Aspen Plus® Workshop
for
Reaction Engineering and Design

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Introduction

What is a Process Flowsheet

Process flowsheet can simply be defined as a blue print of a plant or part of it. It identifies all feed streams, unit operations, streams that inter-connect the unit operations and finally the product streams. Operating conditions and other technical details are included depending on the detail level of the flowsheet. The level can vary from a rough sketch to a very detailed design specification of a complex plant.

For steady-state operation, any process flowsheet leads to a finite set of algebraic equations. For a case where we have only one reactor with appropriate feed and product streams the number of equations may be manageable by manual hand-calculations or simple computer applications. However, as the complexity of a flowsheet increases and when distillation columns, heat exchangers, absorbers with many purge and recycle streams come into the picture the number of equations easily approach many ten thousands. In these cases, solving the set of algebraic equations becomes a challenge in itself. However, there are computer applications called process flowsheet simulators specialized in solving these kinds of large equation sets. Some well known process flowsheet simulators are Aspen Plus™, ChemCad™ and PRO/II™. These products have highly refined user interfaces and on-line component databases. They are used in real world applications from interpreting laboratory scale data to monitoring a full scale plant.

Advantages of using a process flowsheet simulator

The use of a process flowsheet simulator is beneficial in all the three stages of a plant: research & development, design and production. In research & development they help to cut down on laboratory experiments and pilot plant runs. In design stage they enable a speedier development with simpler comparisons of various alternatives. Finally, in the production stage they can be used for risk-free analysis of various what-if scenarios.

Disadvantages of using a process flowsheet simulator

Manual solution of a problem usually forces someone to think deeper on the problem, find novel approaches to solve it, and evaluate and reevaluate the assumptions closer. A drawback of process flowsheet simulators may be cited as the lack of this detailed interaction with the problem. This might act as a double edged sword. On one side it hides the complexities of a problem so you can concentrate on the real issues at hand. On the other side this hiding may also hide some important understanding of the problem as well.

History

In 1970s the researchers at MIT's Energy Laboratory developed a prototype for process simulation. They called it Advanced System for Process Engineering (ASPEN). This software has been commercialized in 1980's by the foundation of a company named AspenTech. AspenTech is now a publicly traded company that employs 1800

people worldwide and offers a complete integrated solution to chemical process industries.

This sophisticated software package can be used in almost every aspect of process engineering from design stage to cost and profitability analysis. It has a built-in model library for distillation columns, separators, heat exchangers, reactors, etc. Custom or propriety models can extend its model library. These user models are created with Fortran subroutines or Excel worksheets and added to its model library. Using Visual Basic to add input forms for the user models makes them indistinguishable from the built-in ones. It has a built-in property databank for thermodynamic and physical parameters. During the calculation of the flow sheet any missing parameter can be estimated automatically by various group contribution methods.

In this workshop we will only scratch the surface of this tool. We will discuss its advantages and disadvantages. Our focus will be on reactors and our goal is to provide you with a smooth and simple introduction to Aspen Plus. Let's start our workshop by learning how to access Aspen Plus™ at The University of Michigan.

Aspen Plus® at The University of Michigan

The current version supported by CAEN is 10.2. Files generated in older versions are upward compatible and will be converted automatically to the newer version. Aspen Plus™ has an extensive on-line documentation library. All on-line documentation is available either as standard Windows help file or as PDF documents. PDF documents are located at the following network neighborhood address "S:\bin\aspentech\AES 10.2 Documentation".

Aspen Plus™ can be invoked by following this path:

From `Programs` menu find

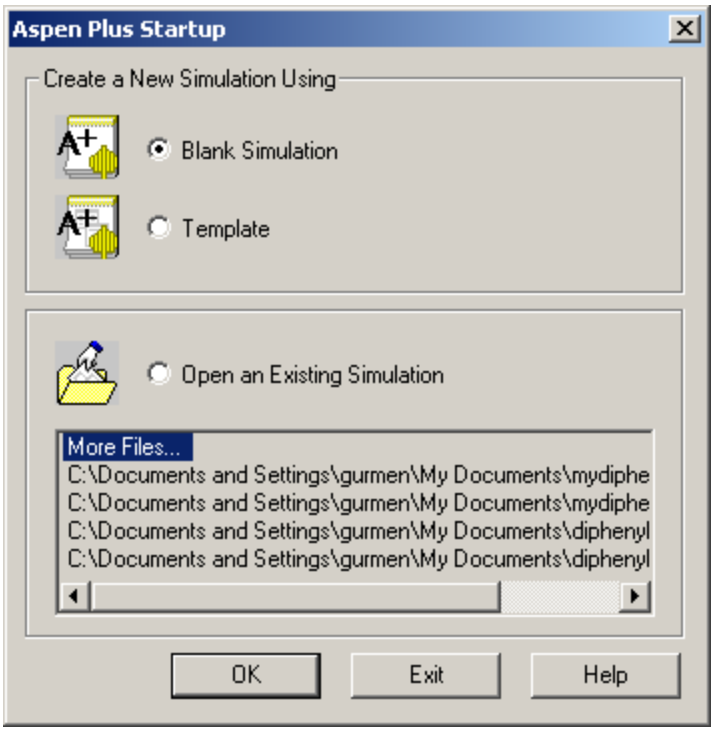
`Engineering Applications -> Aspen Plus 10.2 -> Aspen Plus 10.2`

And click

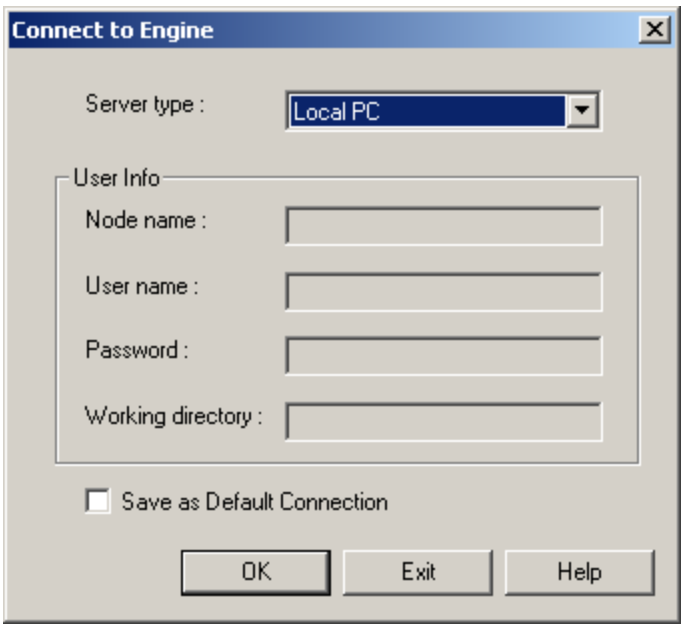
`Aspen Plus User Interface`

Interface basics

After invoking Aspen Plus™ , it will present you the *Aspen Plus Startup* dialog. There are three choices for starting a new Aspen Plus™ session. You can open an existing simulation, start from a template or create your work from scratch using a blank simulation. Let's select the option with blank simulation and click ok.

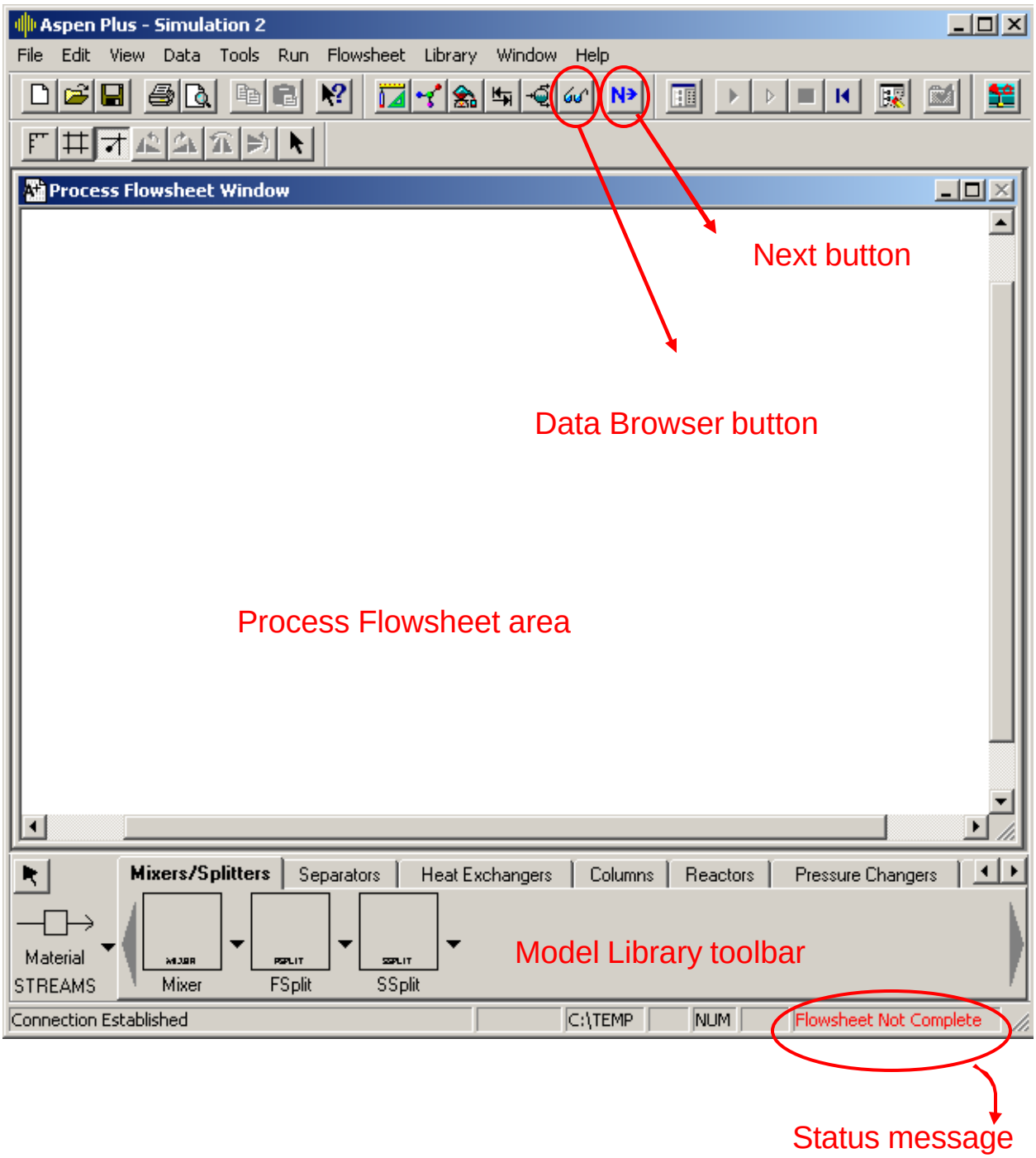


Aspen Plus™'s simulation engine is independent from its graphical user interface (GUI). You can create your simulations using the GUI at one computer and run them



connecting to the simulation engine at another computer. For this workshop we will use the simulation engine at Local PC. Default values should be ok. Click ok at the *Connect to Engine* dialog.

The next screen will be the main Aspen Plus™ application window with a blank *Process Flowsheet Window* in it. Let's familiarize ourselves with the interface.

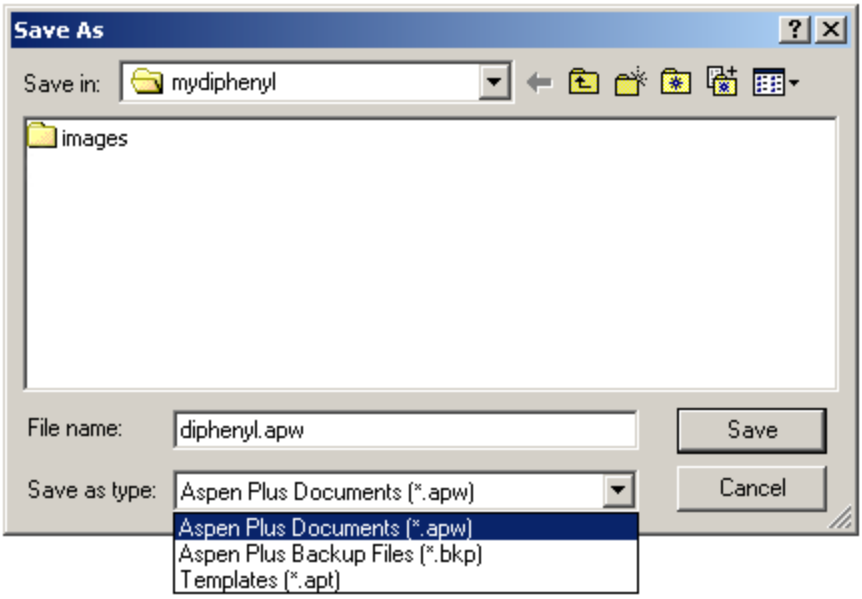


Flowsheet Not Complete message is shown until a full flowsheet description is entered in the *Process Flowsheet Window.* When the flowsheet is complete the status

message changes to *Required Input Incomplete*. A simulation can only be run when the status message shows *Required Input* Complete. For a minimalist flowsheet there has to be at least two streams, one for FEED and one for PRODUCT, connected to a unit operation equipment, say a REACTOR.

Under the process flowsheet window there is the Model Library toolbar. This toolbar contains the built-in Aspen Plus™'s models for various unit operations.

As with any other complex software application it is a good practice to save your work frequently. For the first save operation select *Save* or *Save As* from *File* menu and save your work. There are three saving modes: the Aspen Plus Document, Aspen Plus Backup file and Template.



The Aspen Plus Document format can retain your results and run information, but it is a propriety binary file format. In backup mode your work is saved as a standard ASCII text file. If you are an expert Aspen Plus™ user you can make changes directly on this file and send it as input to the simulation engine from the command line. It is easy to transfer this file from one machine to another. However, it does not retain the results or run information in it. Finally, a project can be saved as a Template and be a starting point for another simulation. While you are working on a project it is a good idea to save your simulation in Aspen Plus Document format. A file in backup format will be created automatically.

Reactor models

There are 7 built-in reactor models, RSTOIC, RYIELD, REQUIL, RGIBBS, RPLUG, RCSTR and RBATCH, in Aspen Plus™. RPLUG, RCSTR and RBATCH are rigorous models for plug flow, CSTR and batch reactors, respectively.

RSTOICH should be used in cases where the stoichiometry is known but the reaction kinetics is either unknown or negligible. If both, the reaction kinetics and stoichiometry is unknown RYIELD should be incorporated into the simulations. For single phase chemical equilibrium or simultaneous phase and chemical equilibrium calculations the reactor model of choice should be either REQUIL or RGIBBS. REQUIL bases its calculations on simultaneous solution of stoichiometric chemical and phase equilibrium calculations whereas RGIBBS solves its model by minimizing Gibbs free energy.

All reactor models except RPLUG and RBATCH can have any number of material feed streams. These streams are mixed internally. The rigorous models can incorporate built-in power law or Langmuir-Hinschelwood-Hougen-Watson kinetics or custom kinetics specified by user. Custom kinetics can be defined either in Fortran subroutines or in excel worksheets.

Table 1 Summary of reactor models in Aspen Plus®

Model	Stoichiometry	Kinetics	Rigorous	Feed
RSTOIC	Yes	No	No	Any
RYIELD	No	No	No	Any
REQUIL	No	No	No	Any
RGIBBS	No	No	No	Any
RBATCH	Yes	Yes	Yes	1
RCSTR	Yes	Yes	Yes	Any
RPLUG	Yes	Yes	Yes	1

Example Problem - Pyrolysis of Benzene

Aspen Plus will be introduced with benzene pyrolysis reaction in a plug flow reactor in this tutorial. The next three pages will present the details and the data.

Diphenyl ($C_{12}H_{10}$) is an important industrial intermediate. One production scheme involves the pyrolytic dehydrogenetation of benzene (C_6H_6) [1]. During the process, triphenyl ($C_{18}H_{14}$) is also formed by a secondary reaction.

The reactions are as follows:

(1) $$2\,C_6H_6 \rightleftarrows C_{12}H_{10} + H_2$$

(2) $$C_6H_6 + C_{12}H_{10} \rightleftarrows C_{18}H_{14} + H_2$$

Substituting the symbolic IDs A = C_6H_6, B = $C_{12}H_{10}$, C = $C_{18}H_{14}$ and D = H_2

(3) $$2\,A \rightleftarrows B + D$$

(4) $$A + B \rightleftarrows C + D$$

Murhpy, Lamb and Watson presented some laboratory data regarding these reactions originally carried out by Kassell [2]. In these experiments, liquid benzene was vaporized, heated to the reaction temperature and fed to a plug flow reactor (PFR). The product stream is condensed and analyzed for various components. The results are tabulated in Table 1.

Table 2 Laboratory data for P = 1 atm.

Temperature (°F)	Flow rate (lbmole/hr)	y_A	y_B	y_C	y_D
1400	0.0682	0.8410	0.0695	0.00680	0.0830
1265	0.0210	0.8280	0.0737	0.00812	0.0900
1265	0.0105	0.7040	0.1130	0.02297	0.1590
1265	0.0070	0.6220	0.1322	0.03815	0.2085
1265	0.0053	0.5650	0.1400	0.05190	0.2440
1265	0.0035	0.4990	0.1468	0.06910	0.2847
1265	0.0030	0.4820	0.1477	0.07400	0.2960
1265	0.0026	0.4700	0.1477	0.07810	0.3040
1265	0.0007	0.4430	0.1476	0.08700	0.3220
1265	0.0003	0.4430	0.1476	0.08700	0.3220

Additional data

A = C_6H_6 B = $C_{12}H_{10}$ C = $C_{18}H_{14}$ D = H_2

The reactor tube dimensions:

L = 37.5 in, D = 0.5 in

Rate laws

$$-r_{1A} = k_{1A}\left(p_A^2 - \frac{p_B p_D}{K_{1A}}\right)$$

$$-r_{2B} = k_{2B}\left(p_A p_B - \frac{p_C p_D}{K_{2B}}\right)$$

Specific reaction rate constants

$$k_{1A} = A_1 \exp(-\frac{E_1}{RT})$$

$$k_{2B} = A_2 \exp(-\frac{E_2}{RT})$$

Equilibrium constants

$$\ln K_{1A} = A' + \frac{B'}{T} + C' \ln(T) + D'T + E'T^2$$

$$\ln K_{2B} = A'' + \frac{B''}{T} + C'' \ln(T) + D''T + E''T^2$$

Parameter values

E_1 = 30190 cal/mol	A_1 = 7.4652E6 lbmole/h/ft^3/atm^2
E_2 = 30190 cal/mol	A_2 = 8.6630E6 lbmole/h/ft^3/atm^2
A’ = -19.76	A’’ = -28.74
B’ = -1692	B’’ = 742
C’ = 3.13	C’’ = 4.32
D’ = -1.63E-3	D’’ = -3.15E-3
E’ = 1.96E-7	E’’ = 5.08E-7
P = 14.69595 psi	R = 1.987 cal/mol/K

Exercise

Follow the instructions during the lab session and use the handouts to replicate the data presented in Table 1 for T = 1400 °F and P = 1 atm using Aspen Plus. What is the percent difference between experimental and simulated mole fractions?

