

Kinetic Reactors: Aspen Plus 2006

In this session you will learn how to create a tubular reactor model in Aspen Plus with a kinetic reaction rate. In this Aspen Plus run we will specify an irreversible reaction and will ignore the reverse reaction.

Reactors.

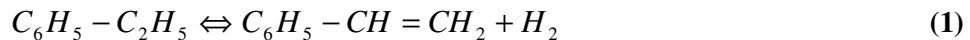
RPlug is a rigorous model for plug flow reactors which assumes that perfect mixing occurs in the radial direction and that no mixing occurs in the axial direction. RPlug can model one-, two-, or three-phase reactors. You can also use RPlug to model reactors with coolant streams (co-current or counter-current). RPlug handles kinetic reactions, including reactions involving solids. You must know the reaction kinetics when you use Rplug to model a reactor. You can provide the reaction kinetics through the built-in Reactions models or through a user-defined Fortran Subroutine.

Use the Reactions form to define the reaction stoichiometry and kinetics parameters for these models. The Aspen Plus formalism allows for specification of irreversible reactions only. To account for the reverse rate, you must enter it as a separate reaction.

Use the Setup Configuration sheet to specify reactor tube length and diameter. If the reactor consists of multiple tubes, you can also specify the number of tubes. You can specify the pressure drop across the reactor on the Setup Pressure sheet, or use a correlation to calculate pressure drop. Additional required input for RPlug depends on the reactor type. You must specify reaction kinetics on the Setup Reactions sheet, by referring to Reaction set that you select. You can specify one-, two-, or three-phase calculations. Specify the reaction phases on the Reactions forms. RPlug can handle only kinetic type reactions.

Aspen Plus PFR Reactors using kinetic rates– Tutorial using Styrene

For this tutorial we will return to the production of styrene from the dehydrogenation of ethylbenzene:



In this reactor we will neglect the fact that equilibrium is important for this reaction, and model this system using a power law expression. The reaction rate expression that you will install is given by the following:

$$r = -k p_{EB} \quad (2)$$

where, $k = A \cdot \exp\left(\frac{-E^*}{R^*T}\right)$, $A = 89.2178 \left[\frac{gmol}{l_{rxr} - kPa - s} \right]$ and $E^* = 21874 \text{ cal / gmol}$.

Notice that the reaction rate has units and the driving force term is partial pressure with units of *kPa*, however the internal unit set for reactions in Aspen is SI units¹.

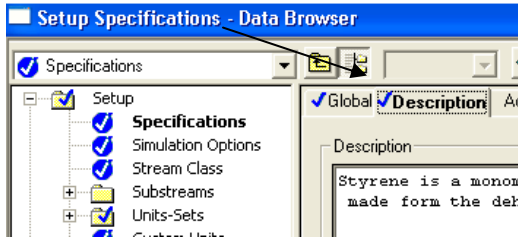
¹ See discussion from Aspen Help on “Rate Controlled Reactions”, posted on the course website.

Units Conversion

Take out a black sheet of paper and perform hand calculations to convert the units specified above to SI units ($\text{kg}\cdot\text{m}^3\cdot\text{s}\cdot\text{Pa}$). *Hand these calculations in with your lab.*

