ASPEN tutorial

Introduction

- ASPEN is a process simulation software package widely used in industry today. Given a process design and an appropriate selection of thermodynamic models, ASPEN uses mathematical models to predict the performance of the process.
- This accurate modeling of thermodynamic properties is particularly important in the separation of non-ideal mixtures, and ASPEN has a large data bases of regressed parameters. ASPEN can handle very complex processes, including multiple-column separation systems, chemical reactors, distillation of chemically reactive compounds.
- ASPEN takes a design that the user supplies and *simulates the performance* of the process specified in that design. Therefore, a solid understanding of the underlying chemical engineering principles is required. A user should have some idea of the column behavior before attempting to use ASPEN. This information could come from an approximate method, such as the McCabe-Thiele approach.

Aspen packages for different simulations

Aspen Adsim - Fixed bed adsorption for pressure swing adsorption, etc.

Aspen Chromatography - Fixed bed adsorption, simulated moving bed chro matography. Runs independent of Aspen Plus.

Aspen Custom Modeler - A utility to permit the creation of user unit operati ons.

Aspen Distil - Aspen's 'Conceptual Engineering Product' for planning for proc essing schemes. Runs independent of Aspen Plus.

Aspen Dynamics - Unsteady-state simulator.

Aspen Plus - Steady-state process simulator.

Aspen Properties - Modeling of properties and phase equilibria. Incorporate d into most other components, though it can be run as a stand-alone subset. All of the phase equilibria and mixture property methods discussed on this si te are accessible in either Aspen Plus or Aspen Properties.

Aspen Polymers - Modeling of polymerization reactors and polymer thermo dynamics. This package is available within Aspen Plus or Aspen Properties rat her than via an external menu.

Process examined

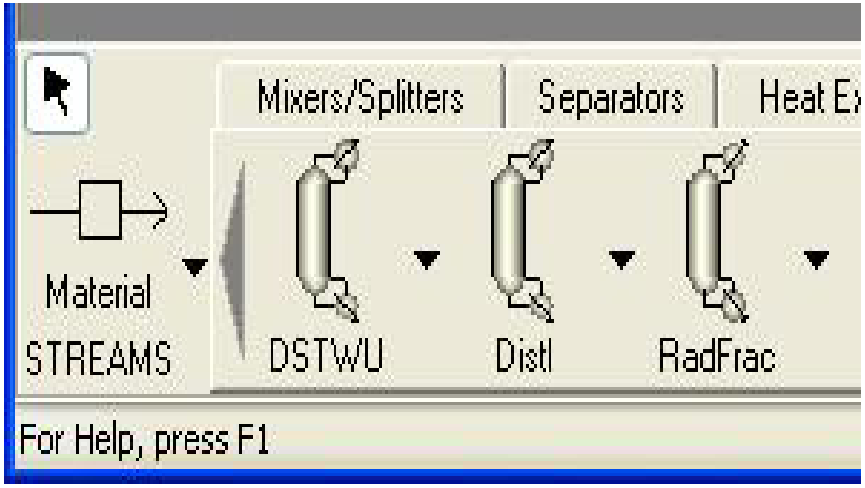
- To demonstrate how to build a process simulation using ASPEN, we will develop a distillation column for separation of ethanol and water.
- The first step in developing a simulation is to develop the process flow diagram (PFD), which consists of the unit operations (blocks) and streams that feed and connect the blocks.
- The blocks are listed by category at the bottom of the main window (columns, reactors, etc.) in a toolbar known as the 'Model Library', a portion is shown in Fig. There are a wide variety of block available. Documentation for the algorithm for each block is provided in the ASPEN documentation.