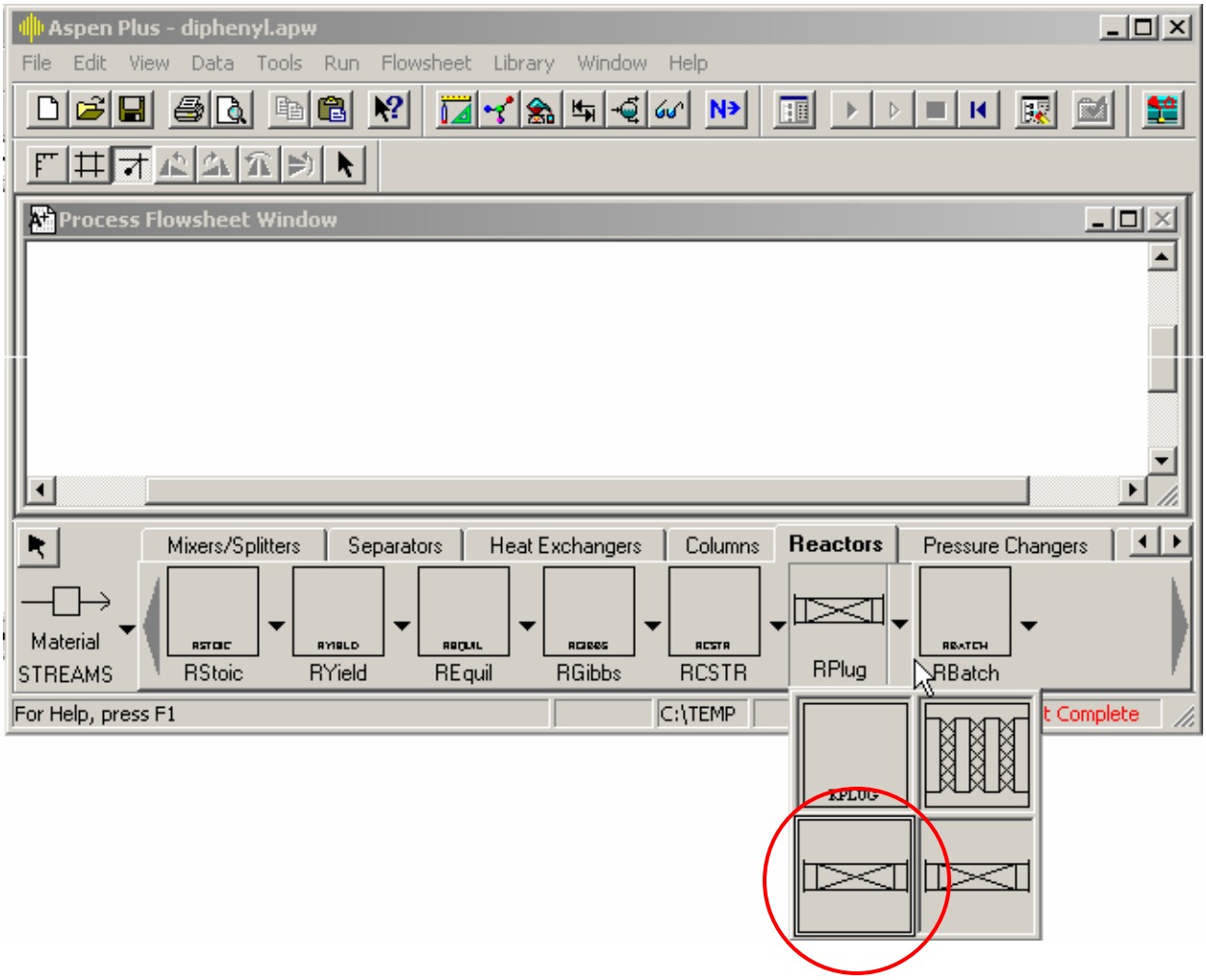
[1] H.S. Fogler, *Elements of Chemical Reaction Engineering*, 3rd ed., p.77-79, Prentice Hall, New Jersey, 1999.

[2] G.B. Murphy, G.G. Lamb, and K.M. Watson, *Trans. Am. Inst. Chem. Engrs.*, (**34**) 429, 1938.

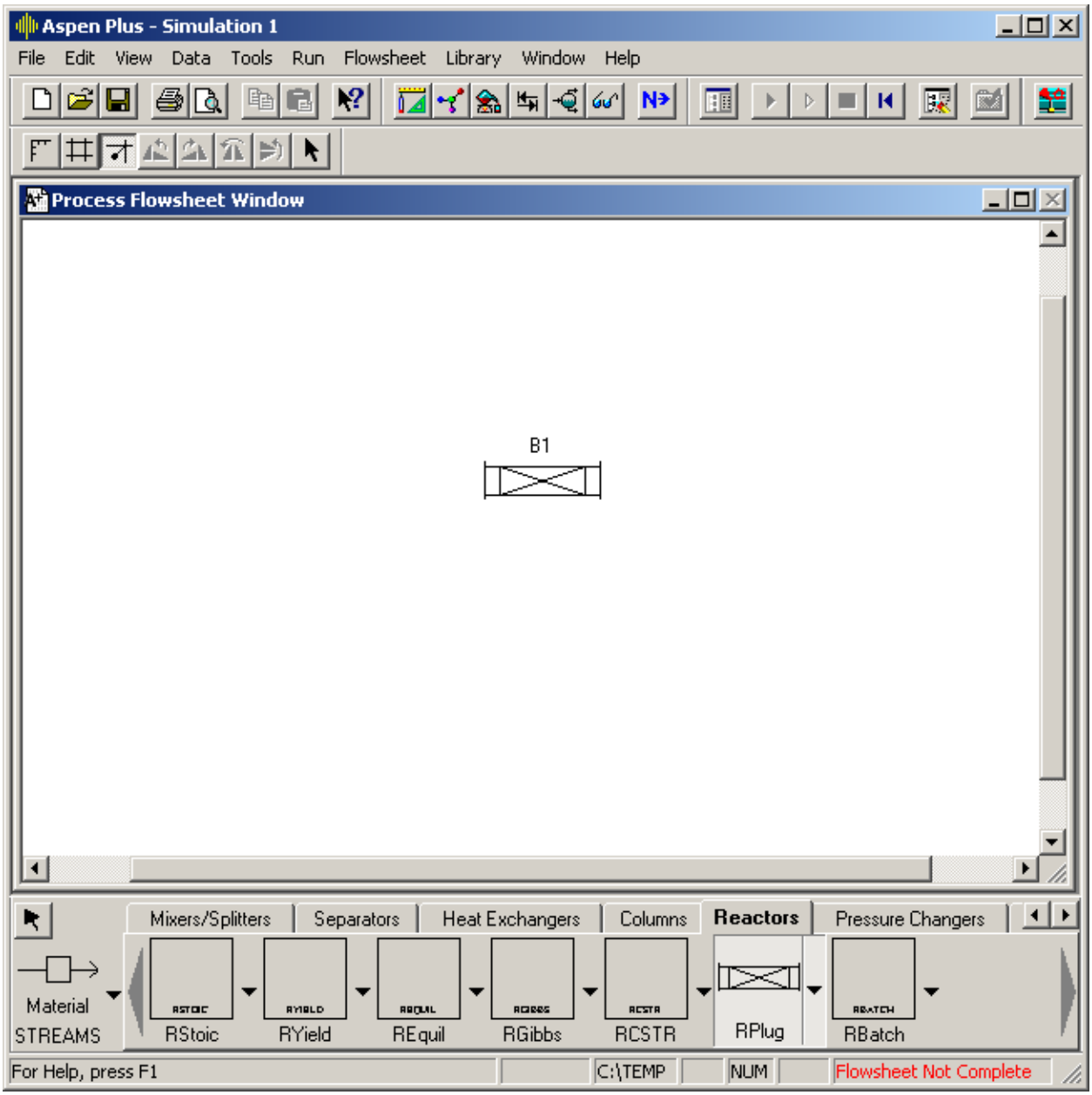
Tutorial

Flowsheet

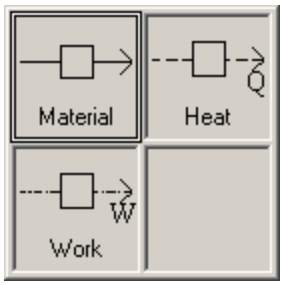
We will start creating our flowsheet by adding a reactor from *Model Library* toolbar to the *Process Flowsheet Window*. Select the *Reactors* tab on the *Model Library* toolbar. The built-in models for reactors are RSTOICH, RYIELD, REQUIL, RGIBBS, RCSTR, RPLUG and RBATCH. Clicking the down arrow to the right of the model gives different symbol choices for the user to insert into the flowsheet.



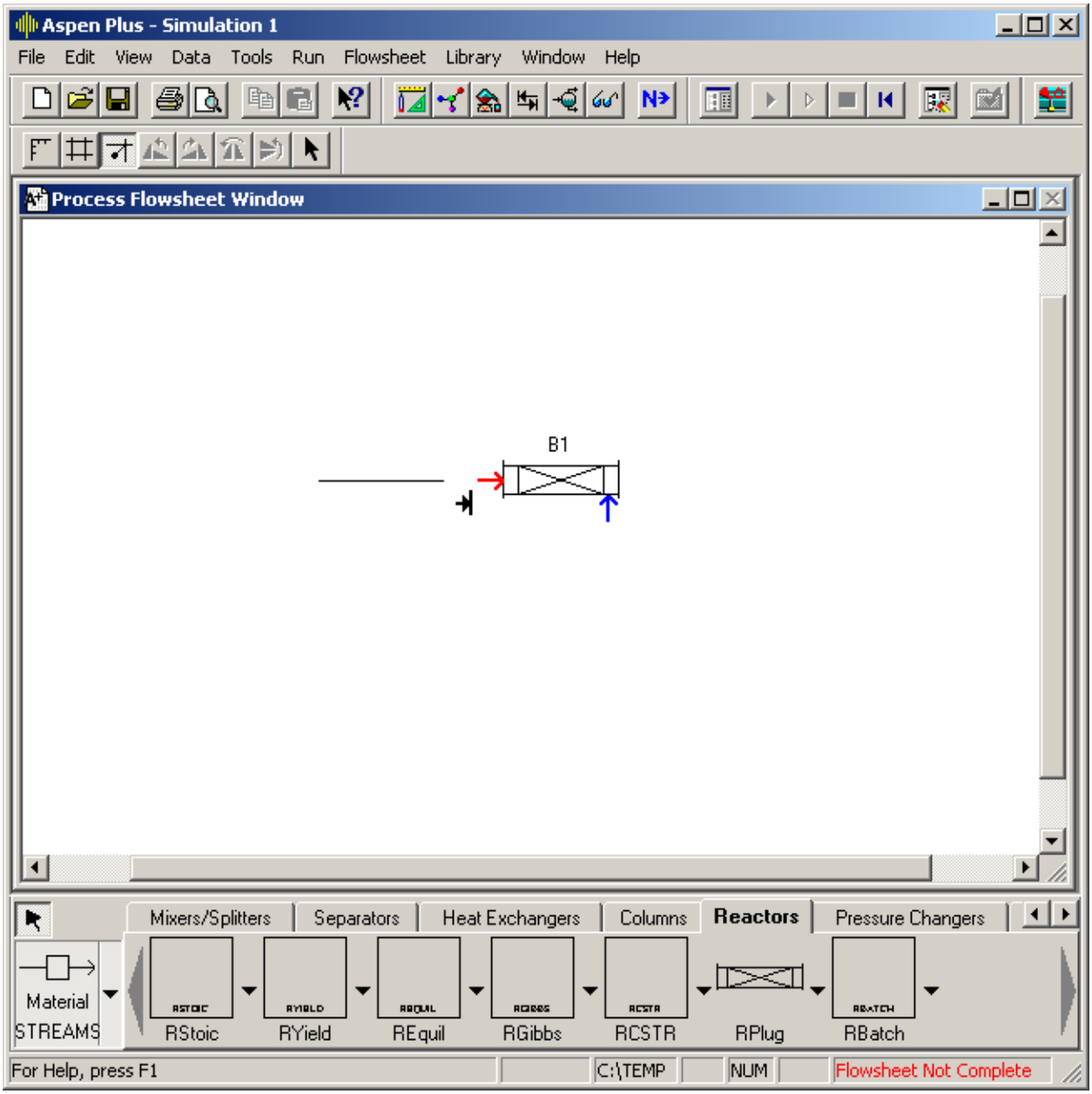
Select the left bottom symbol after expanding the RPLUG symbols and draw a rectangle where you want to insert on the *Process Flowsheet Window*. Now the *Process Flowsheet Window* should have an icon representing your plug flow reactor as shown in the next picture. In Aspen Plus™ terminology it is a Block. Hence, it is named by default as B1.



Now select the STREAMS section of the *Model Library* toolbar. Aspen Plus™ has three different stream categories, Material, Heat and Work, as shown in the next figure. Material Stream is the default icon shown.

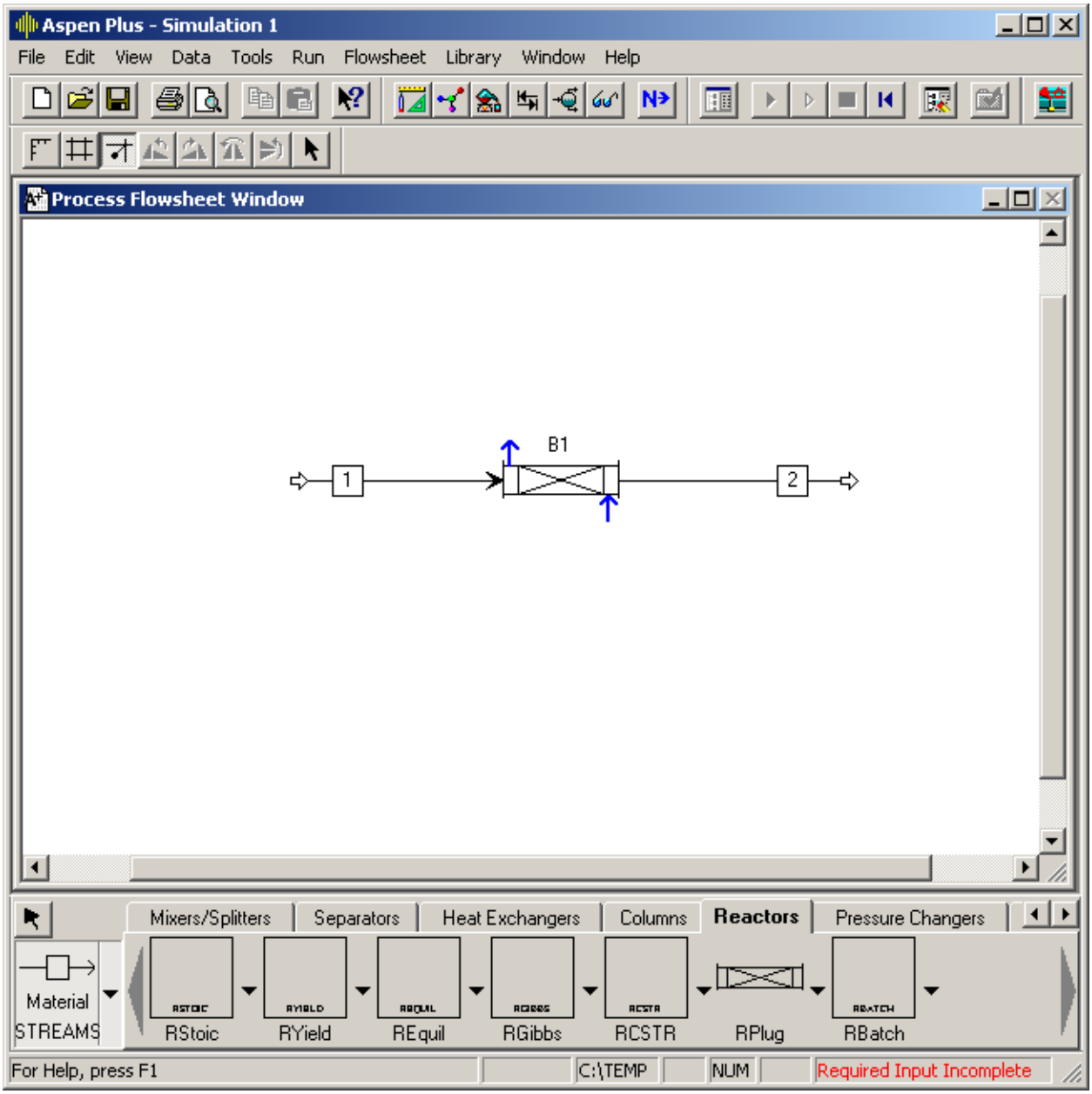


After selecting the Material Stream icon draw a line on the flowsheet from a point to the left of the block B1 towards B1. You will realize two highlighted arrows as you approach the block. The red line is the required FEED connection to RPLUG. The blue line is the optional heating or cooling fluid entrance. Select the red arrow to connect your feed stream.

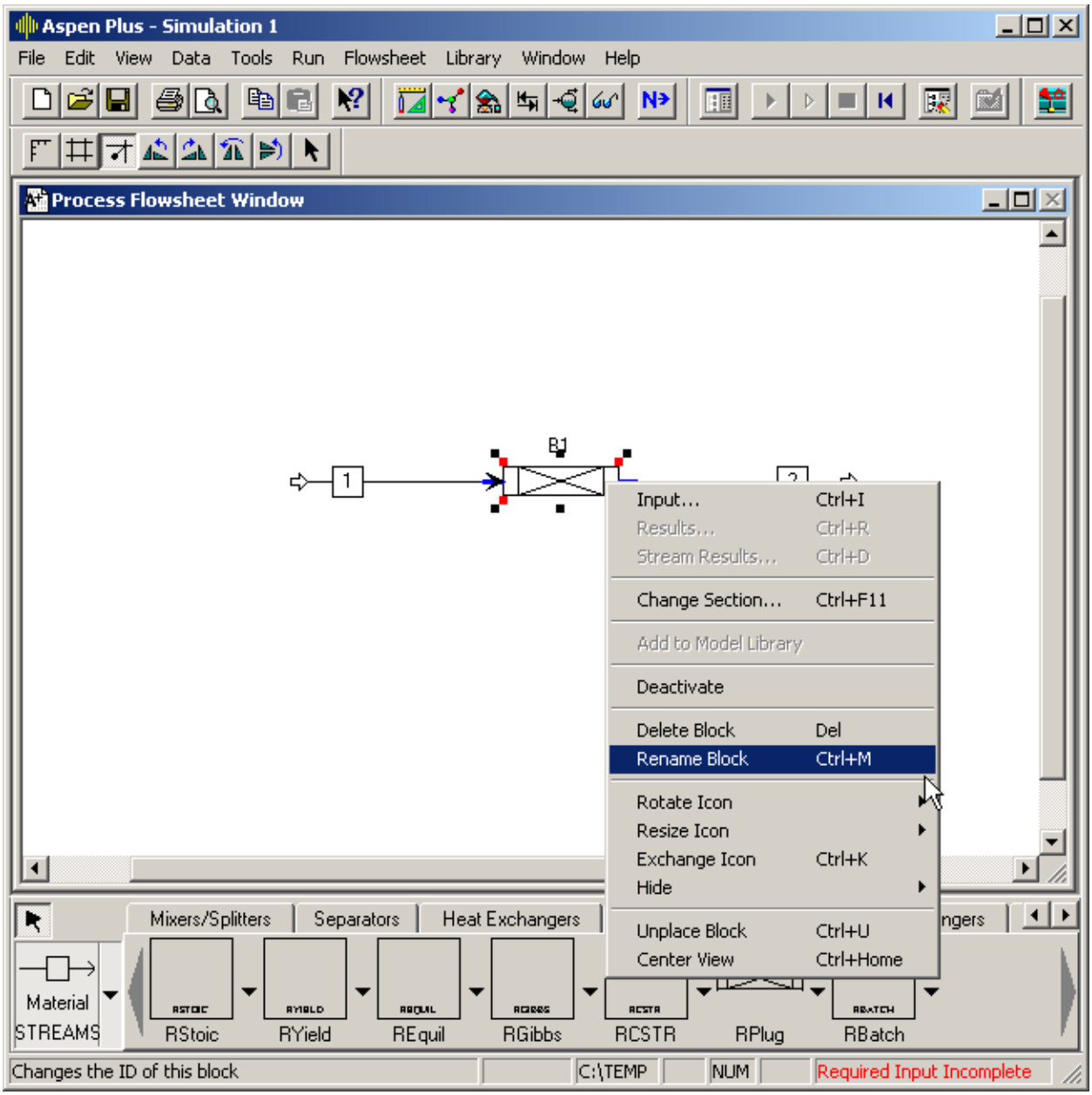


The stream is named as S1 by default. Similarly connect your product stream to the block. When you are done your flowsheet should look like the following picture. There will be still two highlighted blue arrows for heat duty requirements. As these streams are optional we can proceed with the next activity. Note the change in the status message from *Flowsheet Not Complete* to *Required Input Incomplete*. Clicking on the arrow above the streams icon will hide the blue arrows and let you freely move the icons on your flowsheet and arrange them to your liking.