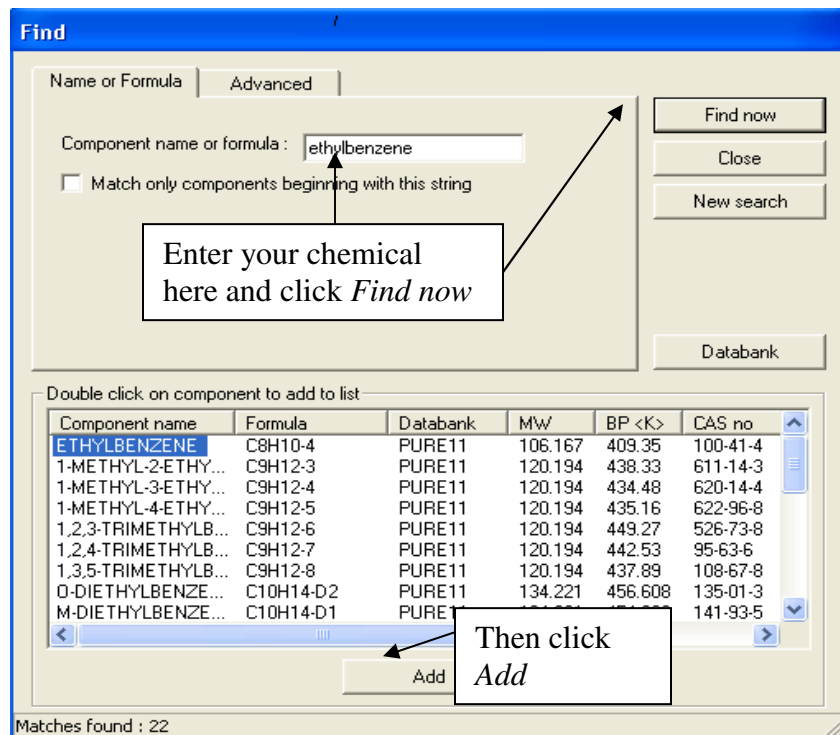
Procedure to Create a Plug-Flow Reactor with Kinetics:

1. Start Aspen Plus 2006.
2. Open a new case by choosing a blank simulation. (Do not use the templates for consistent units when specifying your kinetics. We will use SI units for all reactors with kinetics).
3. Select the data browser and choose 'SI' units for input and output results on the Global tab.



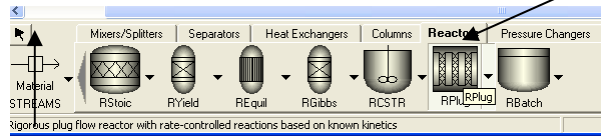
4. Select the databrowser and click *Setup*. You can enter the title and brief description of the process by choosing the *Description* tab.
5. Under the *Report Options, Stream* tab, specify *Mole* and *Mass* for both the *Flow Basis* and the *Fraction Basis*.

6. Choose the *Components* option in the data browser window to start adding chemical components.
7. Select all the chemicals for your reaction system: styrene, ethylbenzene, and hydrogen. Use the *Find* button to find the component ID and then add them.



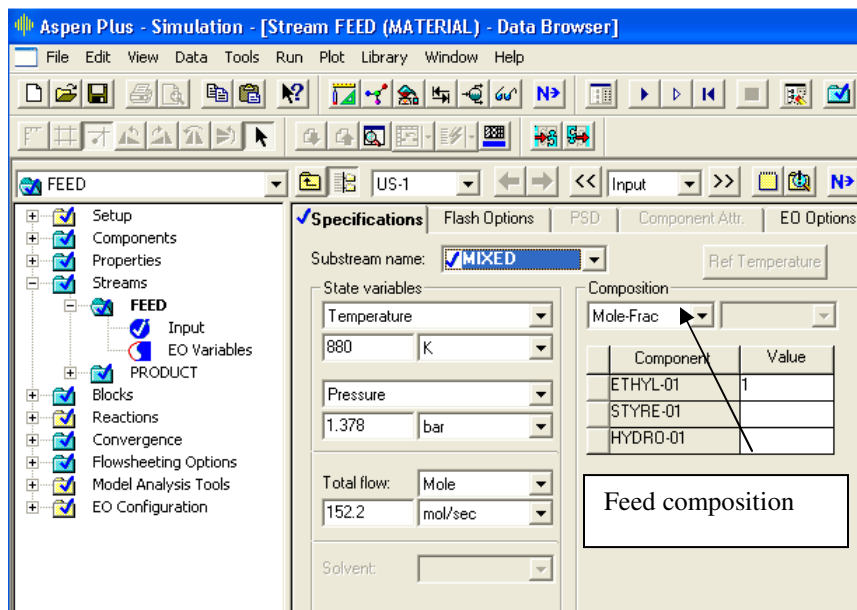
8. Next, under Properties, Specifications, select your base property method. Since these compounds are hydrocarbons, use the Peng-Robinson thermodynamic package.
9. Close the data browser.


- To create RPlug use the Model Library, click on *Reactors* and then choose *RPlug*. Click on the *RPlug* icon, then release left mouse button. Move cursor to pfd screen and then press left mouse button only once.

