ethylene, vinyl chloride and propylene. Styrene is made from the dehydrogenation of ethylbenzene:



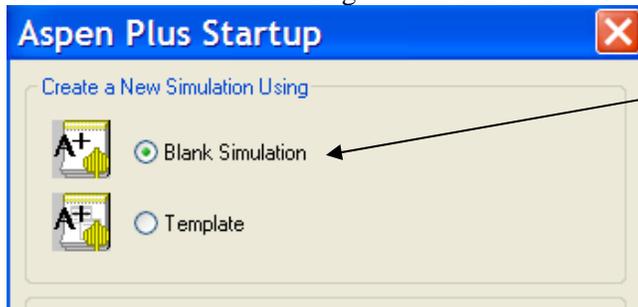
Here we will create a stoichiometric reactor model to be run both isothermally and adiabatically. In this tutorial you will examine material and energy balances of a reacting system.

Procedure to Create a Stoichiometric Reactor Model:

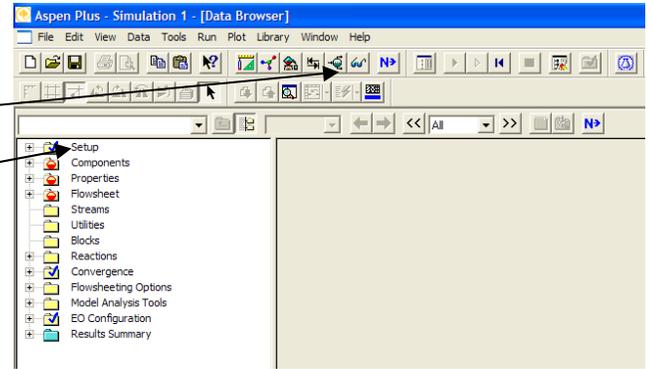
1. Start Aspen Plus User Interface by going through the start menu, Chemical Engineering, AspenTech, Aspen Engineering Suite, Aspen Plus 2006, Aspen Plus User Interface



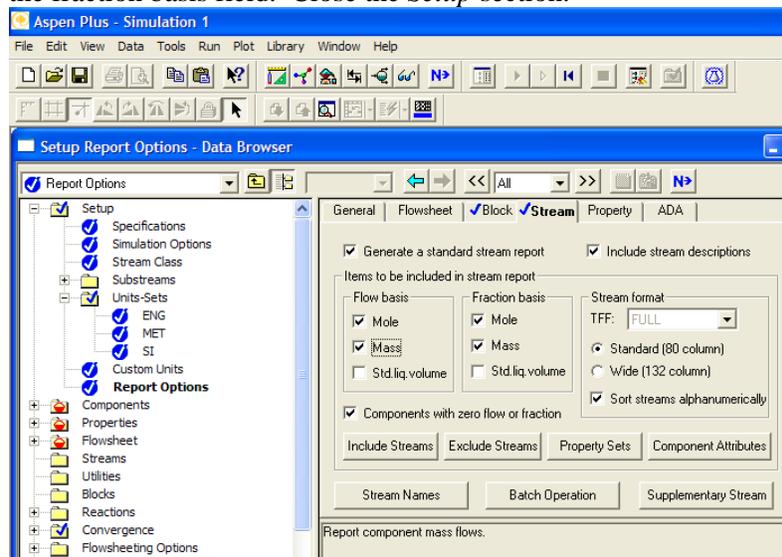
2. Create a new simulation using a blank simulation