One thing that might be useful is to align the streams and blocks. To do that, draw a large rectangle to select all of your icons on the flowsheet and then right click to activate a pop up menu. Select the Align Blocks entry from this pop up menu. If you do not select all icons, but only one, a different pop up menu will be activated.



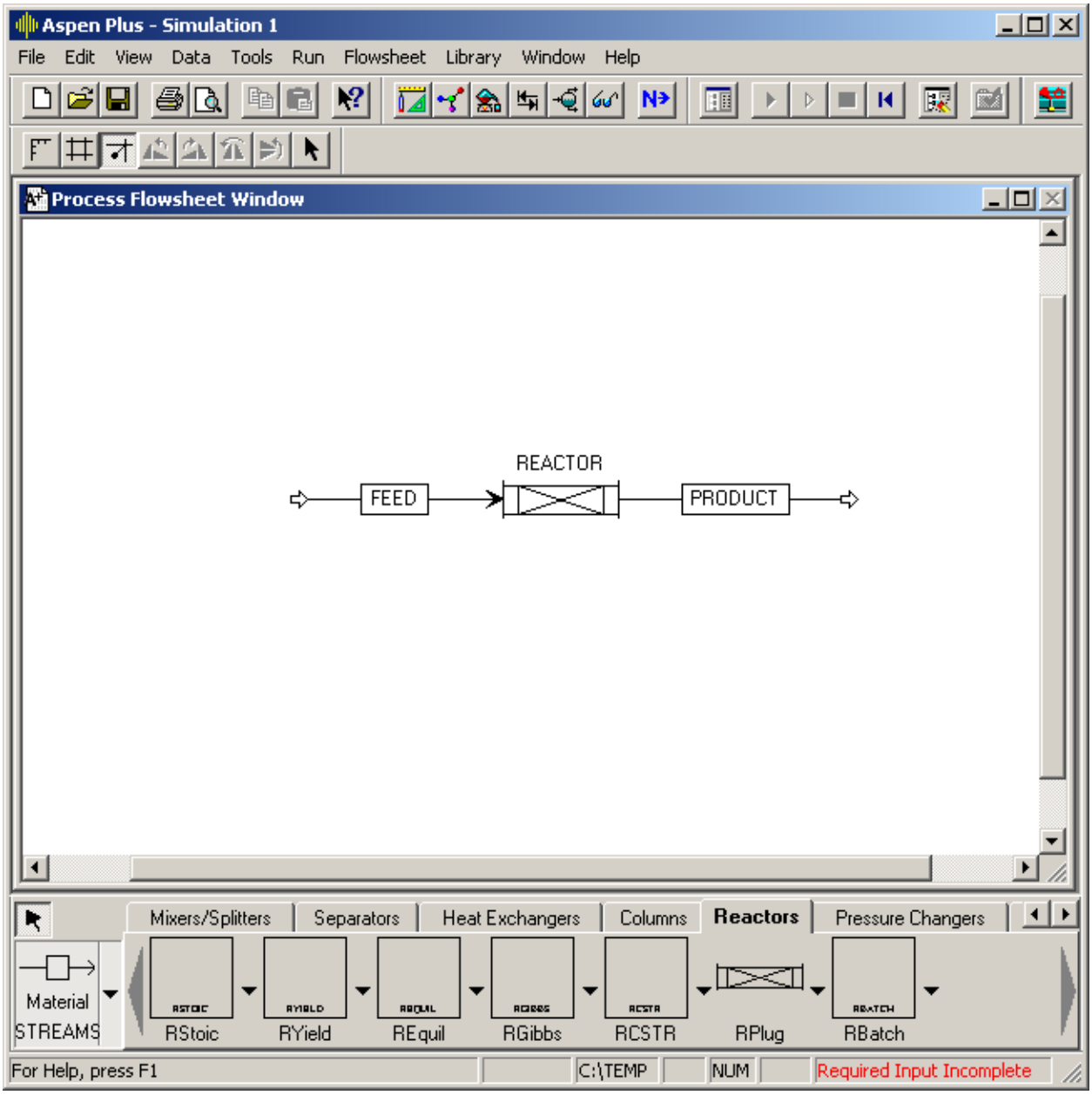
You can also rename the objects you insert onto the flowsheet. To do that highlight the object you want to rename and click the right mouse button. A pop up menu will be activated. Select the Rename Block entry from it. The next picture shows the rename operation for the block B1.



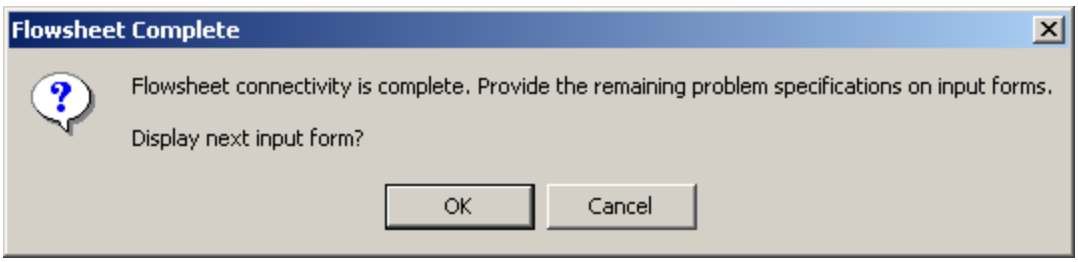
After renaming stream S1 to FEED, stream S2 to PRODUCT and B1 to REACTOR the flowsheet will look like the following picture. At this stage the flowsheet is complete and the rest of the specification is done with *Input Forms*.

Whenever you have doubts on what to do next, the lowest energy action is to click the Next Button.

This button will take you to next part of the specification or tell you what is missing from your specifications.

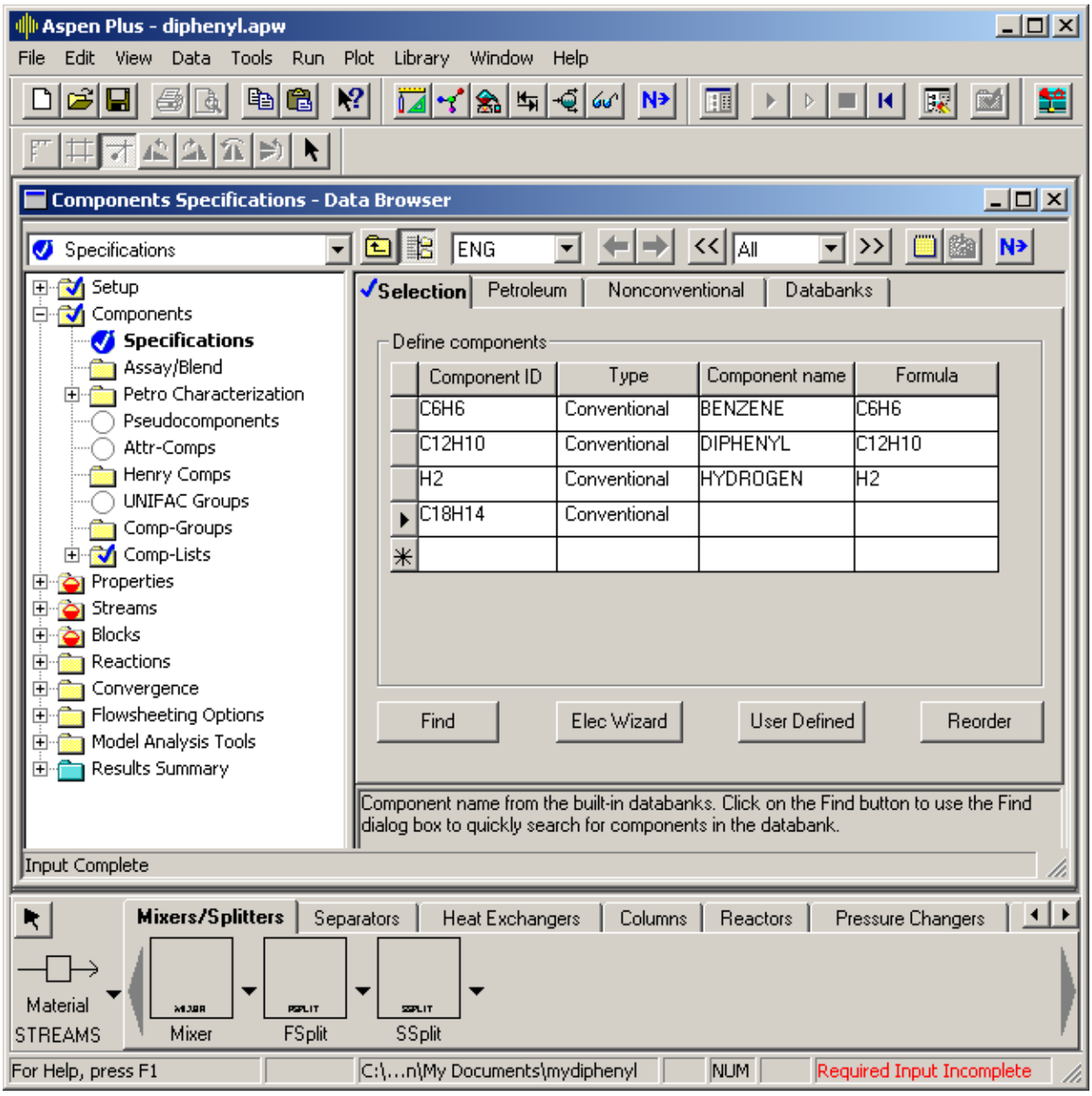


At this point, we know that the flowsheet is complete. However, we also know that parts of the required input are missing. Remember, if we are not sure what to do next we click the Next Button.

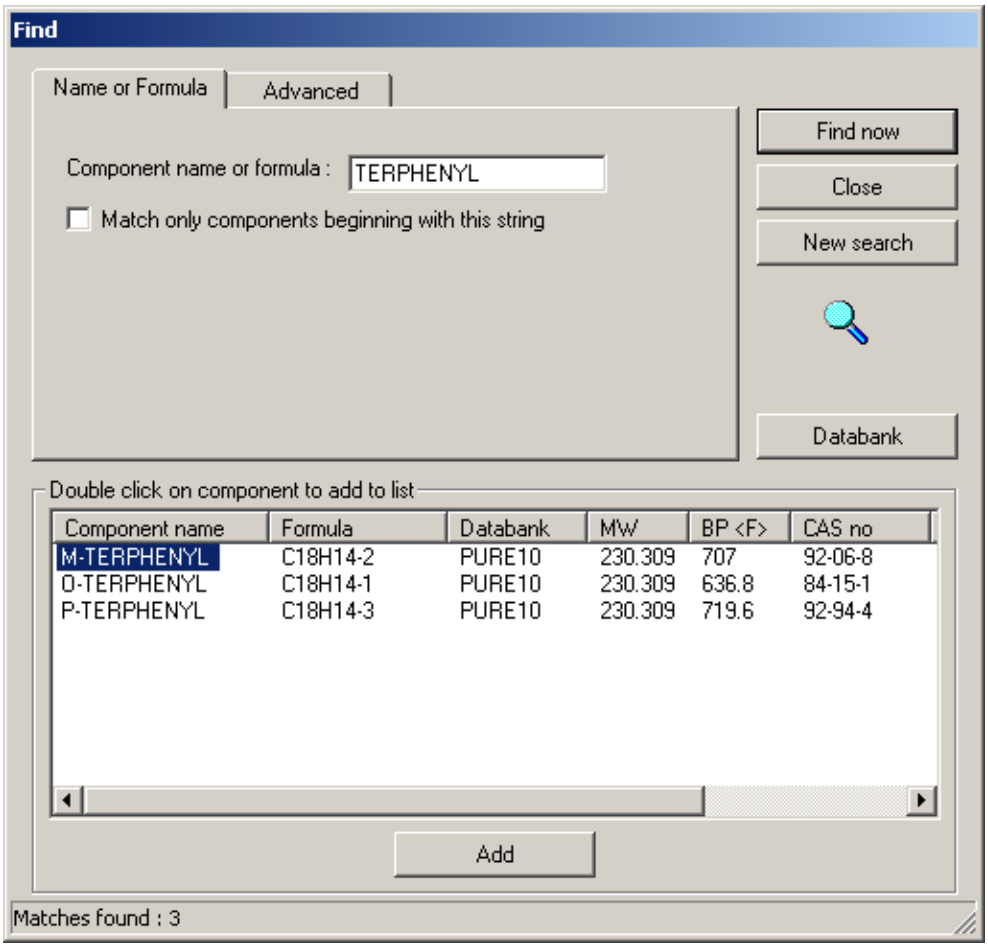


Components input forms

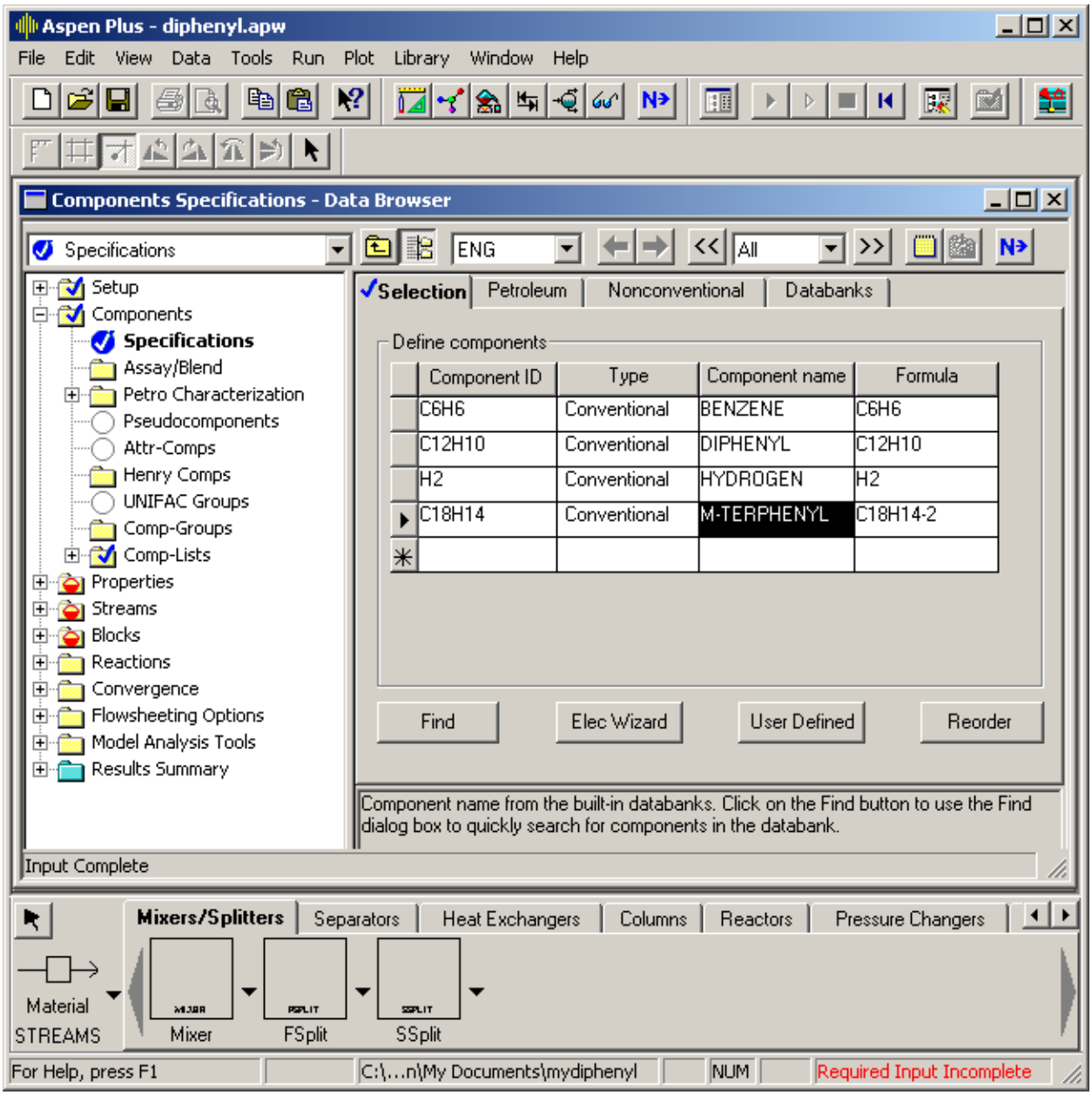
The response will be a message dialog offering to display the next input form. Clicking on ok brings up the Components section of the Data Browser.