Distillation block

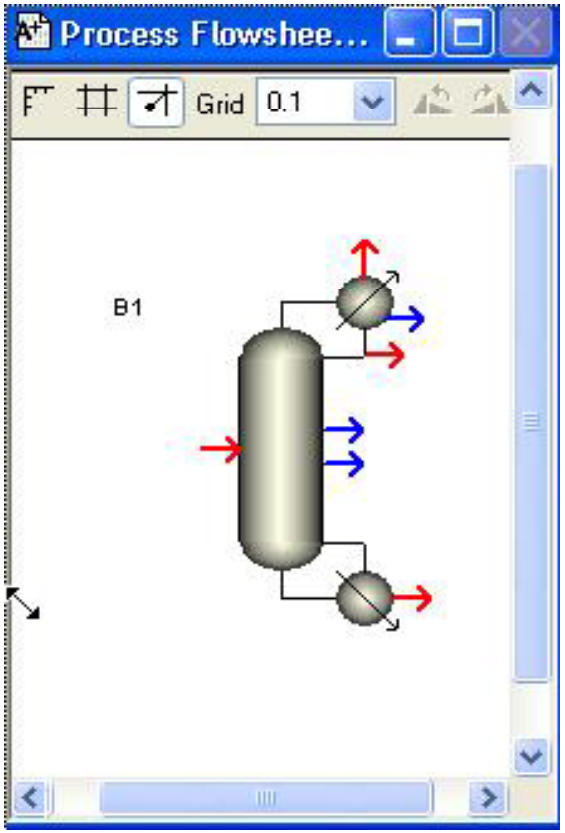
- **The first step is to choose the column type for the ethanol-water separation.**
- **Click on columns to view the different column simulations available.**
- **The two types of common interest are 'DSTWU', which is the multicomponent shortcut distillation method, and 'RadFrac', which is the rigorous simulation of a single column.**

Column and Stream menu

- For the ethanol + water system, the short-cut will not be appropri ate since the system has an azeotrope.
- Choose 'RadFrac'. Click on the small arrow on the right side of 'Ra dFrac' to select the column icon that you want to use on the PFD.
- The menu will disappear; move the crosshairs to the desired loca tion on the main flowsheet window and click the mouse button.

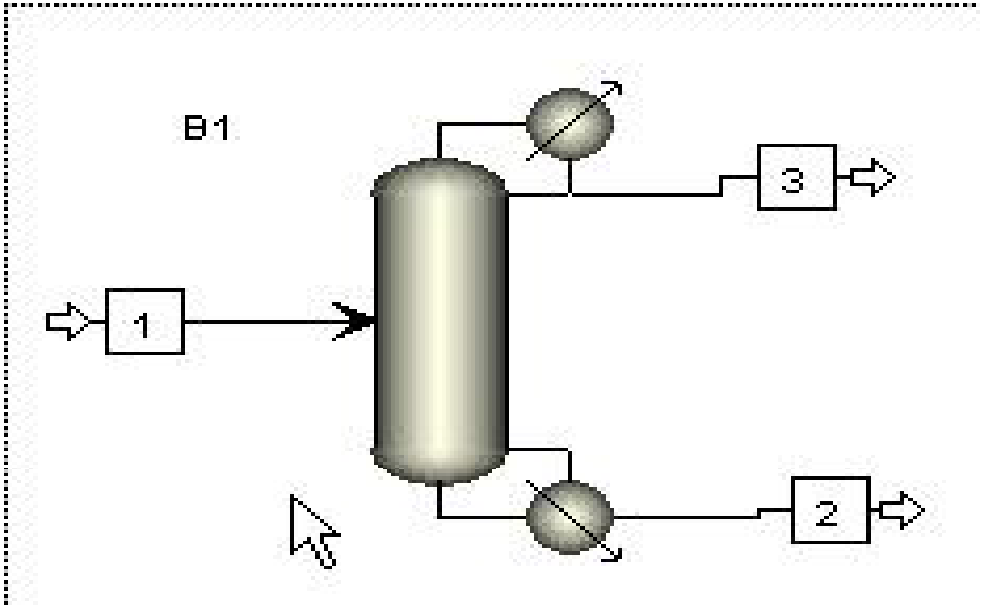


- Next you have to add streams to the block.
- Click on the small arrow to the right of the STREAMS button at the lower left corner of your screen), and choose the stream icon you want from the menu (material, energy or work).
- For this example, set up the feed stream: choose the Material stream by clicking on it. The column will now show arrows where the stream can be connected; red arrows indicate requir ed streams as shown in Fig.