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



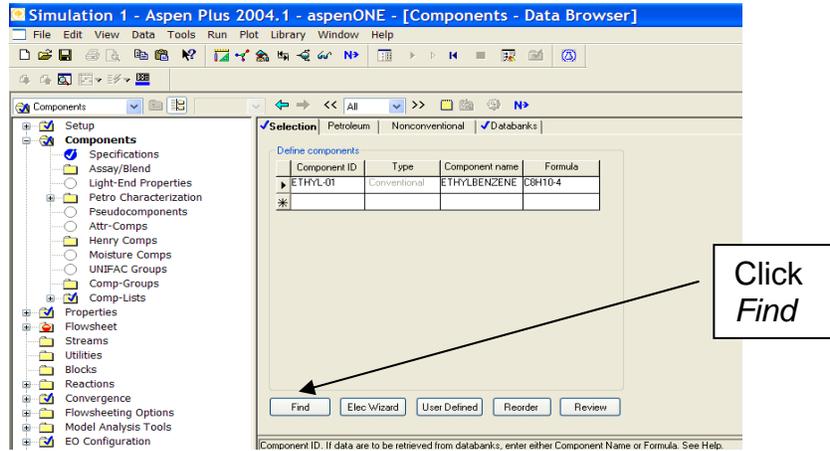
- Select *Specifications*. You may enter a title in the *Title* field, and a brief description of the process by choosing the *Description* tab. You should also specify input and output units for your simulation. **Select metric [MET] units.**
- Before proceeding, move to *Report Options* where you can 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.



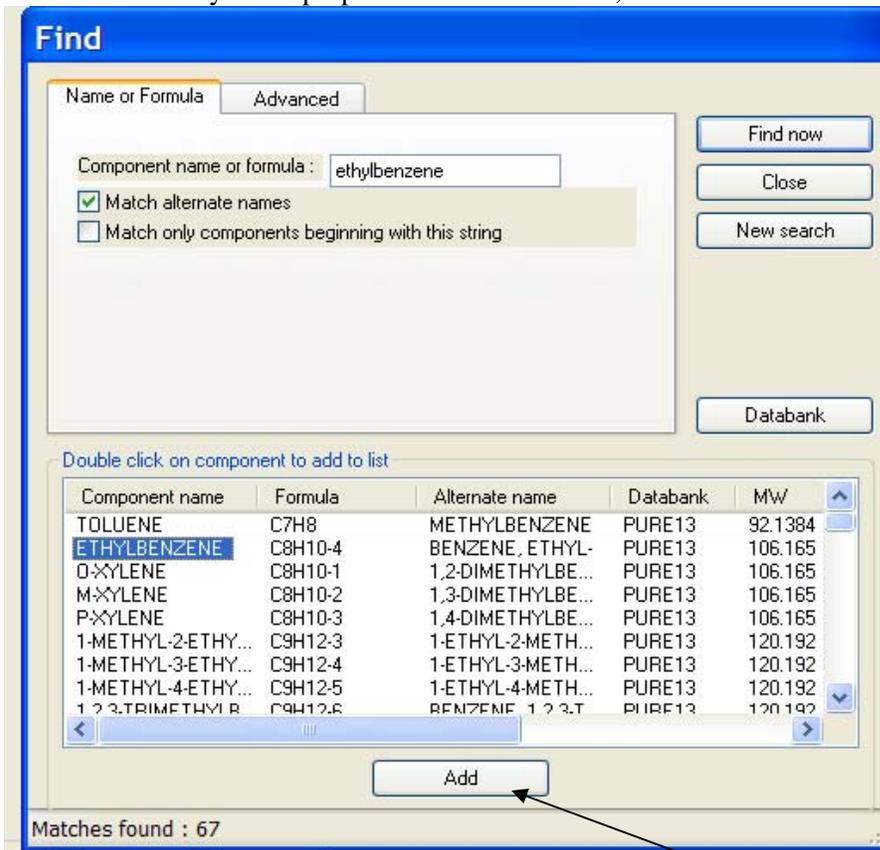
Click  to take you to next Input step.

- Choose the *Components* option in the data browser window to start adding chemical components, and select *Specifications*.