Fill out the table as suggested in the above picture. Component ID is essentially an alias for the components. As the components we are dealing in this problem are simple enough I used their formulas as component IDs. From these component IDs Aspen Plus™ fills out the name and formula columns. However, for the fourth component it will fail because there are three isomers with the same formula: Meta-, Para-, and Ortho-terphenyl. As another hint, enter TERPHENYL in the name column of the fourth component. This will bring up a dialog box as follows:



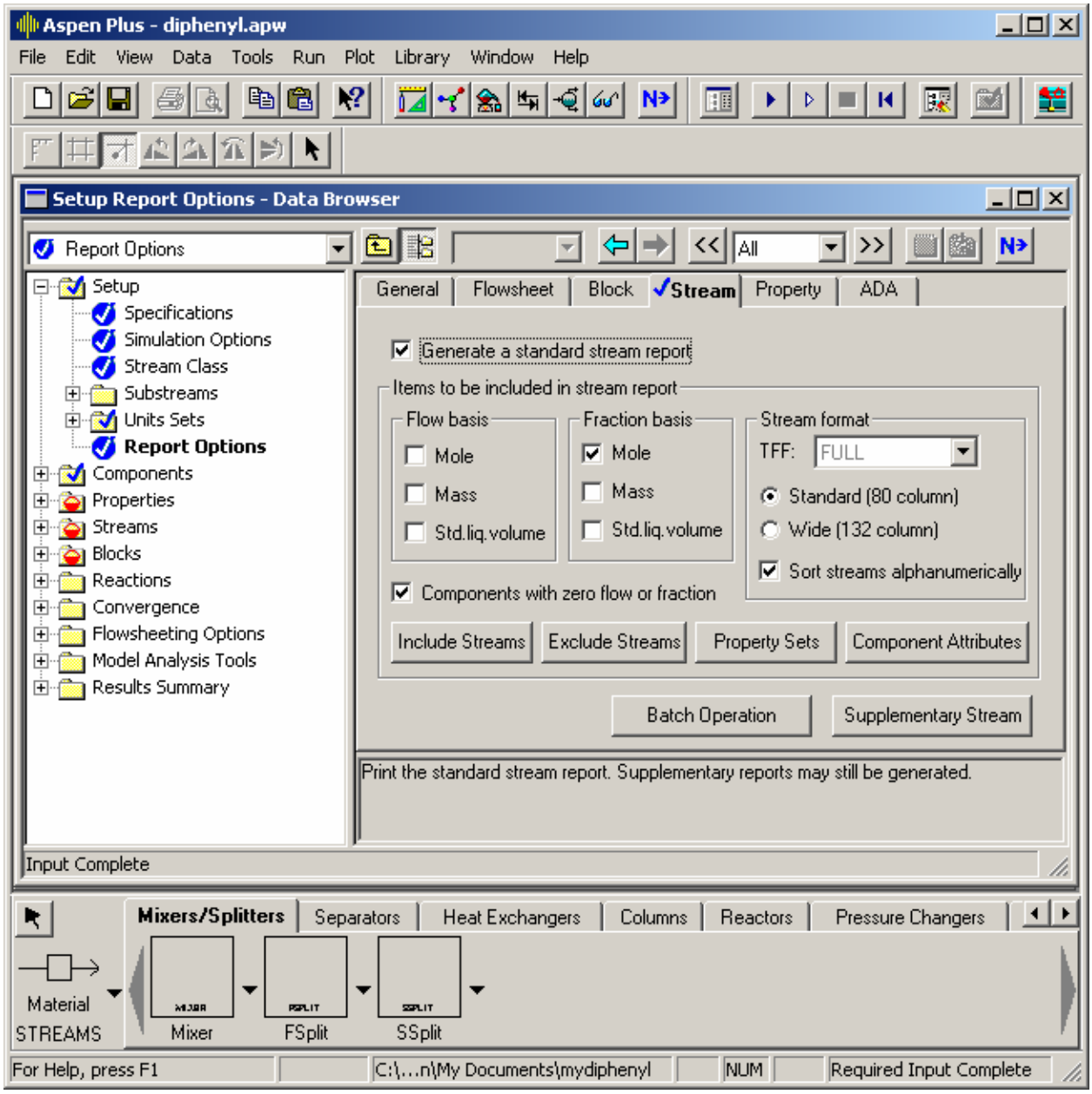
Select M-TERPHENYL, click *Add* and finally, close the dialog. Now the input form should look like the next picture.



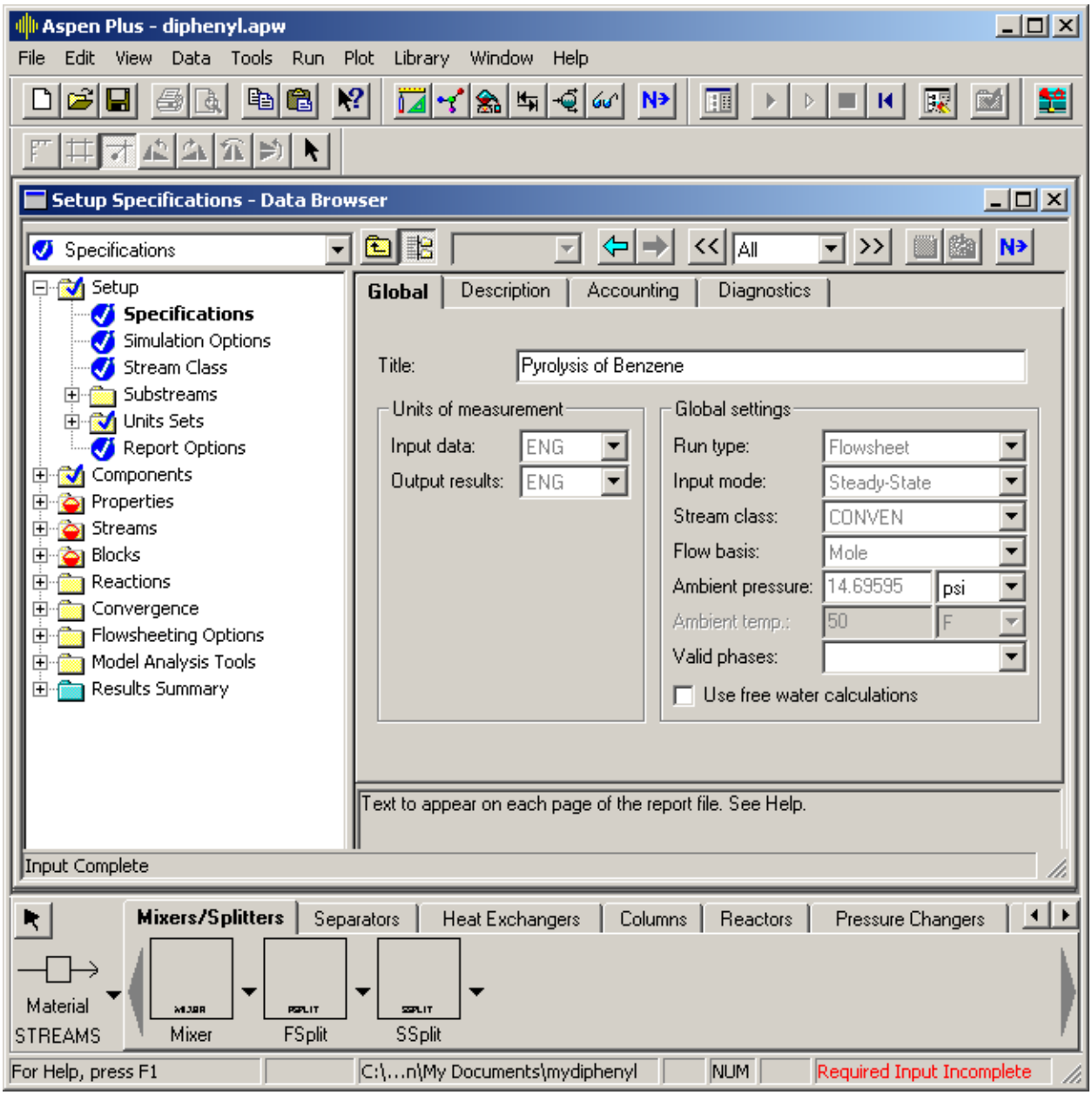
The blue check sign indicates that the minimum requirements for this section are complete. Now, hitting the Next Button will take you to the next input form. However, let's modify the defaults selected by Aspen Plus™ in the Setup section, first. Therefore close the Components section and open the *Setup* section in the *Data Browser*.

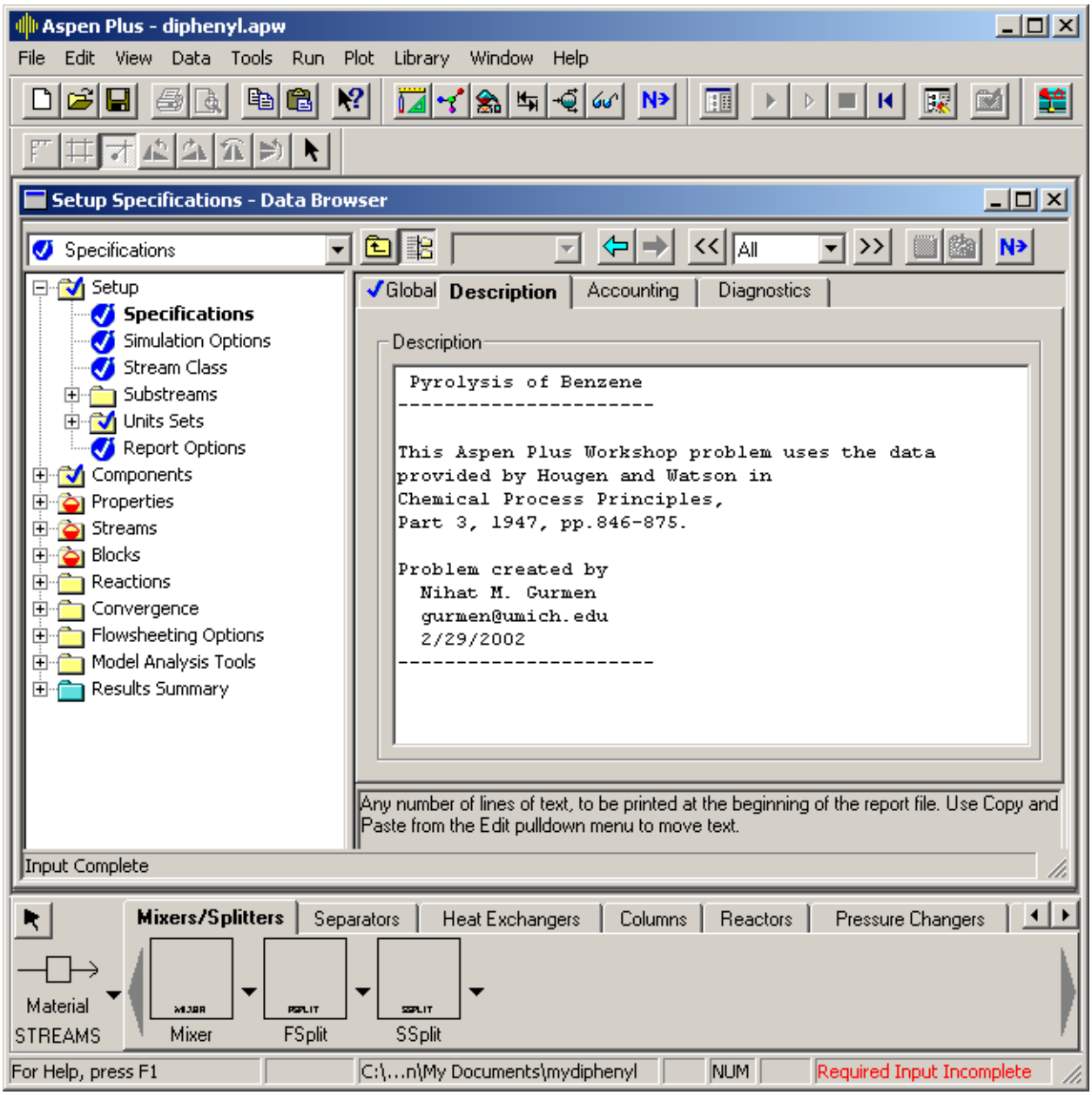
Setup input form

One useful option set to customize is the Report Options. The next picture illustrates my choices.



Although optional, it is also a good idea to fill out a title and description for your project. The next two pages show two suggestions for these entries.

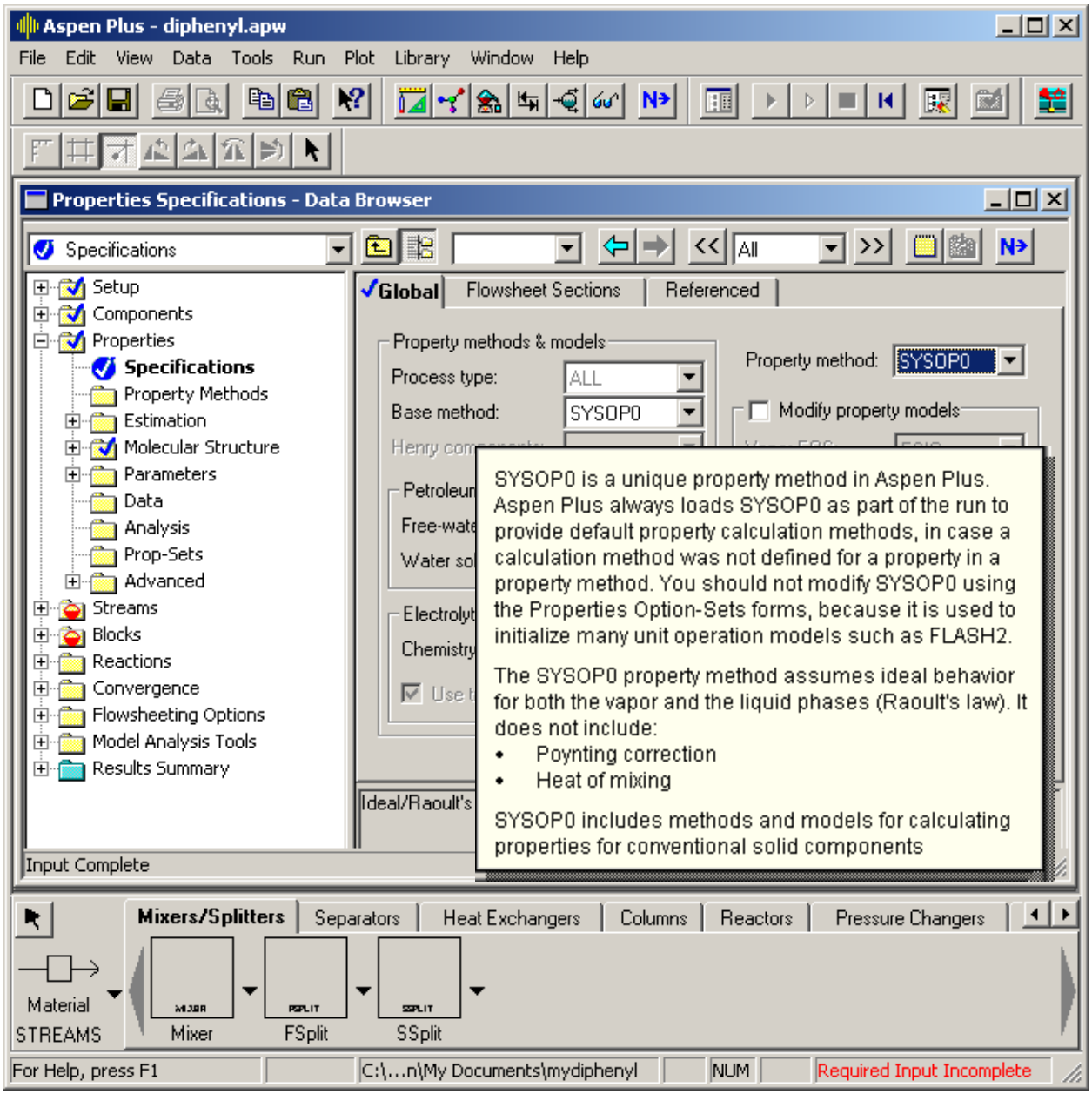

Aspen Plus - diphenyl.apw
File Edit View Data Tools Run Plot Library Window Help
Setup Specifications - Data Browser
Specifications
All
Setup
Specifications
Simulation Options
Stream Class
Substreams
Units Sets
Report Options
Components
Properties
Streams
Blocks
Reactions
Convergence
Flowsheeting Options
Model Analysis Tools
Results Summary
Global
Description
Accounting
Diagnostics
Title:
Pyrolysis of Benzene
Units of measurement
Input data:
ENG
Output results:
ENG
Global settings
Run type:
Flowsheet
Input mode:
Steady-State
Stream class:
CONVEN
Flow basis:
Mole
Ambient pressure:
14.69595
psi
Ambient temp.:
50
F
Valid phases:
Use free water calculations
Text to appear on each page of the report file. See Help.
Input Complete
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Material
STREAMS
Mixer
FSplit
SSplit
For Help, press F1
C:\...n\My Documents\mydiphenyl
NUM
Required Input Incomplete



Next Button will take you to the Properties input forms.

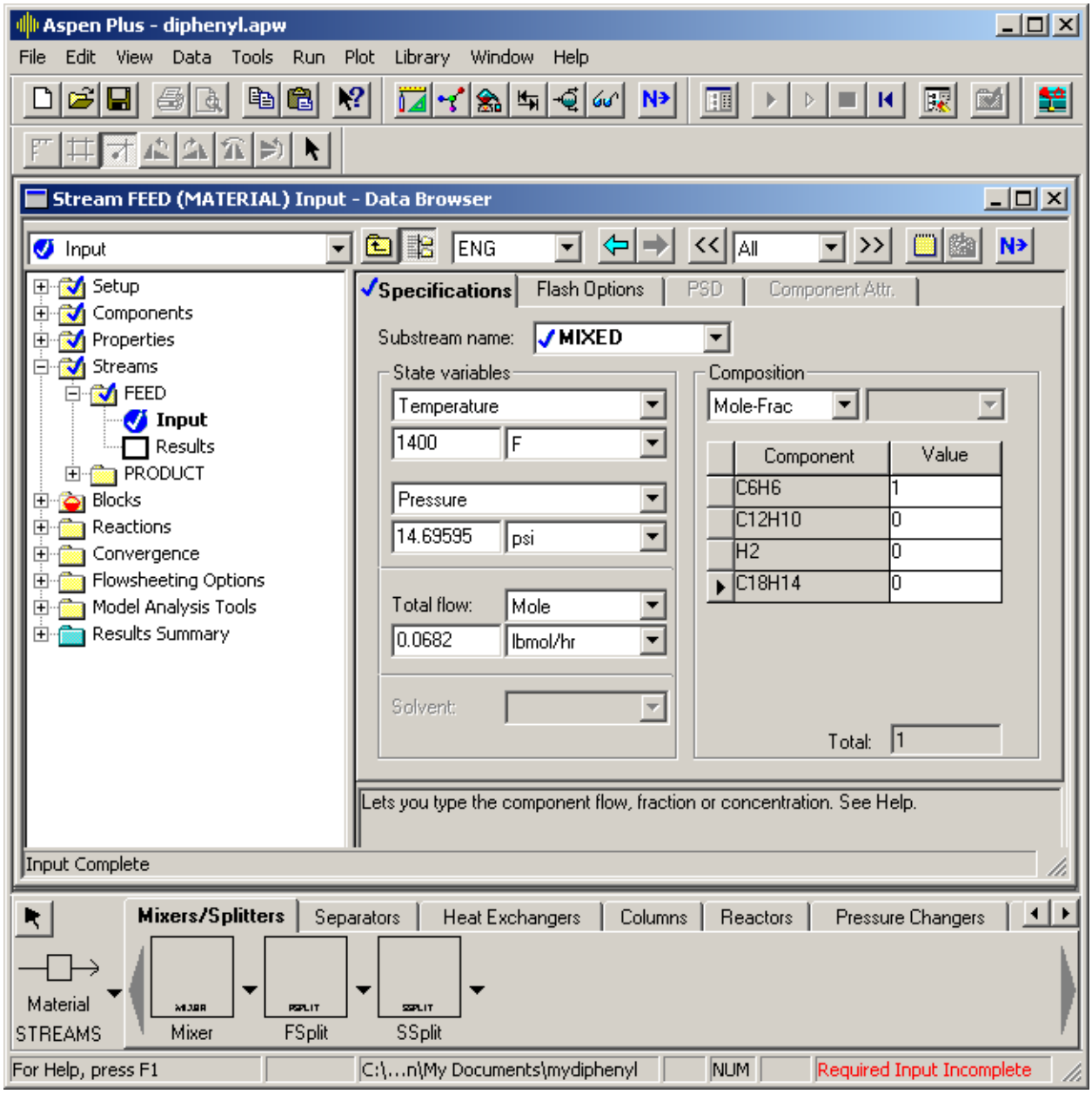
Properties input forms

In this section the parameters for various component properties are set. As the pressure is low enough ideal conditions will be assumed. SYSOP0 is the property method in Aspen Plus™ that provides ideal behavior in liquid and vapor phases. You can get information about a feature by selecting the *What's this?* entry from Help menu and clicking on the feature you are interested in. Most of the time a yellow tool tip box will pop up with a short reasonable description.