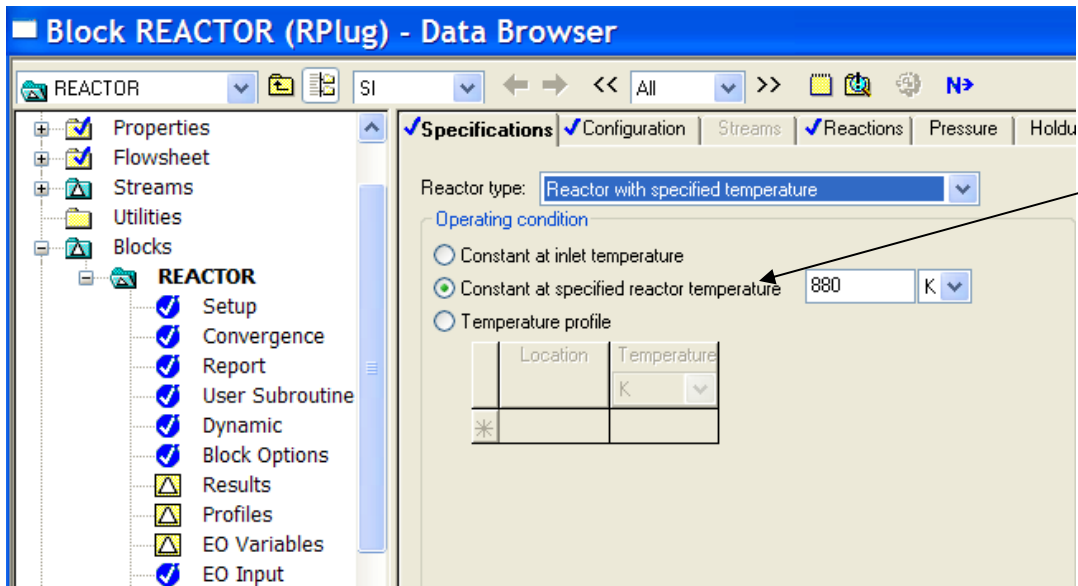


After adding the reactor, click the small arrow on the left bottom corner of the Aspen Plus Process Flowsheet Window.

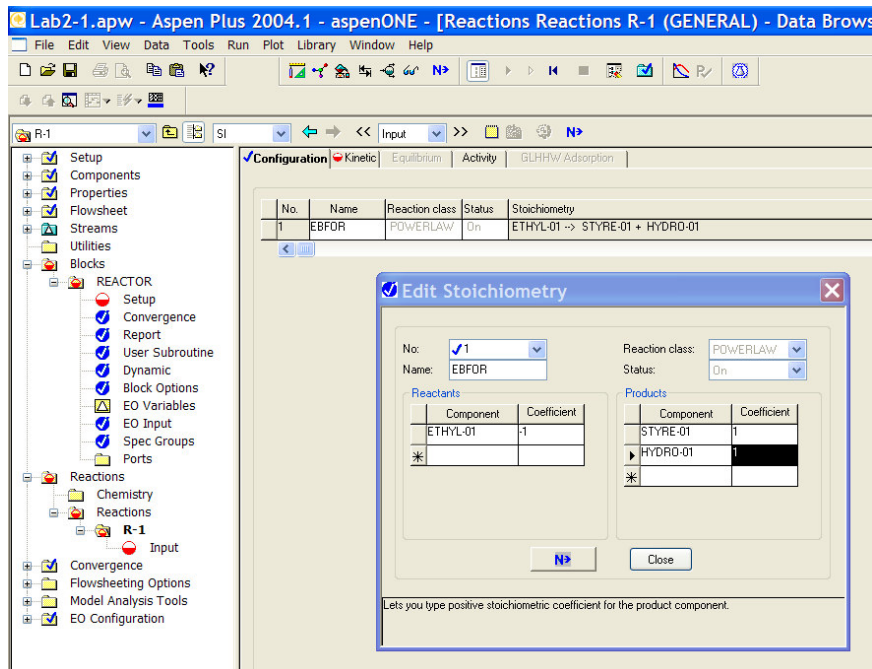
- To add streams, From the Model Library at the bottom of the Aspen Plus Process Flowsheet Window, select the *Material STREAMS* tab and click once. This will allow you to place multiple streams as needed. Move the cursor, now a crosshair, onto the process flowsheet. Click once, drag the cursor to connect 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.
- Specify the feed stream (Double click on the stream or right click on it and then choose input or through *Data, Streams* in the main menu) having a composition of pure ethylbenzene (specified as a mole fraction) at 152.2 gmol/s, 880 K, 1.378 bar.