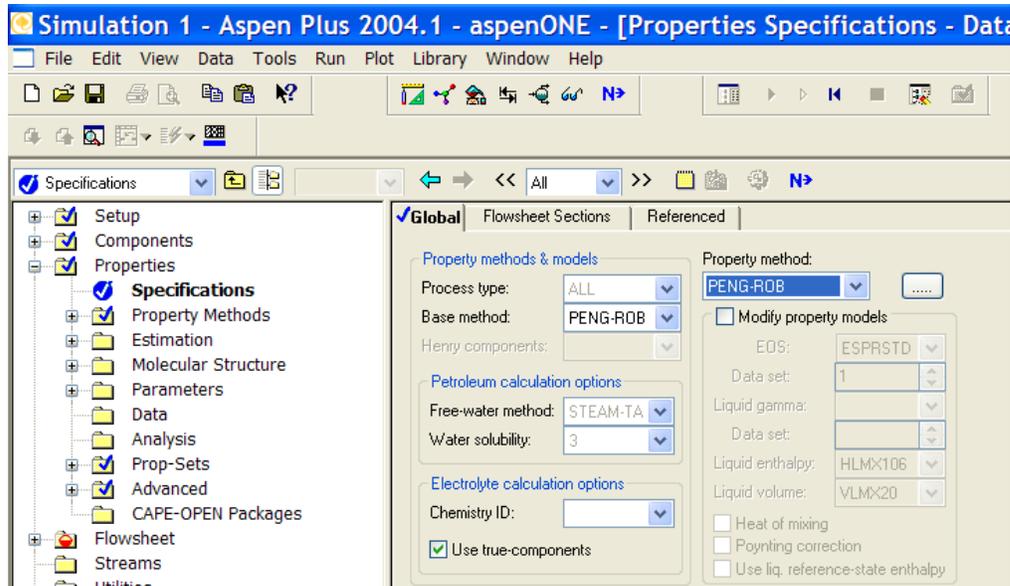
6. Next select the chemicals for your reaction system. Use the *Find* button to search for the components for this problem: styrene, ethylbenzene, and hydrogen. Select your component from the list, and then *Add* it. When finished, close the *Components* section.



7. 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.

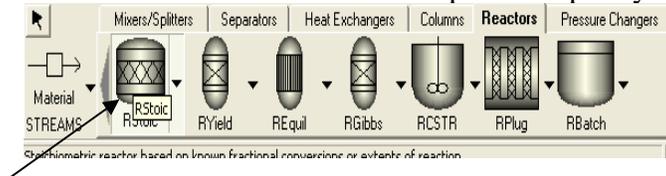


8. Next, select as base method for system properties, by selecting *Properties, Specifications*. Since these compounds are hydrocarbons, use the Peng-Robinson thermodynamics package by selecting PENG-ROB under the *Base method* tab. Close the *Properties* section and the *Data Browser* (and all other windows) revealing the blank Process Flow Window.



Specifying RStoic (From RStoic reference)

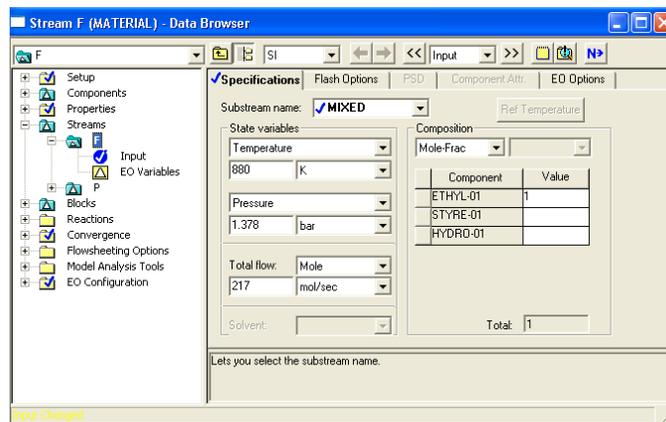
- You are now ready to setup your flowsheet. You should see the blank Process Flow Window. Create a stoichiometric reactor using the RStoic reactor block, by selecting the Reactor tab from the *Model Library* along the bottom of your window. Click on *Reactors* and then choose *RStoic* by clicking on the *RStoic* icon, then releasing the left mouse button. Move cursor onto the Process Flow Window and then press left mouse button only once. Select the arrow in the very left corner of the model library taskbar, and then double click on the reactor to open and specify details.