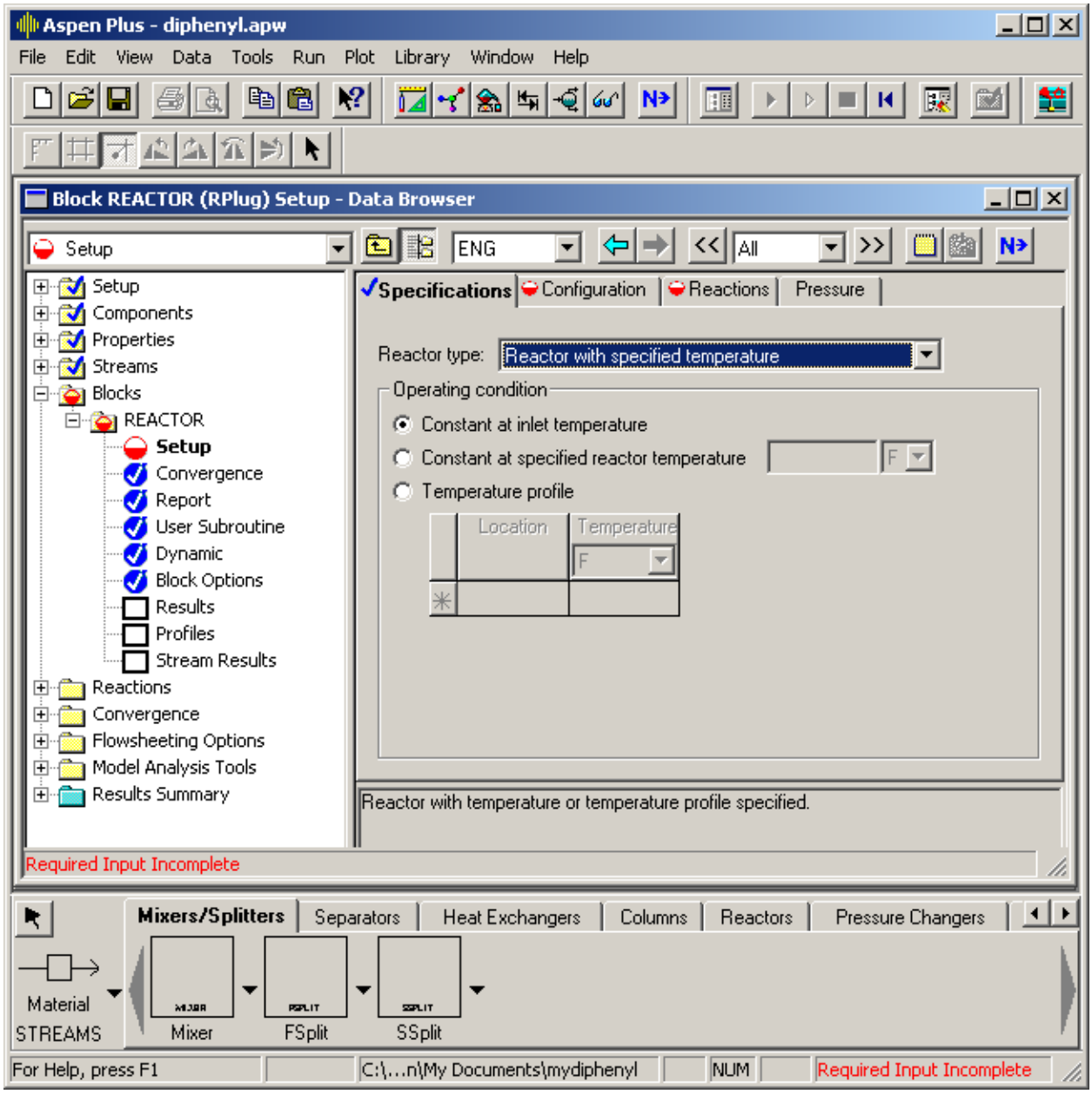
Streams input forms

FEED steam is assumed to consist of pure benzene at atmospheric pressure with conditions specified in the example problem description.

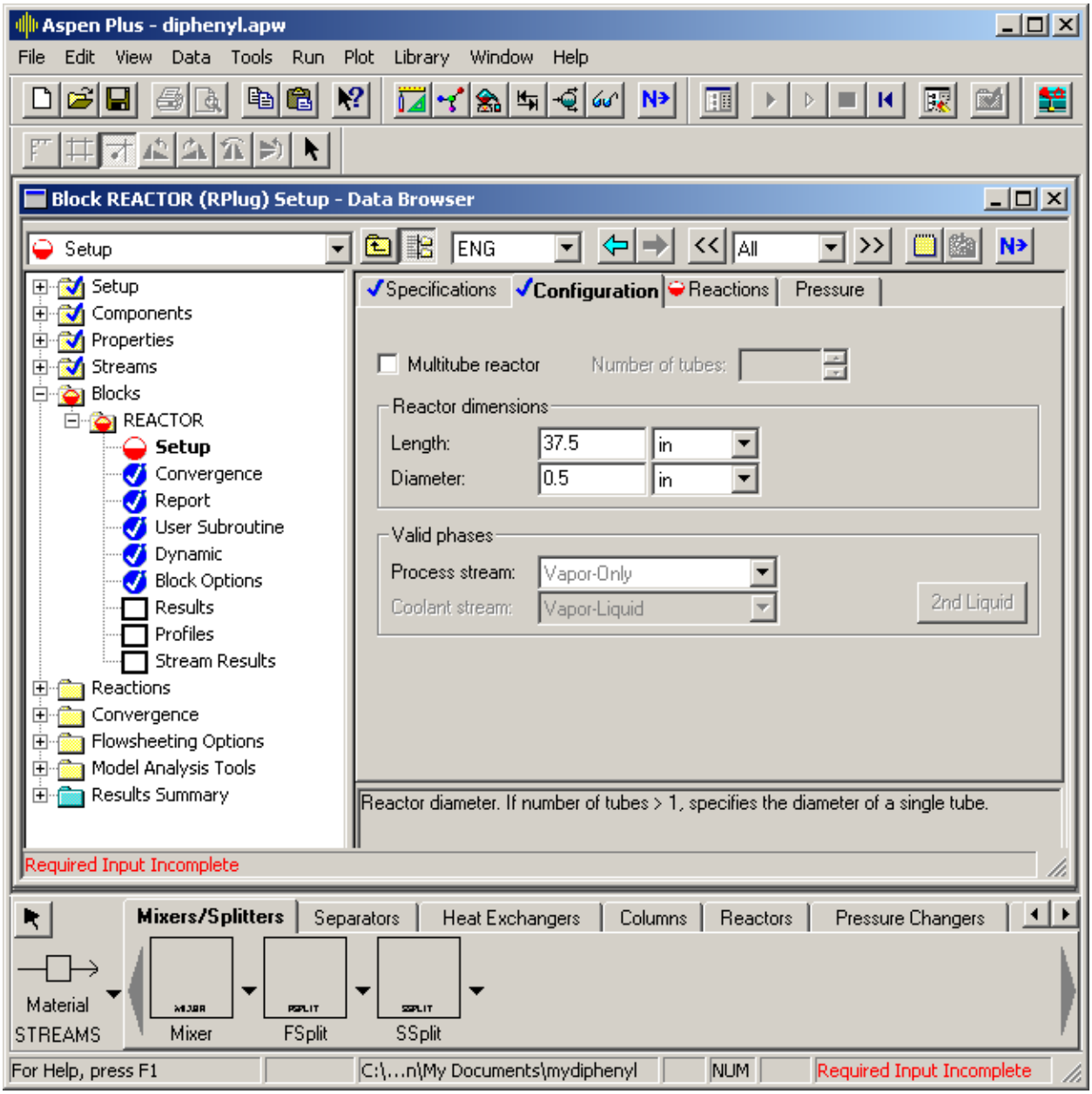


Blocks input forms

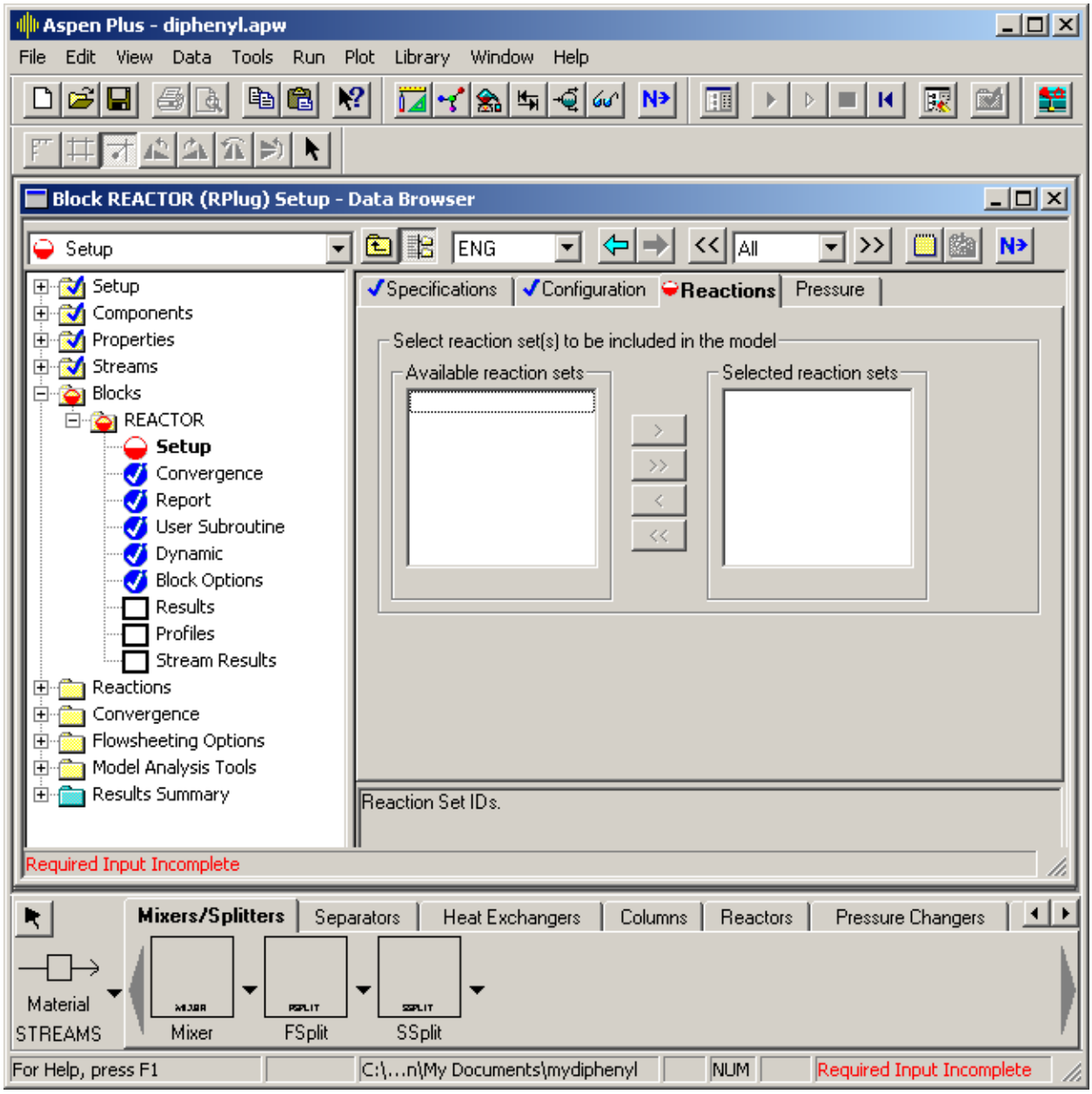
Now we will specify the reactor specifications. First, we assume isothermal operation at inlet conditions.



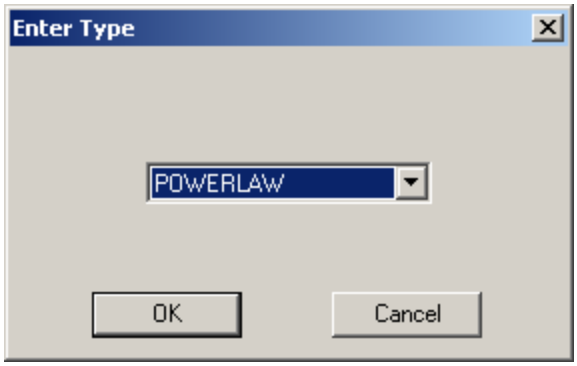
Next, we enter the physical dimensions of the reactor. Note the option about the multitube reactors.

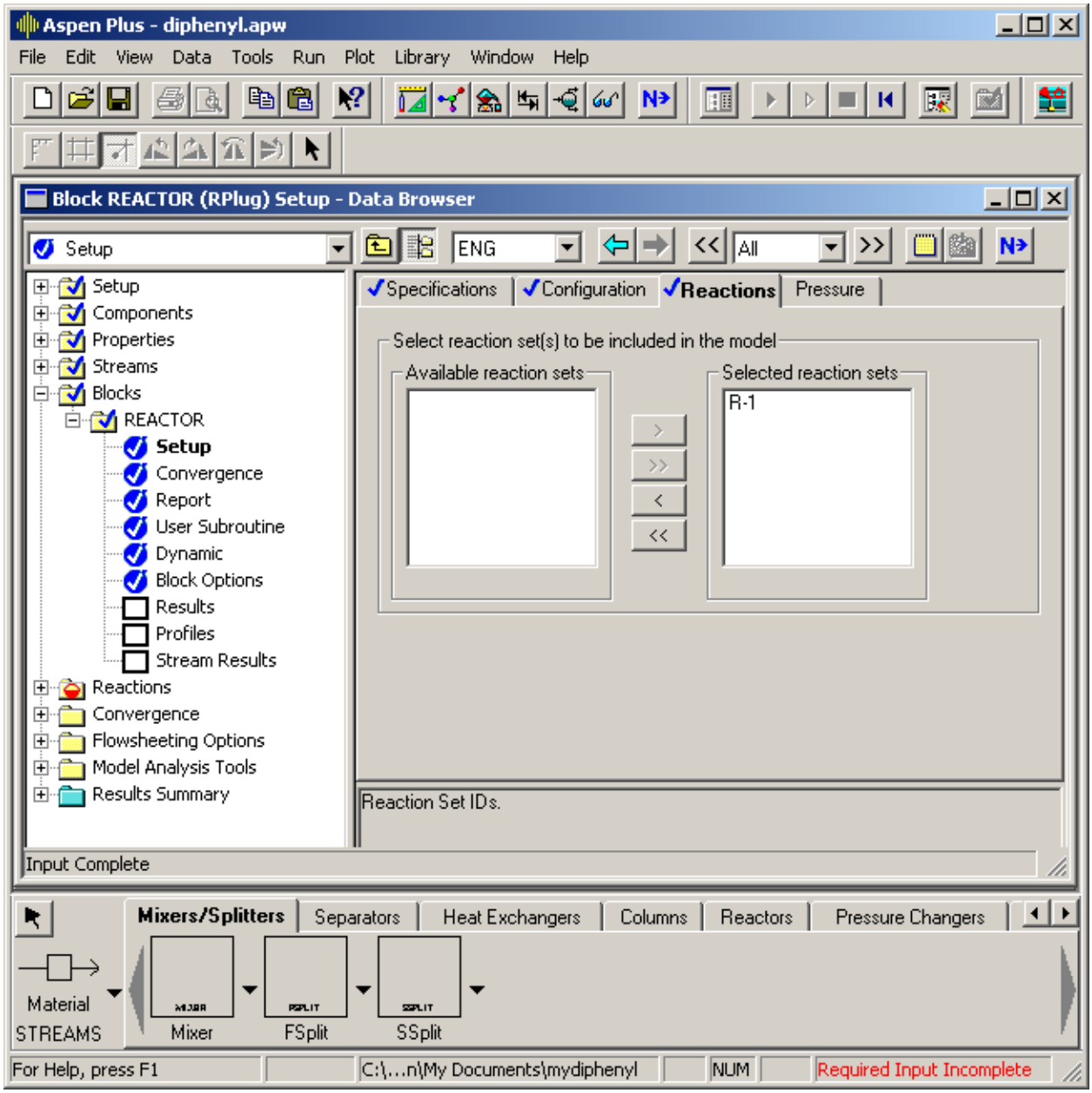


Finally, we define a reaction set for our simulation. The default name R-1 is fine.



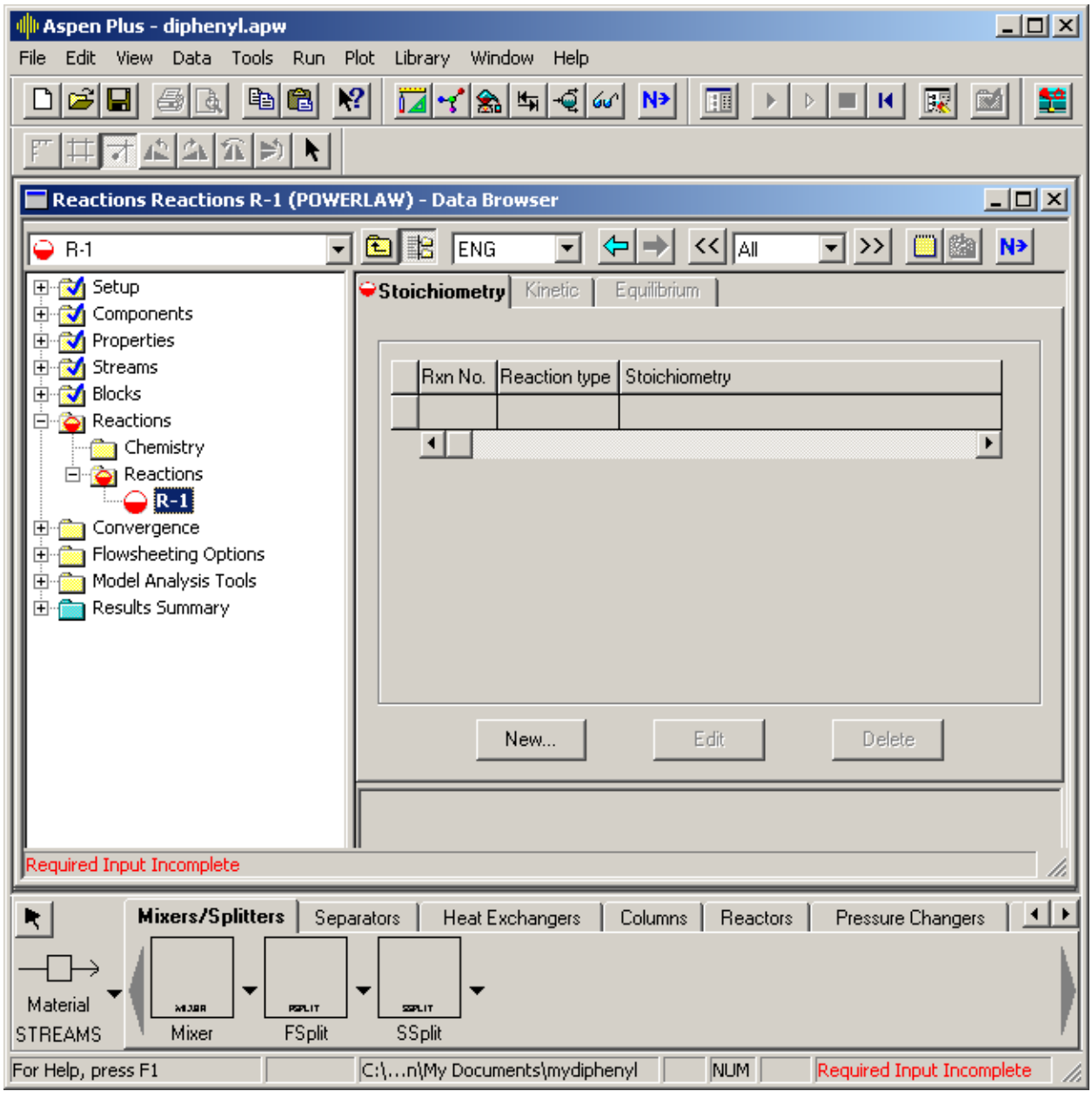
We will represent reactions with power law kinetics in this reaction set.