- To input the reactor specifications, double click on the reactor block. The reactor Data Browser opens. Specify the reactor as an isothermal reactor (reactor with specified temperature) and click . (Use “Constant at specified reactor temperature” option).

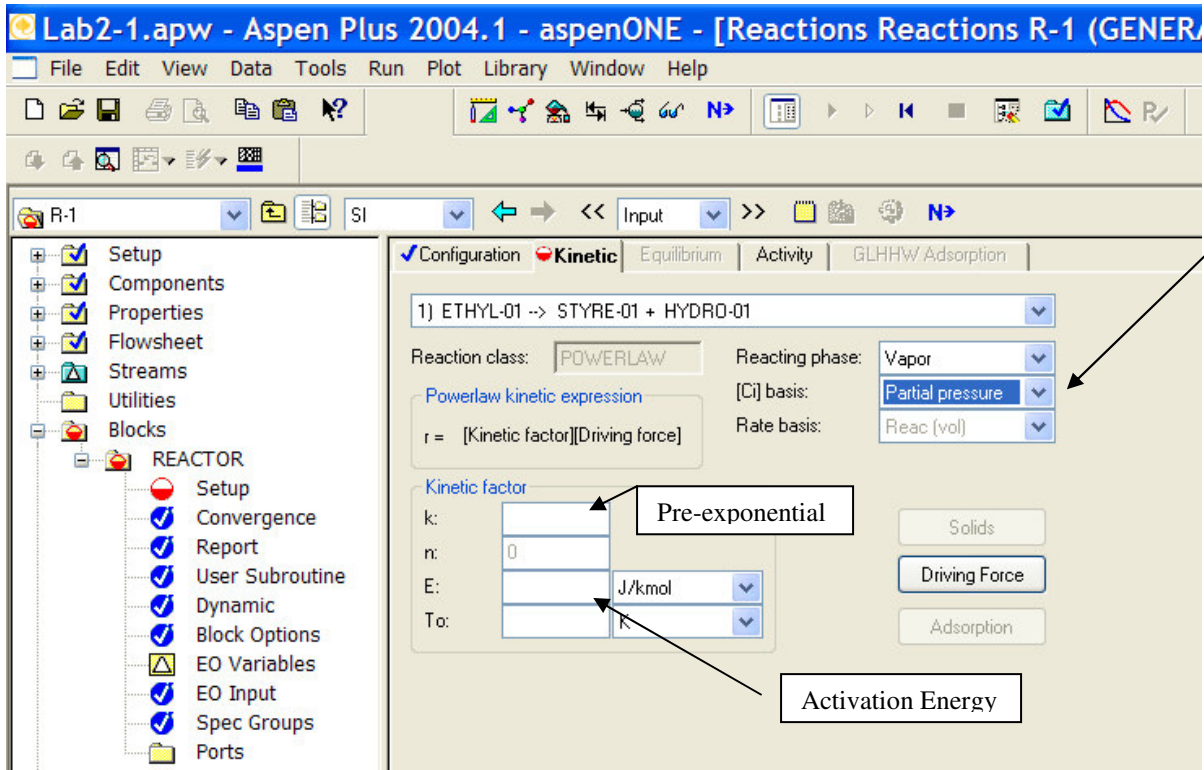


14. In the next *Configuration* page specify the length and diameter of the reactor as 3 m and 0.5717 m respectively (for .77 m³ reactor).
15. Now you need to specify the reaction set to complete the specification for the PFR. Choose the *Reactions* block from the browser window. Then click on *Reactions*. Then click *New* on the window that appears. A new dialog box opens, enter a reaction ID and specify the reaction as *General*. Then click *New*. Give the reaction a name (EBFOR here), and specify the reaction stoichiometry. And the Next button.