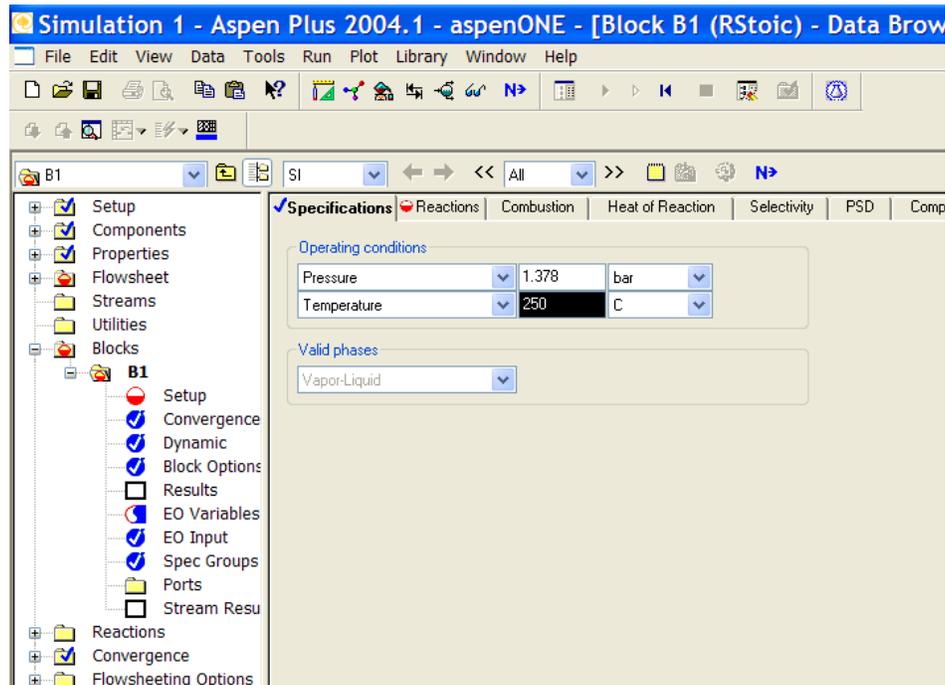
- Rename the reactor using a descriptive name by right clicking and selecting *Rename Block*.
- To add feed and effluent streams, use the *Model Library* to select the *Material STREAMS* tab in the lower left-hand corner and click once. This will allow you to place multiple streams as needed. Move the 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*. You may rename streams by right clicking).



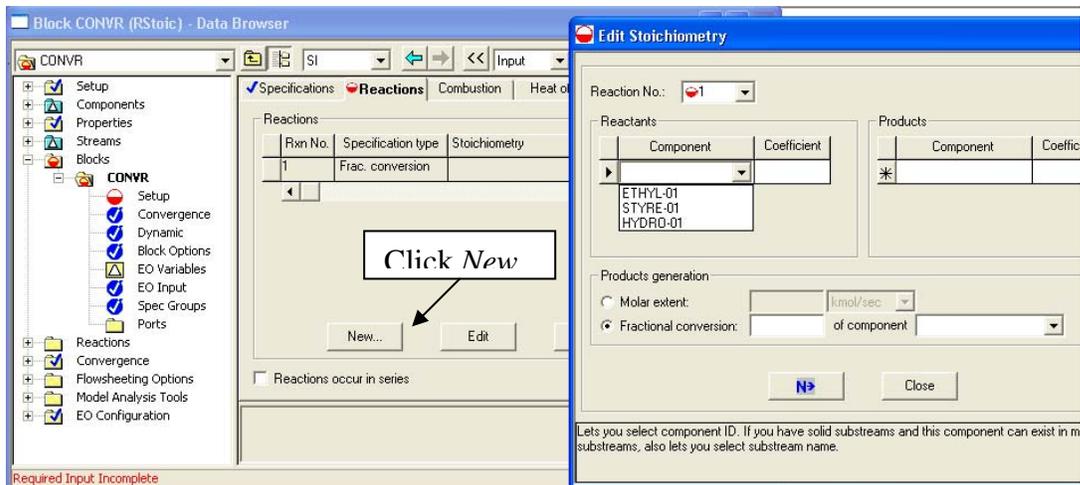
- Specify the feed stream (Double click on the stream or right click on it and then choose input) having a composition of pure ethylbenzene at 217gmol/s, 880 K, 1.378 bar. Specify the feed composition as a mole fraction. Close the *Streams* tab.