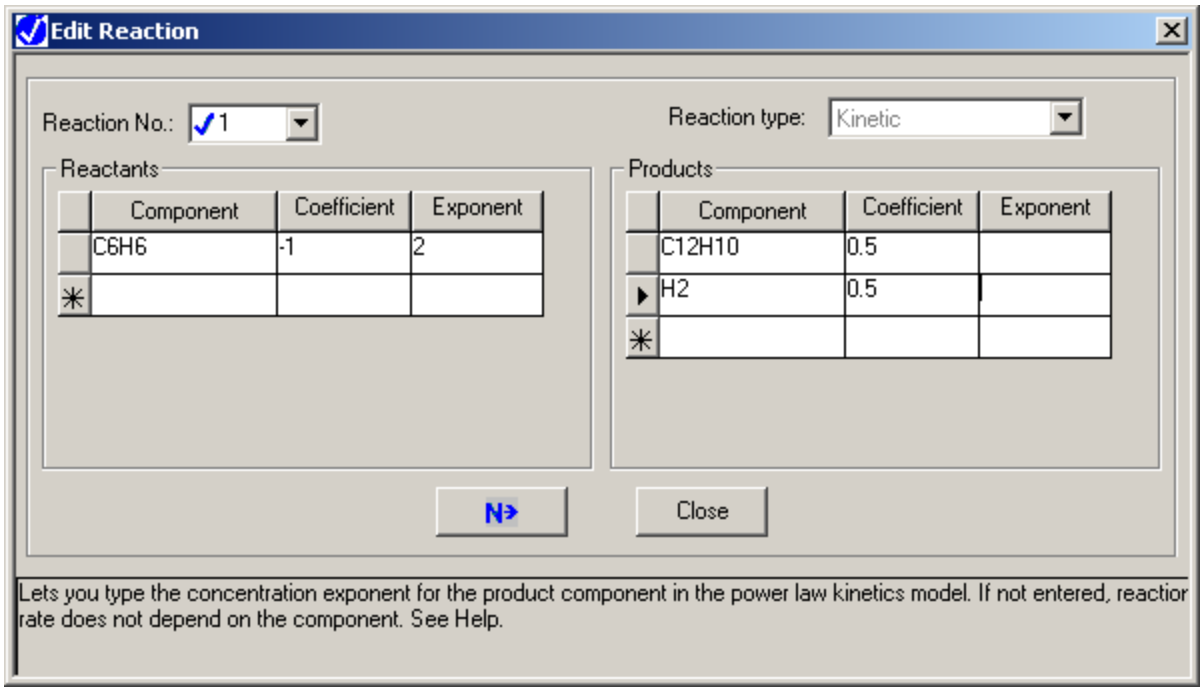




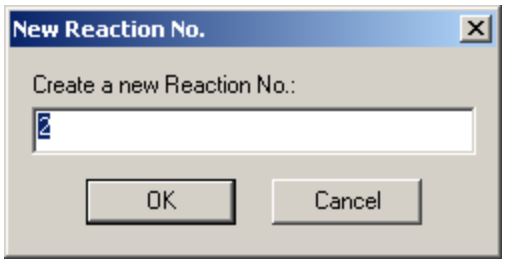
Reactions input forms

In these forms we will first enter the stoichiometric and power law coefficients for all components in each reaction, and then we will move on to kinetics tab. In Aspen Plus™ notation we will represent the two reversible reactions as four separate reactions, each with their own kinetic expression. Select New to proceed and fill the boxes as suggested by the following pictures.



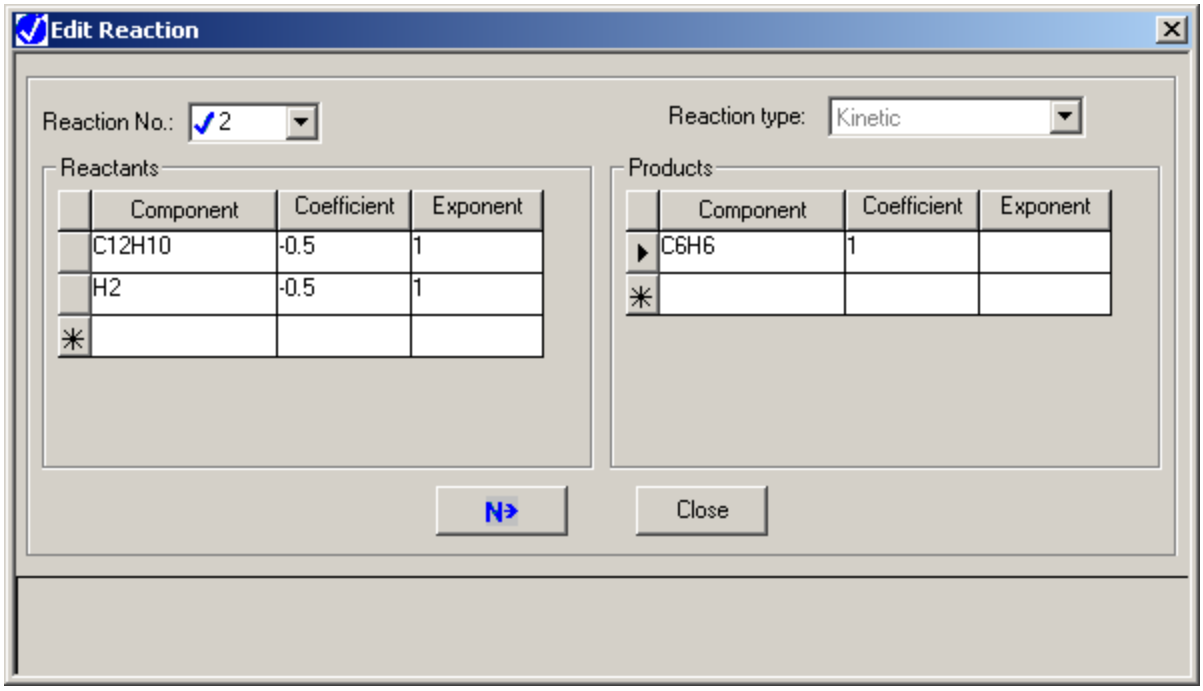


After completing the first reaction select New from Reaction No. list. Enter 2 for reaction number as suggested below.

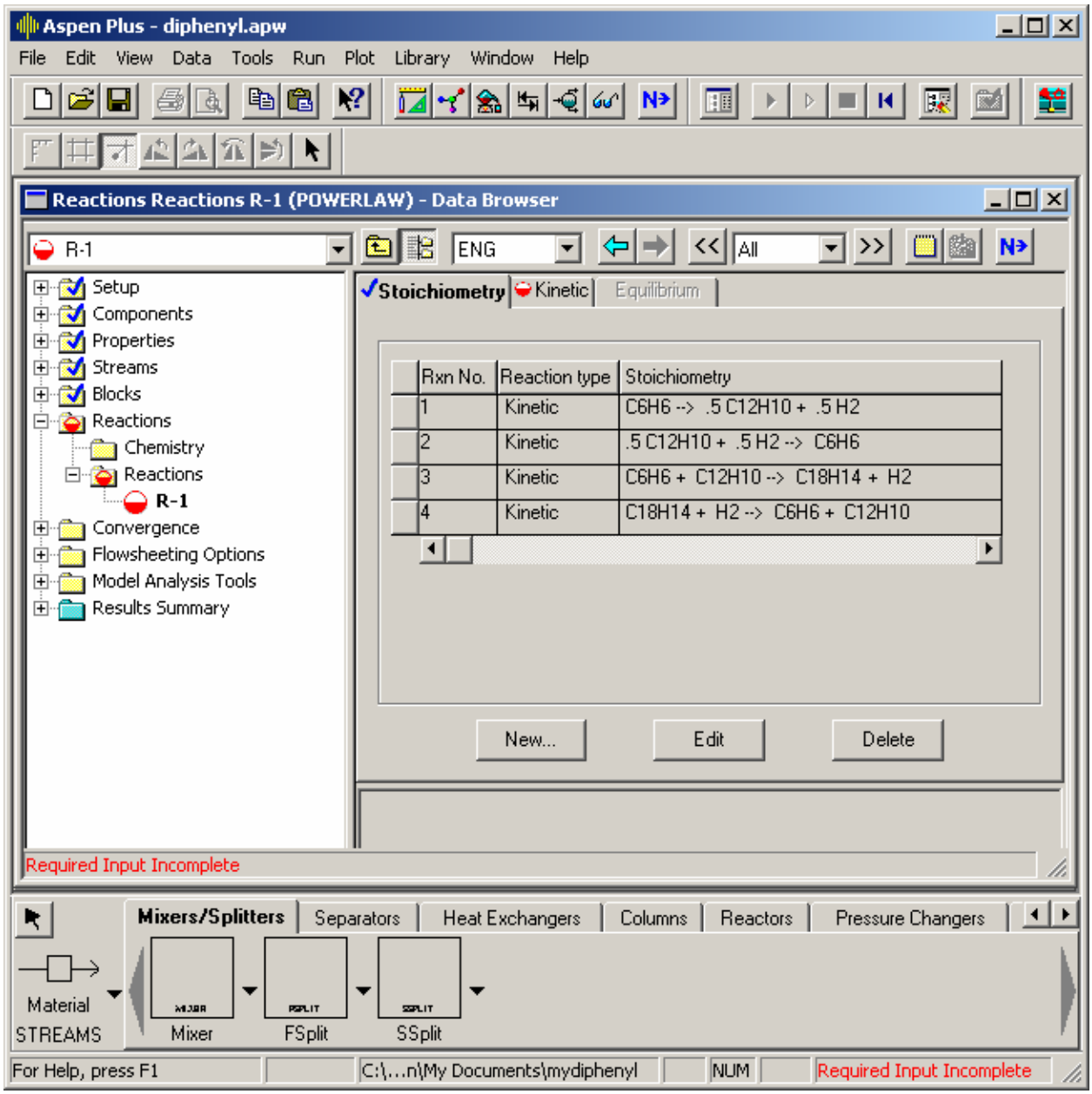


Next picture will show the coefficients for the reversed part of the first reaction. In Aspen Plus™ notation, this will be our 2nd reaction

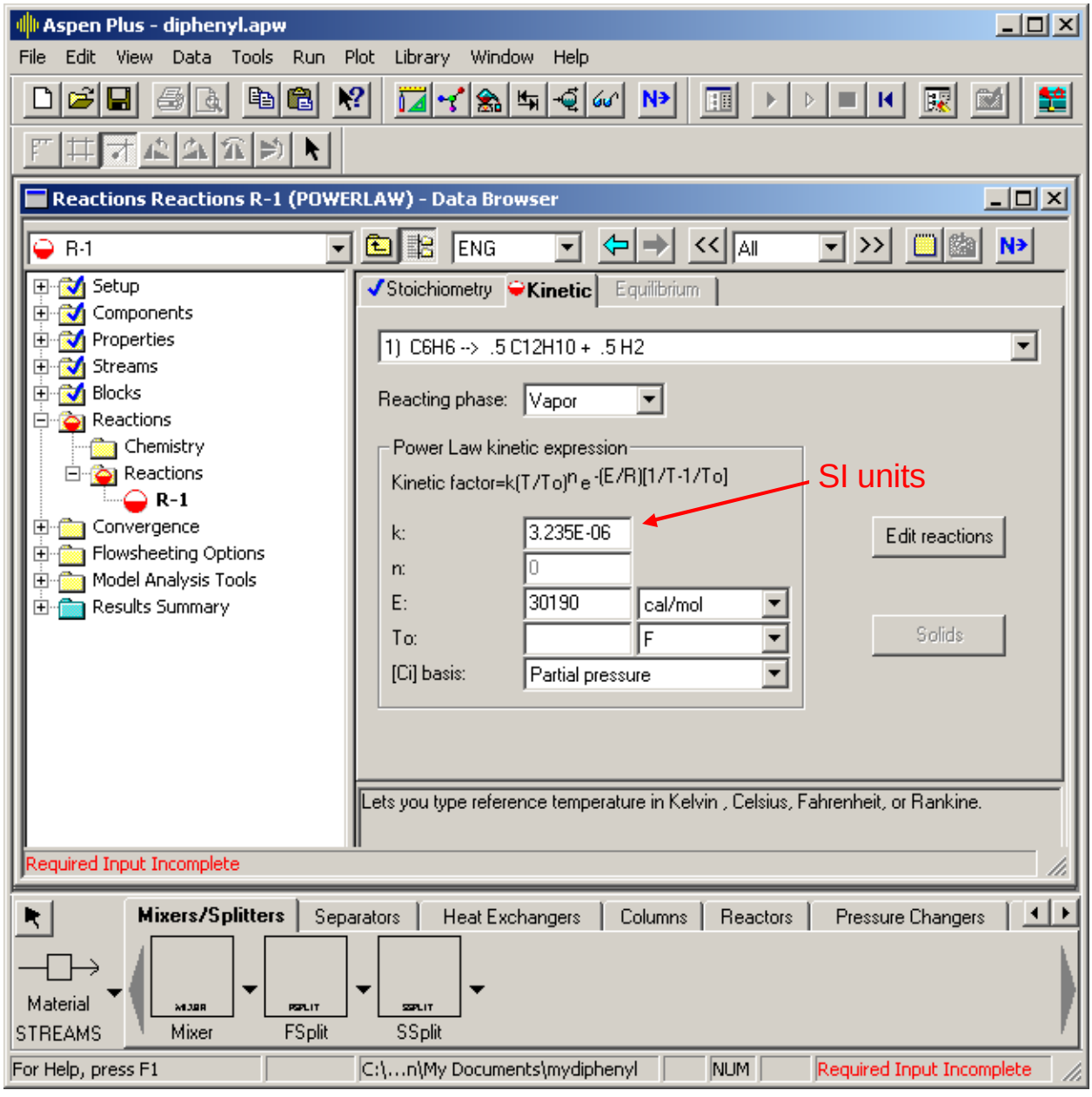
In these entries note that we brought all species on a “per mole of benzene” basis. This is an important detail.