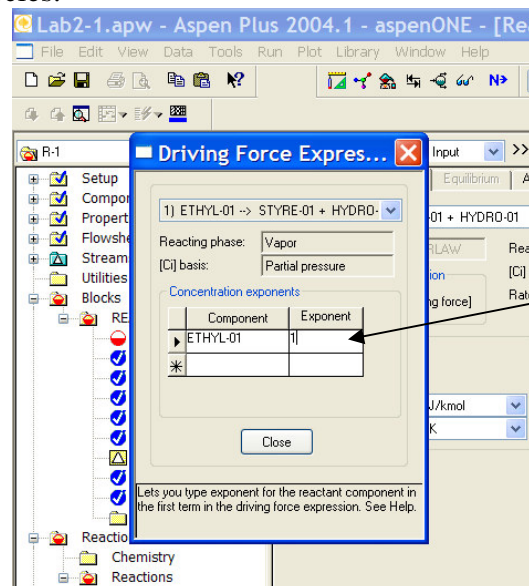


16. Click the *Kinetic* tab to specify the kinetics parameters and reaction driving force.
17. Specify the reacting phase as *vapor*, the concentration basis as *partial pressure* and the rate basis as *reactor volume*.

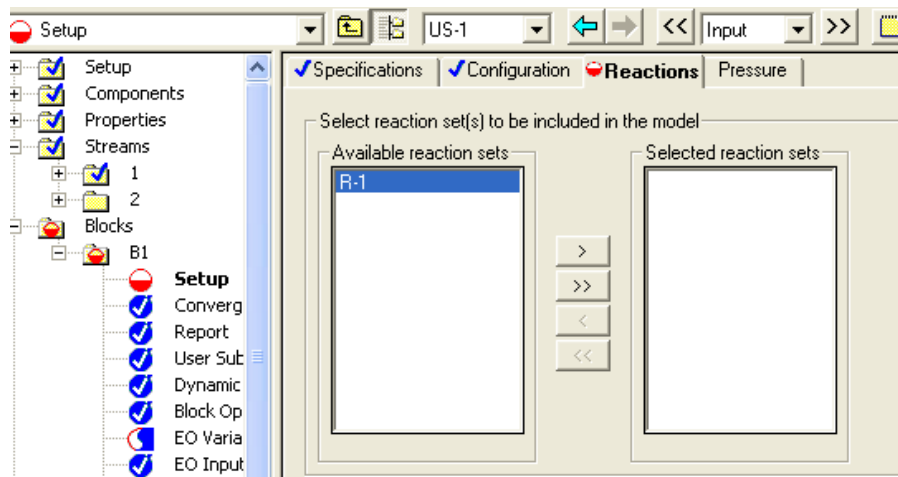
18. Next add the kinetics parameters. **How you enter the reaction parameters are critical to getting your simulation to work properly** The pre-exponential factor **MUST BE** in SI units (as derived earlier), but you have a choice for units for the activation energy.




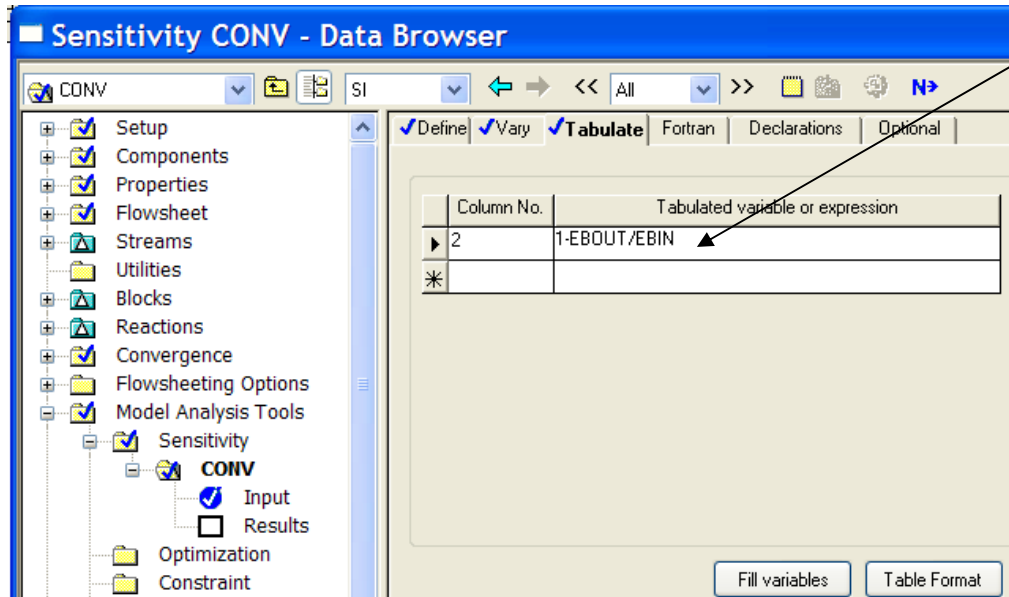
19. Finally, click on the driving force tab, to enter the 'power' dependence of the rate on your reacting species.