- 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 are required to input values for two variables. Use the drop-down list). For an isothermal reactor (Case 1) specify the outlet temperature and pressure. For Case 1, enter pressure and temperature of 1.378 bar and 880K. (250°C is shown and is incorrect)



- Click  or the *Reactions* tab.
- Use the Setup Reactions sheet to define the reaction occurring in the reactor. You must specify the stoichiometry for each reaction and in addition, you must specify either the molar extent or the fractional conversion for all reactions. Click *New*, to choose the reactants and products using the drop down list, input the stoichiometric coefficients and specify the fractional conversion (0.8) and the species on which the conversion is based (ethylbenzene) and then click .



16. Close the reactor window to find your way back to the Process Flow Window.
17. Click  in the Data Browser window. A dialog box opens saying "All required input is complete". Run the simulation by clicking OK.
18. To view the results click  again, and then OK to display Run- Status form. The summary sheet should indicate that 'Simulation calculations completed...'. You can view the reactor results by selecting the reactor block on the left.
19. Select the block. And then view report (View menu, Report election).
20. View stream results (from the block results) from the data browser. Select these results by clicking in the upper right hand corner of your browser and paste into an Excel spreadsheet. (This is for a temperature of 250°C you did 880K)

	1	2	
Substream: MIXED			
Mole Flow kmol/hr			
STYRE-01	0.0	624.9600	
ETHYL-01	781.2000	156.2400	
HYDRO-01	0.0	624.9600	
Mole Frac			
STYRE-01	0.0	.4444444	
ETHYL-01	1.000000	.1111111	
HYDRO-01	0.0	.4444444	
Mass Flow kg/hr			
STYRE-01	0.0	65090.53	
ETHYL-01	82937.97	16587.59	

21. Save this simulation as case 1.
22. For the base case 2, the adiabatic reactor, you should specify the heat duty (as zero) and the pressure. Specify the pressure as 1.378 bar and the heat duty of zero. Run your simulation, and save as case 2.
23. Next, simulate the cases done in class for case 2 through 4. You may need to refer to the lecture notes that are on line..
 - Case 1) 880 K Isothermal at X=0.69
 - Case 2) 880 K inlet with an adiabatic reactor and X=0.2
 - Case 3) 880 K Isothermal with steam at a flowrate of 1736 mol/s at X=0.69 (For this case you will need to go back to step 7 and add water. Do not add this to the reaction, because it does not take place in the reaction.

Case 4) 880 K inlet into a adiabatic reactor with steam at a flowrate of 1736 mol/s at $X=0.39$ an

24. Now run at least 5 adiabatic cases with molar feed ratios of steam to ethylbenzene between 0 and 8. Make a plot of the outlet temperature as a function of the feed ratio for a constant conversion of ethylbenzene of $X=0.69$. Make observations and explain the behavior shown in this plot.
25. To create a report file for both cases 1 & 2, for printing, select the File menu & Export. Under the Export screen choose Report Files (*.rep) as your file type and save.

Submit a word document and aspen file to blackboard of the following on or before 4/24/09:

- **Into a word document paste in the stream results (from the block results) for all for cases**
- **Submit the aspen file (*.apw) that contains case 4.**
- **Make a plot of the outlet temperature as a function of the feed ratio for a constant conversion of ethylbenzene of $X=0.69$. Paste this plot in the word document and type your observations. Also explain the behavior shown in this plot.**