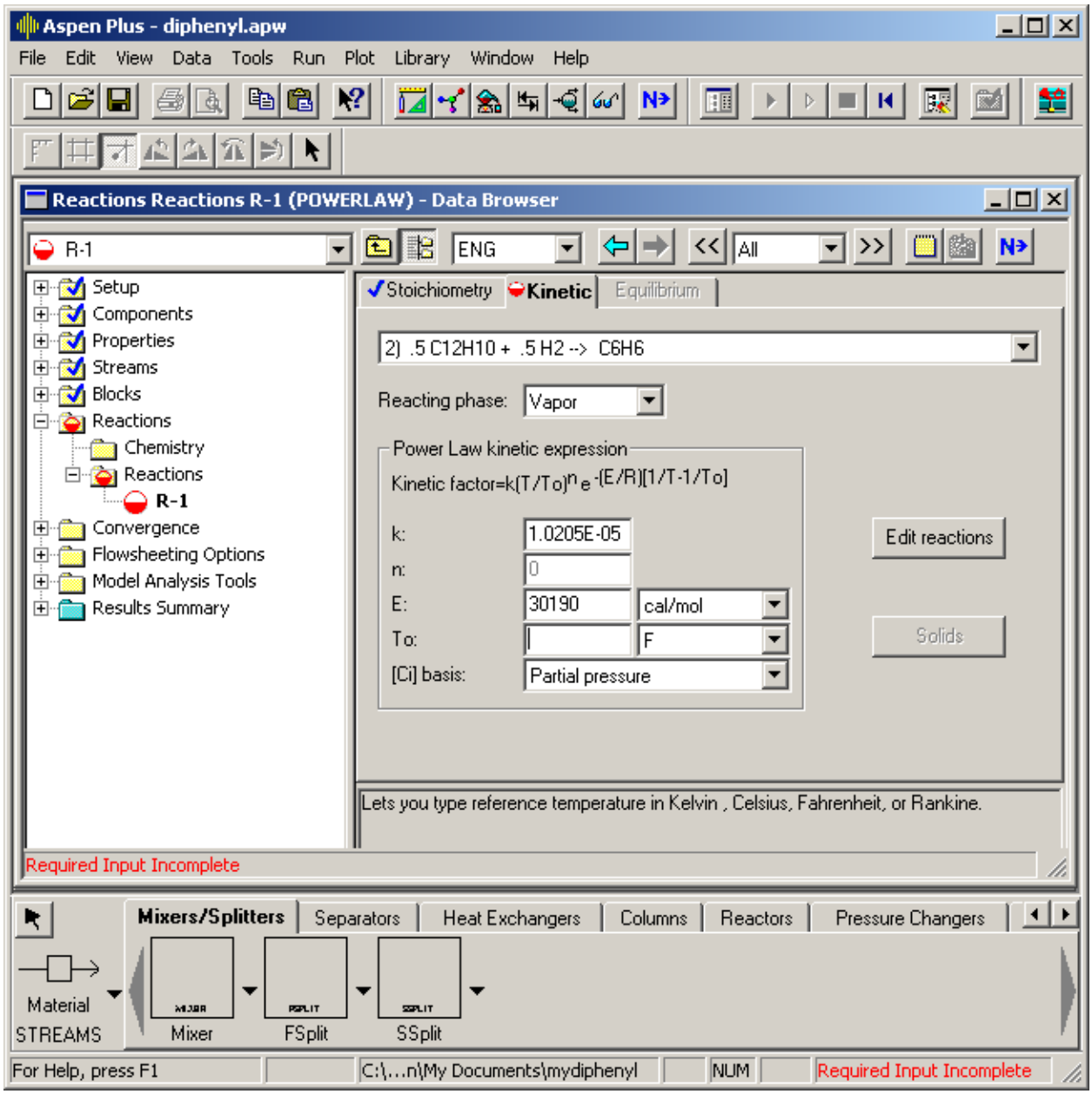


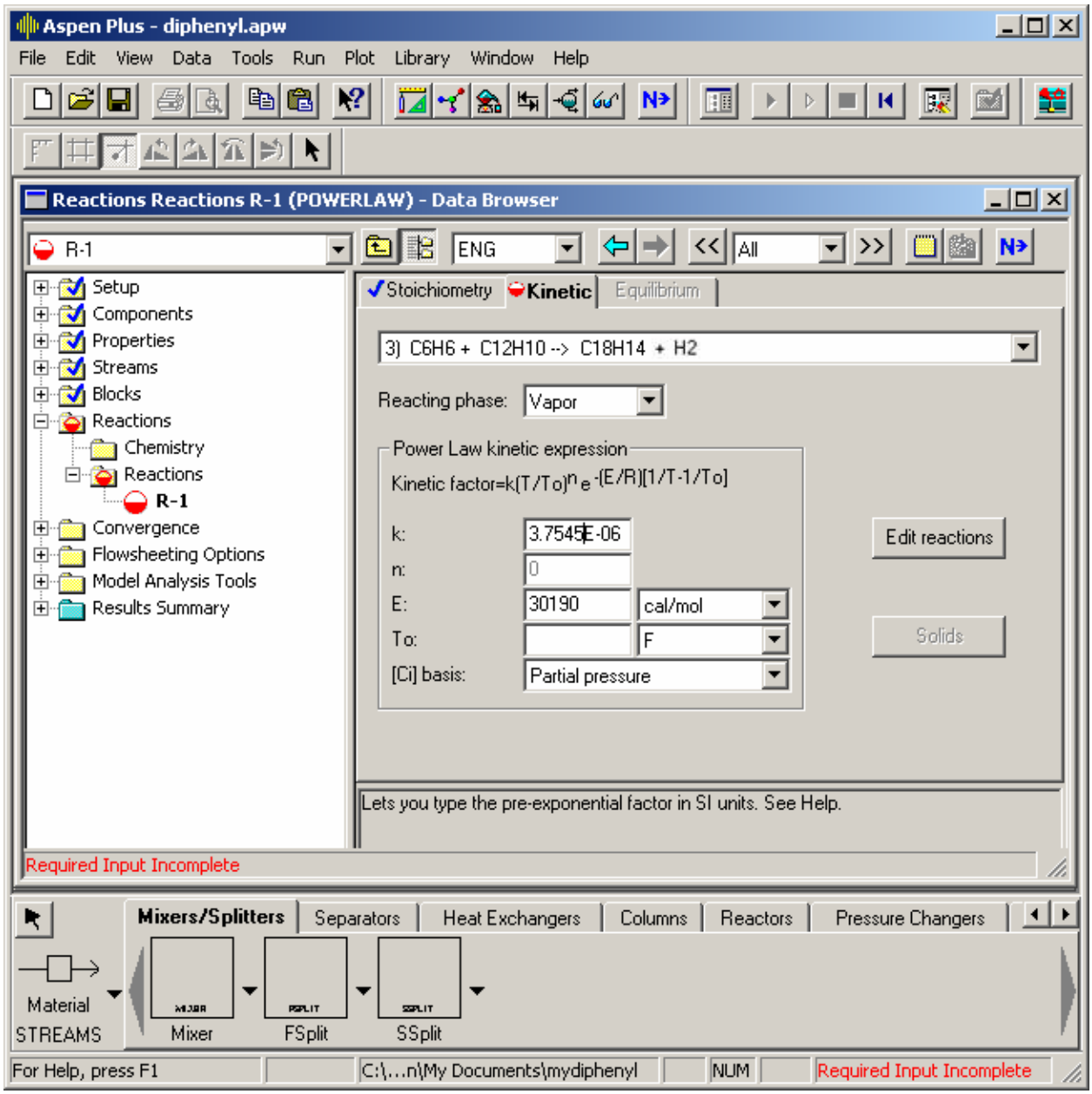
Similarly, enter the last two equations. The next screen will show the resulting stoichiometric relations.

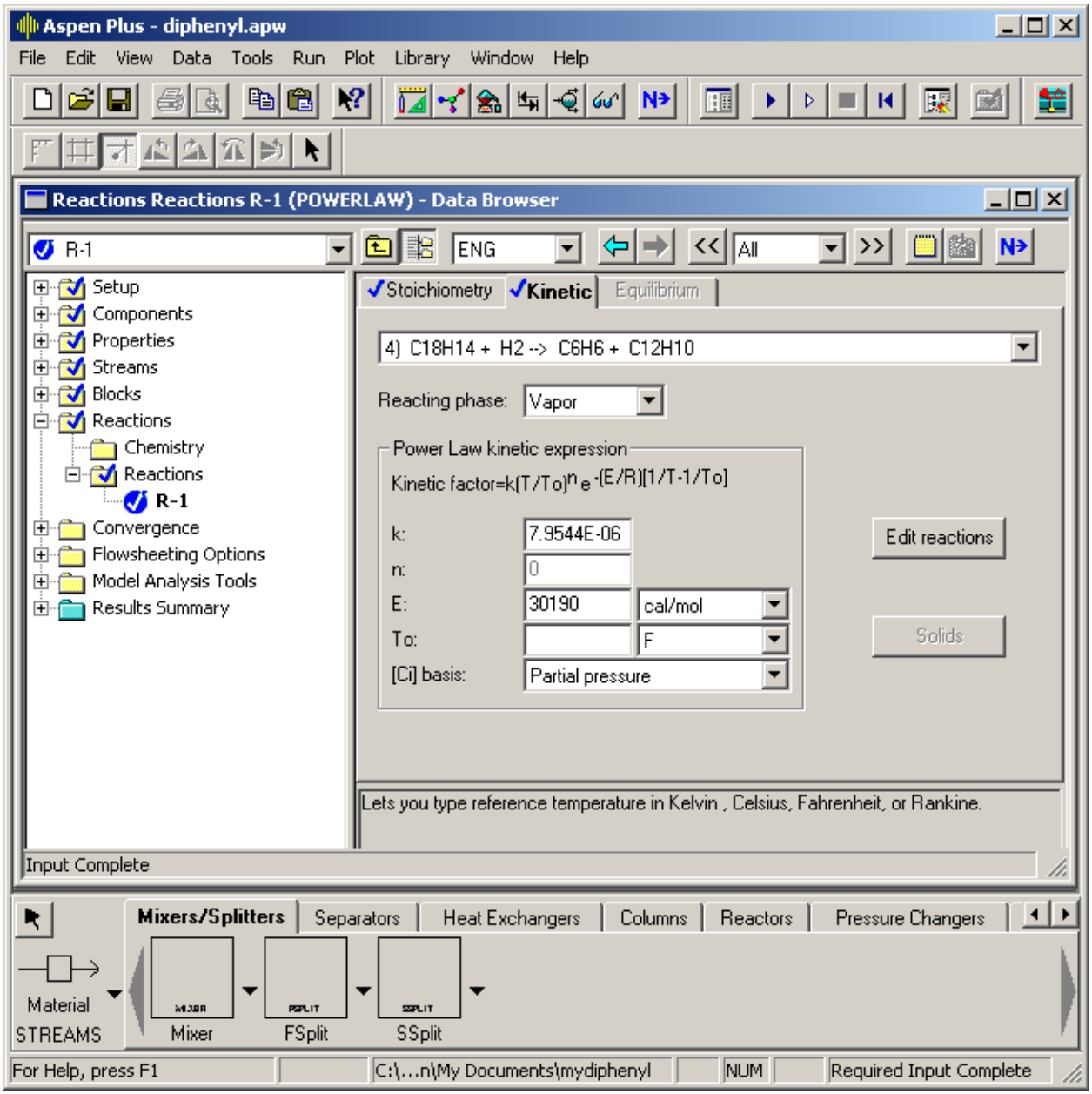

Aspen Plus - diphenyl.apw
File Edit View Data Tools Run Plot Library Window Help
Reactions Reactions R-1 (POWERLAW) - Data Browser
R-1
ENG
All
Setup
Components
Properties
Streams
Blocks
Reactions
Chemistry
Reactions
R-1
Convergence
Flowsheeting Options
Model Analysis Tools
Results Summary
Stoichiometry
Kinetic
Equilibrium
Rxn No. Reaction type Stoichiometry
1 Kinetic C6H6 --> .5 C12H10 + .5 H2
2 Kinetic .5 C12H10 + .5 H2 --> C6H6
3 Kinetic C6H6 + C12H10 --> C18H14 + H2
4 Kinetic C18H14 + H2 --> C6H6 + C12H10
New...
Edit
Delete
Required Input Incomplete
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Material
STREAMS
Mixer
FSplit
SSplit
For Help, press F1
C:\...n\My Documents\mydiphenyl
NUM
Required Input Incomplete

The kinetics coefficients are specified in the following four pages. Note that the definition of the kinetic factor expression is a little different. It is a more general definition for the specific reaction rate constant. When T_o is ignored Aspen Plus™ defaults back to simpler Arrhenius Equation. Also note that k should be specified in SI units regardless of the units used elsewhere.

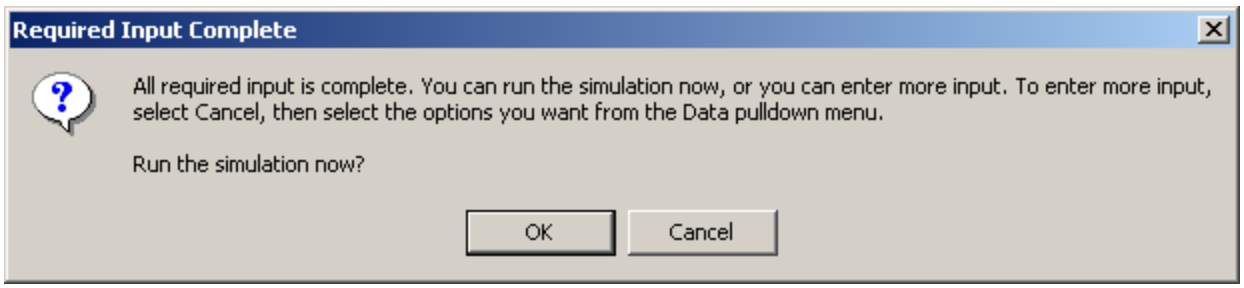



Aspen Plus - diphenyl.apw
File Edit View Data Tools Run Plot Library Window Help
Reactions Reactions R-1 (POWERLAW) - Data Browser
R-1
ENG
All
Setup
Components
Properties
Streams
Blocks
Reactions
Chemistry
Reactions
R-1
Convergence
Flowsheeting Options
Model Analysis Tools
Results Summary
Stoichiometry
Kinetic
Equilibrium
2) .5 C12H10 + .5 H2 --> C6H6
Reacting phase: Vapor
Power Law kinetic expression
Kinetic factor=k(T/To)^n e^-(E/R)[1/T-1/To]
k: 1.0205E-05
n: 0
E: 30190 cal/mol
To: F
[Ci] basis: Partial pressure
Edit reactions
Solids
Lets you type reference temperature in Kelvin , Celsius, Fahrenheit, or Rankine.
Required Input Incomplete
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Material
STREAMS
Mixer
FSplit
SSplit
For Help, press F1
C:\...n\My Documents\mydiphenyl
NUM
Required Input Incomplete


Aspen Plus - diphenyl.apw
File Edit View Data Tools Run Plot Library Window Help
Reactions Reactions R-1 (POWERLAW) - Data Browser
R-1
ENG
All
Setup
Components
Properties
Streams
Blocks
Reactions
Chemistry
Reactions
R-1
Convergence
Flowsheeting Options
Model Analysis Tools
Results Summary
Stoichiometry
Kinetic
Equilibrium
3) C6H6 + C12H10 --> C18H14 + H2
Reacting phase: Vapor
Power Law kinetic expression
Kinetic factor=k(T/To)^n e^-(E/R)[1/T-1/To]
k: 3.7545E-06
n: 0
E: 30190 cal/mol
To: F
[Ci] basis: Partial pressure
Edit reactions
Solids
Lets you type the pre-exponential factor in SI units. See Help.
Required Input Incomplete
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Material
STREAMS
Mixer
FSplit
SSplit
For Help, press F1
C:\...n\My Documents\mydiphenyl
NUM
Required Input Incomplete

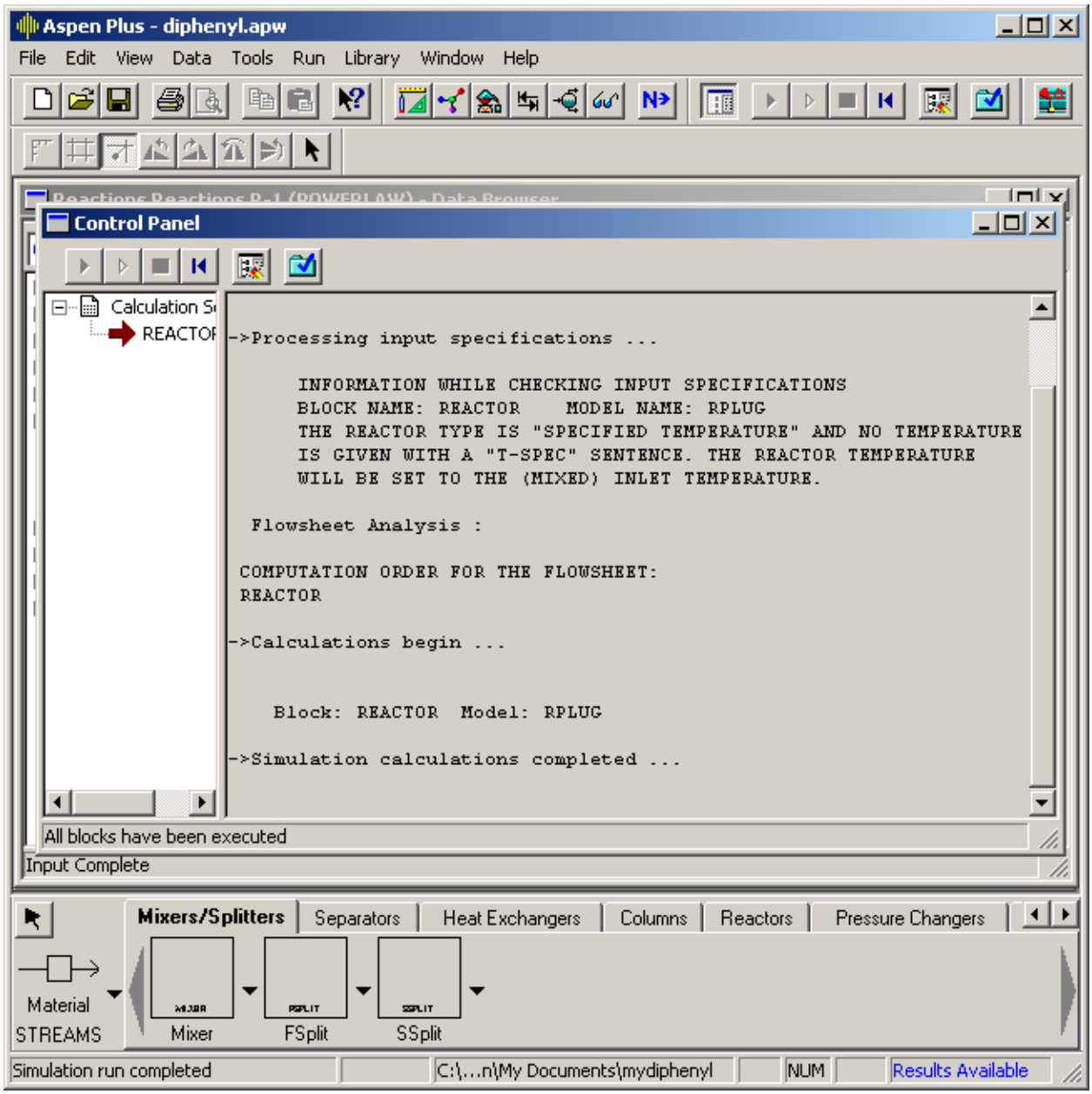


All required input is now complete. We are ready to run the simulation. Clicking the Next Button will invoke the following dialog.



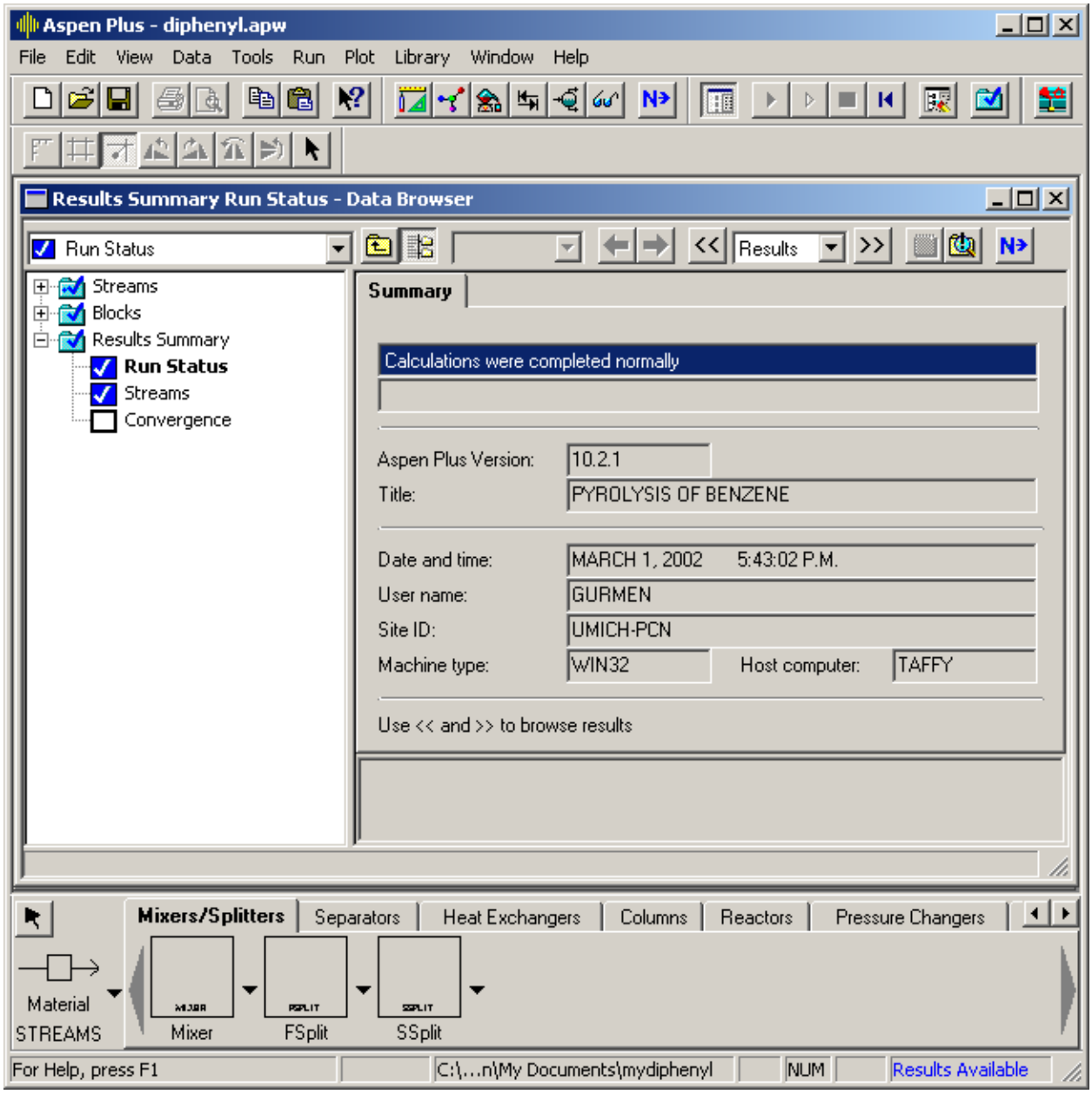
Control Panel

Control panel will show the progress of our simulation. All warning, error, and status messages will also be presented in this screen. After the simulation completes successfully we can analyze them pressing the blue folder icon with check mark on the Control Panel toolbar.