20. Click . It automatically goes to the *Reactions* page under Reactor specifications.



21. The reaction set you specified will be in the *available reaction sets*, now transfer it to the *selected reaction sets* and click .
22. A dialog box opens saying “All required input is complete’. Run the simulation by clicking OK. To view the results right click on the reactor block and choose *Stream Results*. **Save these results to a spreadsheet file.**
23. In the first lab, we explored the effects of some variable on our reactor performance. In this case, we will examine a more realistic case using real kinetics. We will explore the effect of reactor temperature on the conversion of ethylbenzene for an isothermal reactor using a Sensitivity Block.
 - a) Click New to create a new *Sensitivity Block* under *Model Analysis Tools*
 - b) Define variables: Since conversion is not an output variable of the simulation, we’ll need to define variables to calculate this output for tabulation. Your ethylbenzene conversion will need to be calculated from species molar flow rates in the inlet and outlet streams.
 - i) Define EBIN as Type: Mole-flow, Stream: Inlet, Component: Ethylbenzene.
 - ii) Define EBOUT as Type: Mole-flow, Stream: Outlet, Component: Ethylbenzene.
 - c) Next, determine the manipulated variable (RX) using the VARY tab, and provide a range (600-1000K) for variation. This will be a Block-Var, and the variable name is SPEC-TEMP. Select ID1 as 1 to specify a location.
 - d) Finally, to specify output variable for tabulation, define an expression in the Tabulate field for calculated conversion, based on your defined variables. For example: $(1-EBOUT/EBIN)$.



- e) Run your simulation.
- f) Generate a graph of Reactor T versus EB Conversion using Excel to hand in today.

Next let's compare these results with a parallel simulation in POLYMATH.

24. Create a plug flow reactor Polymath model for our reaction on a volume basis, using species molar flows, as shown below. (You may use these units, or change to match your Aspen model. In either case, be sure to make a comparison).

$$\begin{aligned}
 d(\text{FEB})/d(V) &= r_{\text{EB}} \text{ \#mol/l-s} \\
 d(\text{FS})/d(V) &= -r_{\text{EB}} \text{ \#mol/l-s} \\
 d(\text{FH})/d(V) &= -r_{\text{EB}} \text{ \#mol/l-s} \\
 \text{FT} &= \text{FEB} + \text{FS} + \text{FH} \text{ \#mol/s} \\
 P &= 137.8 \text{ \#kPa} \\
 T &= 880 \text{ \#K} \\
 k &= 89.2178 * \exp(-21874/1.987/T) \text{ \#mol/l-s-kPa} \\
 p_{\text{EB}} &= \text{FEB}/\text{FT} * P \text{ \#kPa} \\
 r_{\text{EB}} &= -k * p_{\text{EB}} \text{ \#mol/l-s} \\
 V(0) &= 0 \\
 \text{FEB}(0) &= 152.2 \text{ \#mol/s} \\
 \text{FS}(0) &= 0 \text{ \#mol/s} \\
 \text{FH}(0) &= 0 \text{ \#mol/s} \\
 V(f) &= 770 \text{ \#l}
 \end{aligned}$$

25. Run the model to generate the default report. Compare these results with your Aspen results. Comment.

HAND IN THE FOLLOWING:

1. Hand calculations on units conversion.
2. Aspen stream results.
3. Aspen table of results from sensitivity analysis and associated graph.
4. POLYMATH results report and discussion of comparison with Aspen results.