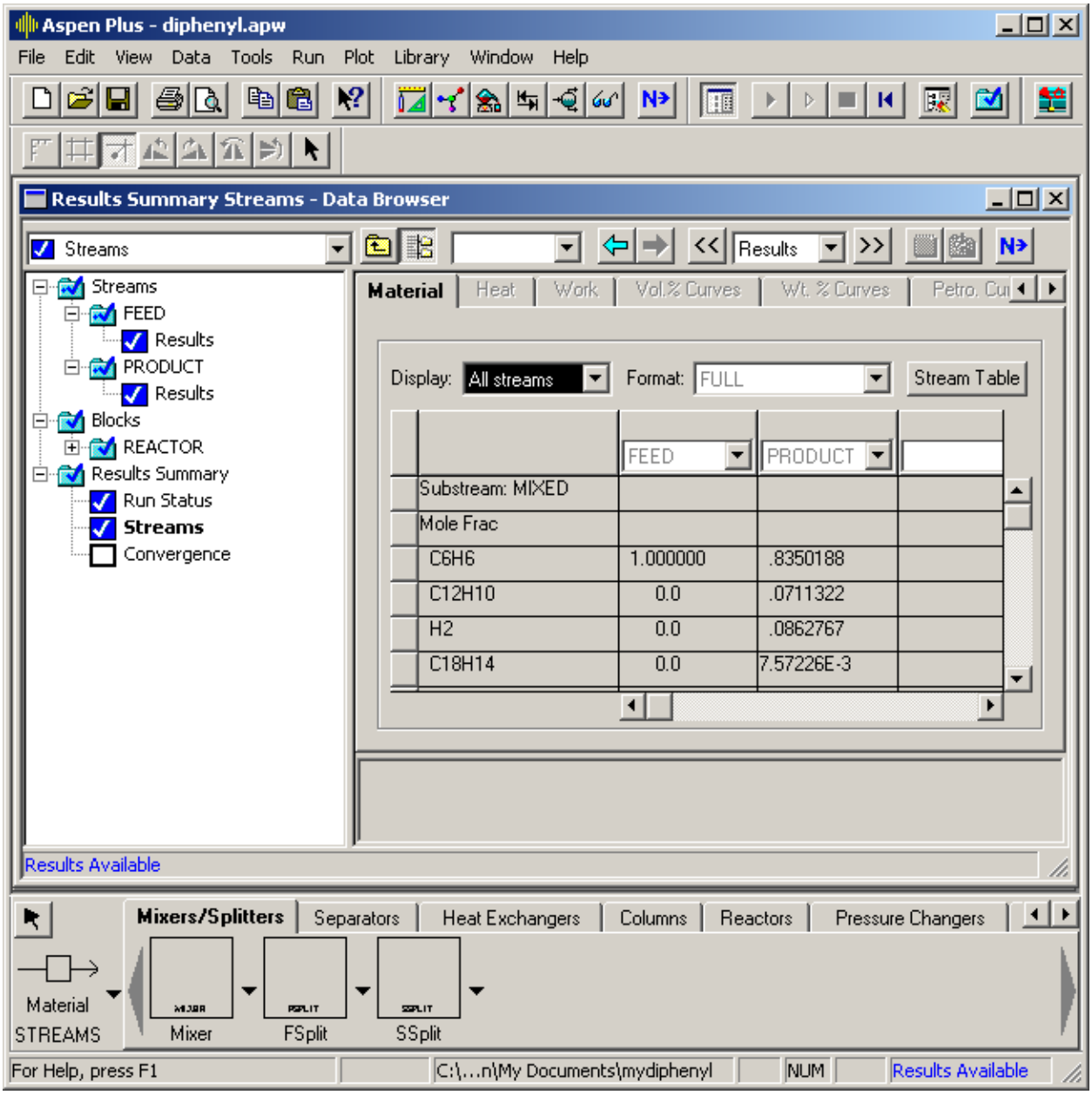


Results

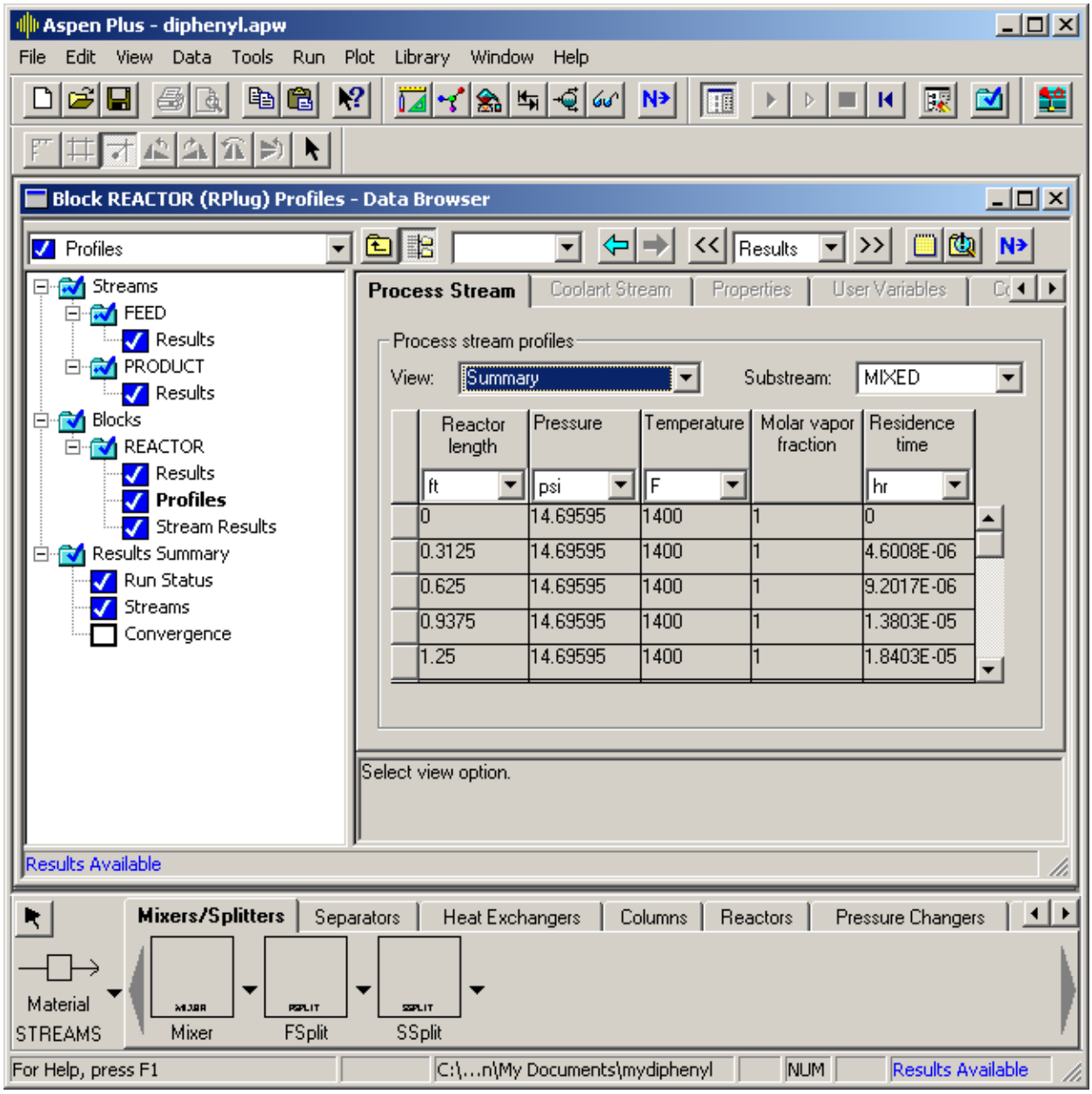
The results summary is shown by default. The first page is the run status screen.



The streams screen gives the results for all streams. You can compare the mole fractions to the one reported in the original problem specification.

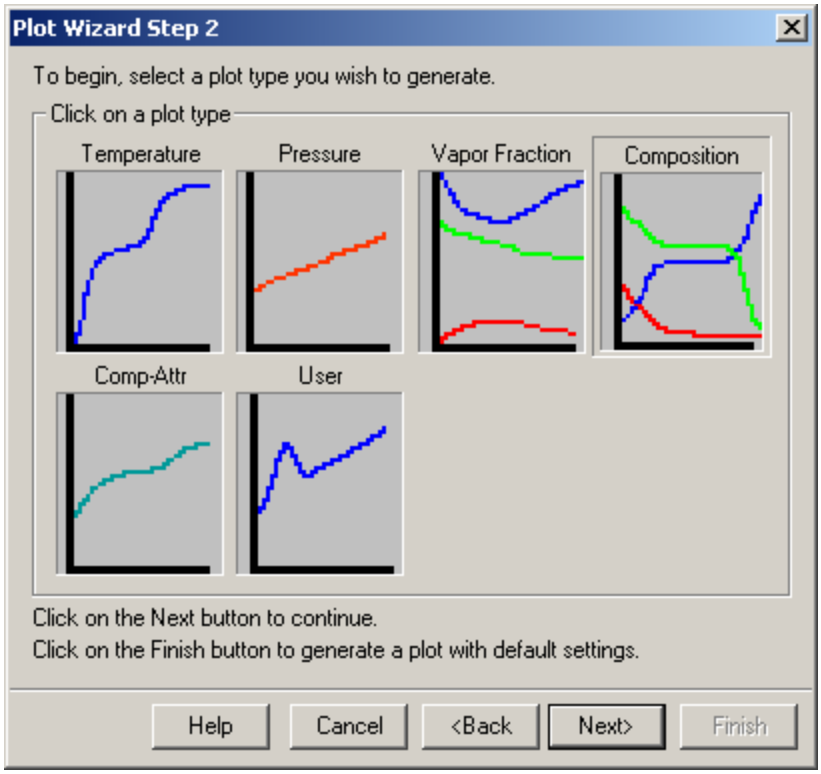


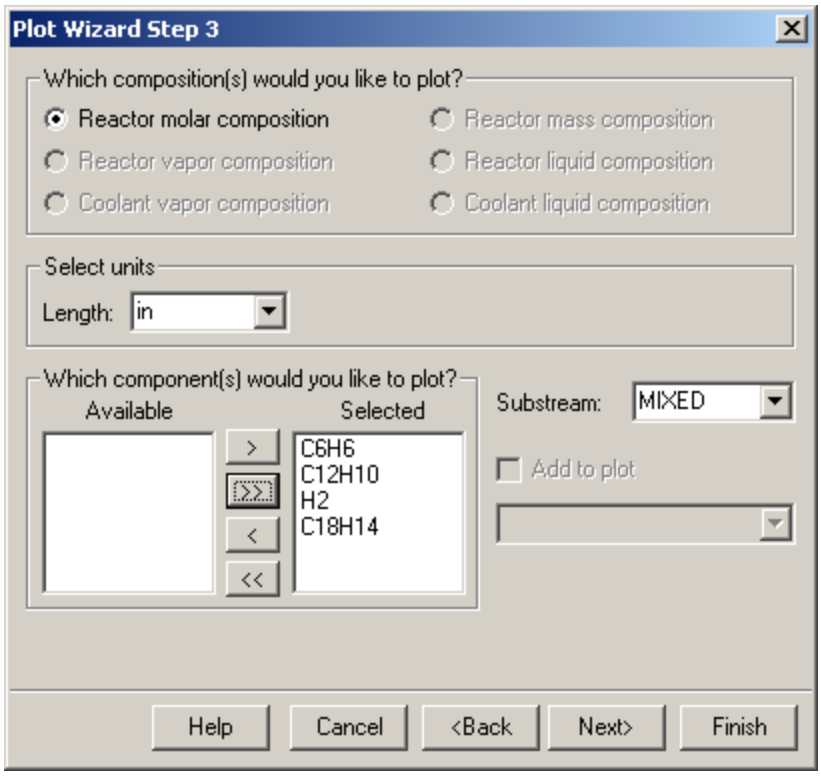
The profiles screen is where you will find concentration, temperature, etc. profiles along the reactor. These results can be analyzed by the Plot Wizard entry from the Plot menu.

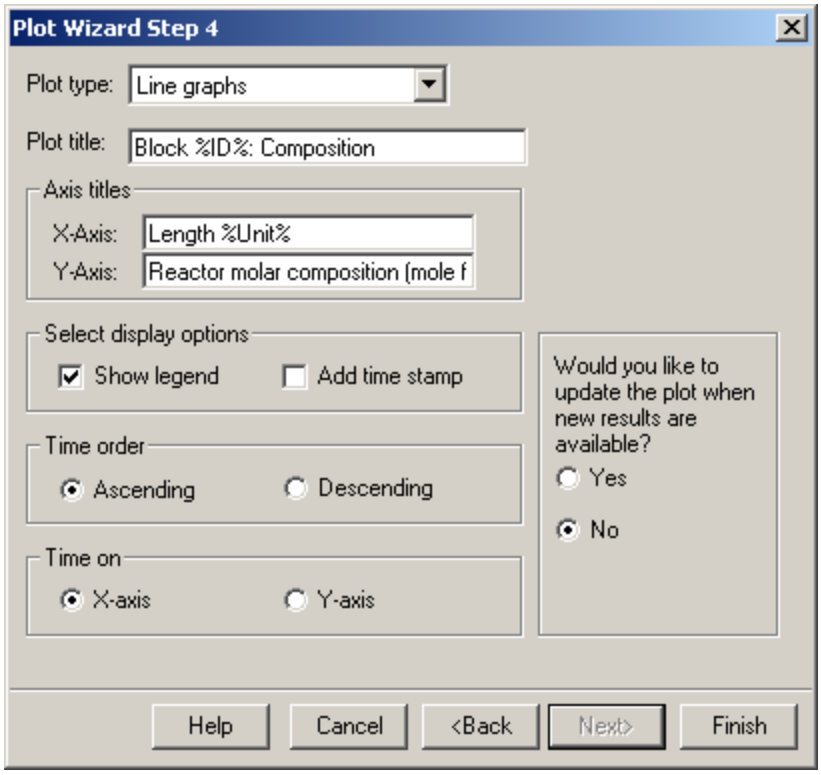


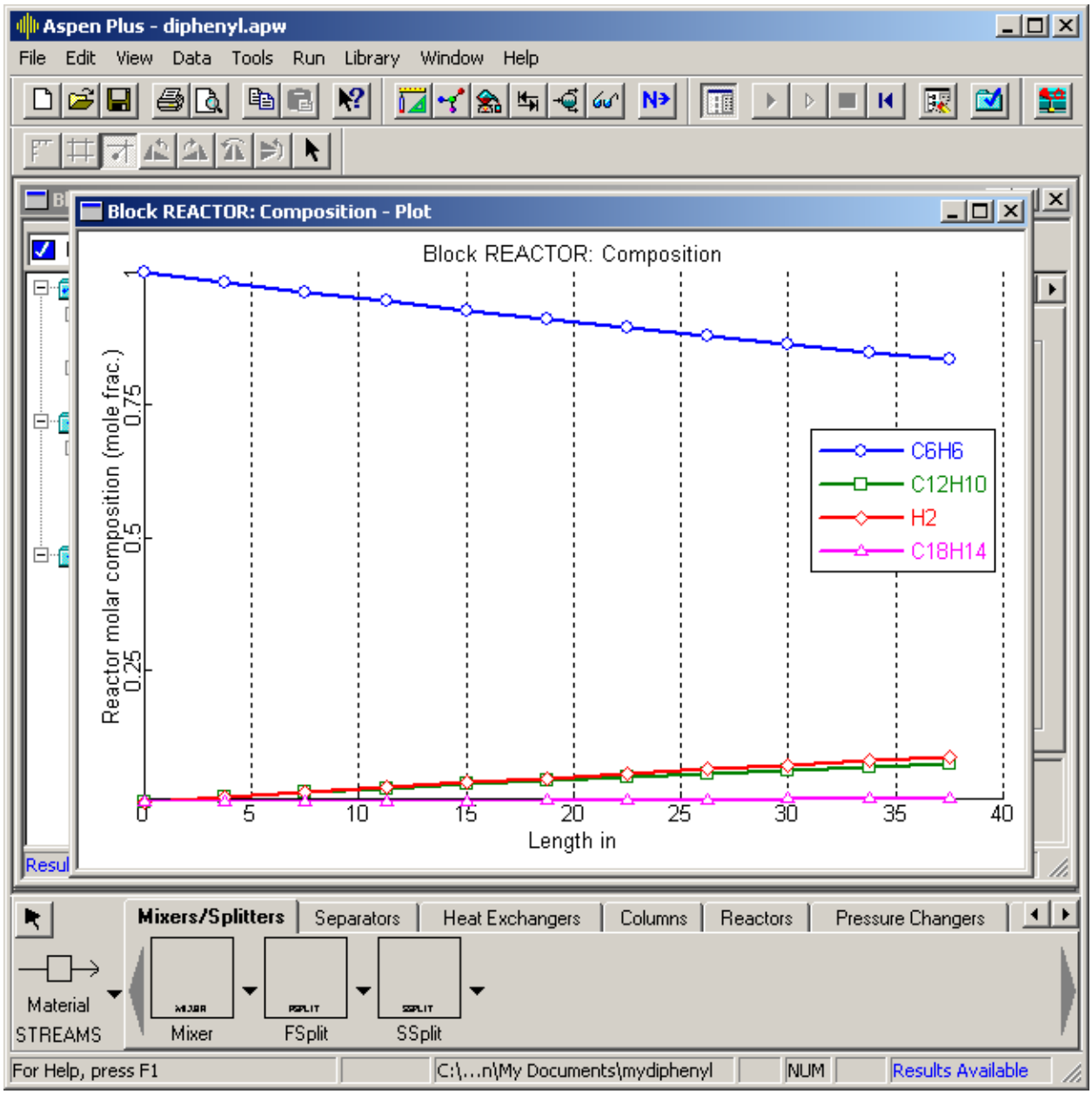
To plot the molar concentration profiles follow the steps outlined in the next three pages.


Plot Wizard Step 1
Welcome to Aspen Plus Plot Wizard!
The wizard guides you through the basic operations in generating a plot.
To continue, click on the Next button at the bottom of the wizard.
To accept all the default values and generate a plot, click on the Finish button when it is activated.
Help
Cancel
<Back
Next>
Finish


Plot Wizard Step 2
To begin, select a plot type you wish to generate.
Click on a plot type
Temperature
Pressure
Vapor Fraction
Composition
Comp-Attr
User
Click on the Next button to continue.
Click on the Finish button to generate a plot with default settings.
Help
Cancel
<Back
Next>
Finish


Plot Wizard Step 3
Which composition(s) would you like to plot?
Reactor molar composition
Reactor mass composition
Reactor vapor composition
Reactor liquid composition
Coolant vapor composition
Coolant liquid composition
Select units
Length: in
Which component(s) would you like to plot?
Available
Selected
C6H6
C12H10
H2
C18H14
Substream: MIXED
Add to plot
Help
Cancel
<Back
Next>
Finish


Plot Wizard Step 4
Plot type: Line graphs
Plot title: Block %ID%: Composition
Axis titles
X-Axis: Length %Unit%
Y-Axis: Reactor molar composition (mole f
Select display options
Show legend
Add time stamp
Time order
Ascending
Descending
Time on
X-axis
Y-axis
Would you like to update the plot when new results are available?
Yes
No
Help
Cancel
<Back
Next>
Finish



This concludes our introductory tutorial on Aspen Plus™.