Required and optional stream connection points

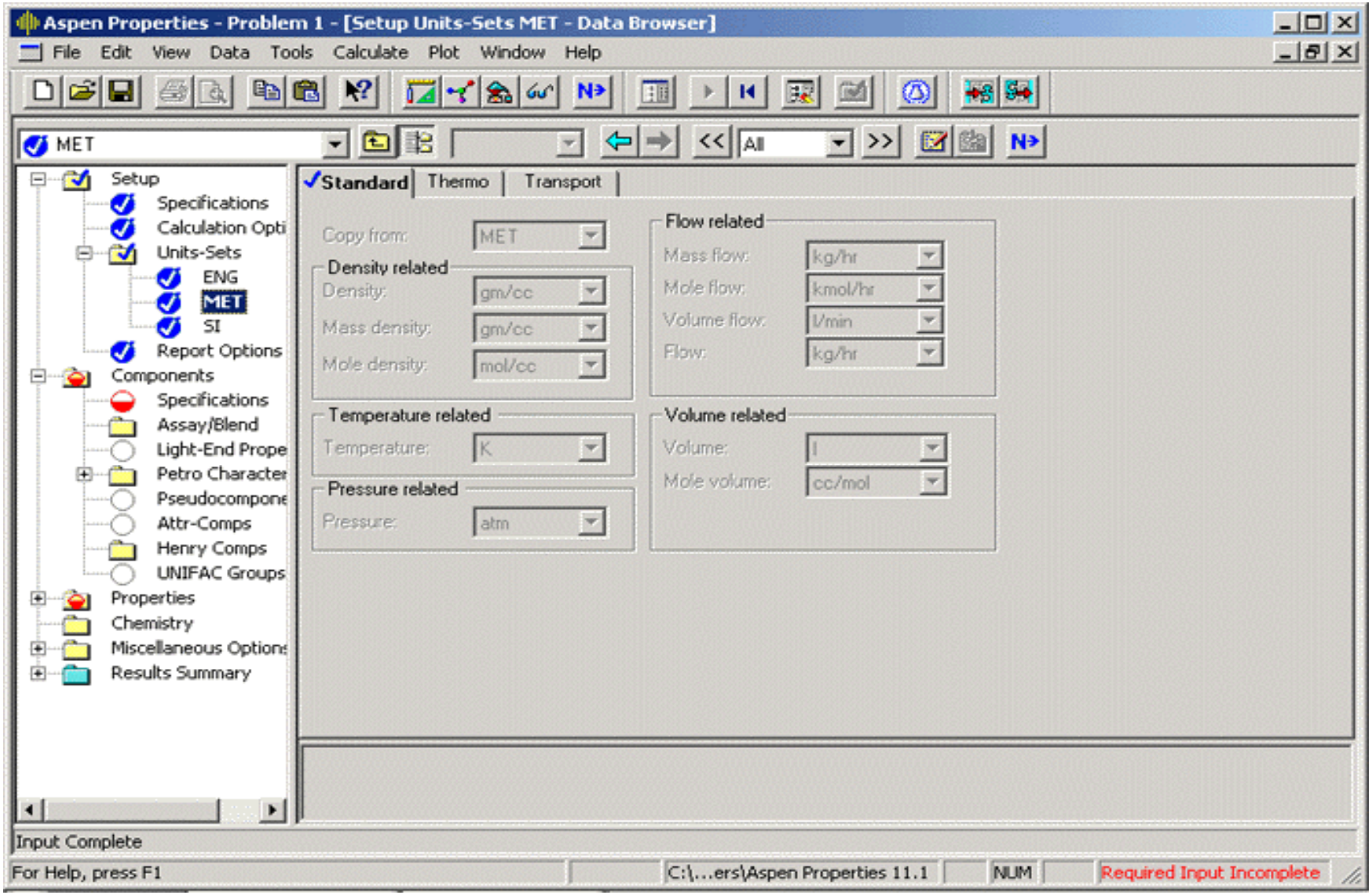
- To set up the feed stream to the column, move the crosshair on top of the red feed position and left click once.
- Now, move the mouse to the left and click again. You should now have a defined feed stream (Stream 1). For the outlet streams click the column outlet first to connect the bottoms (Stream 2) and liquid distillate (Stream 3).



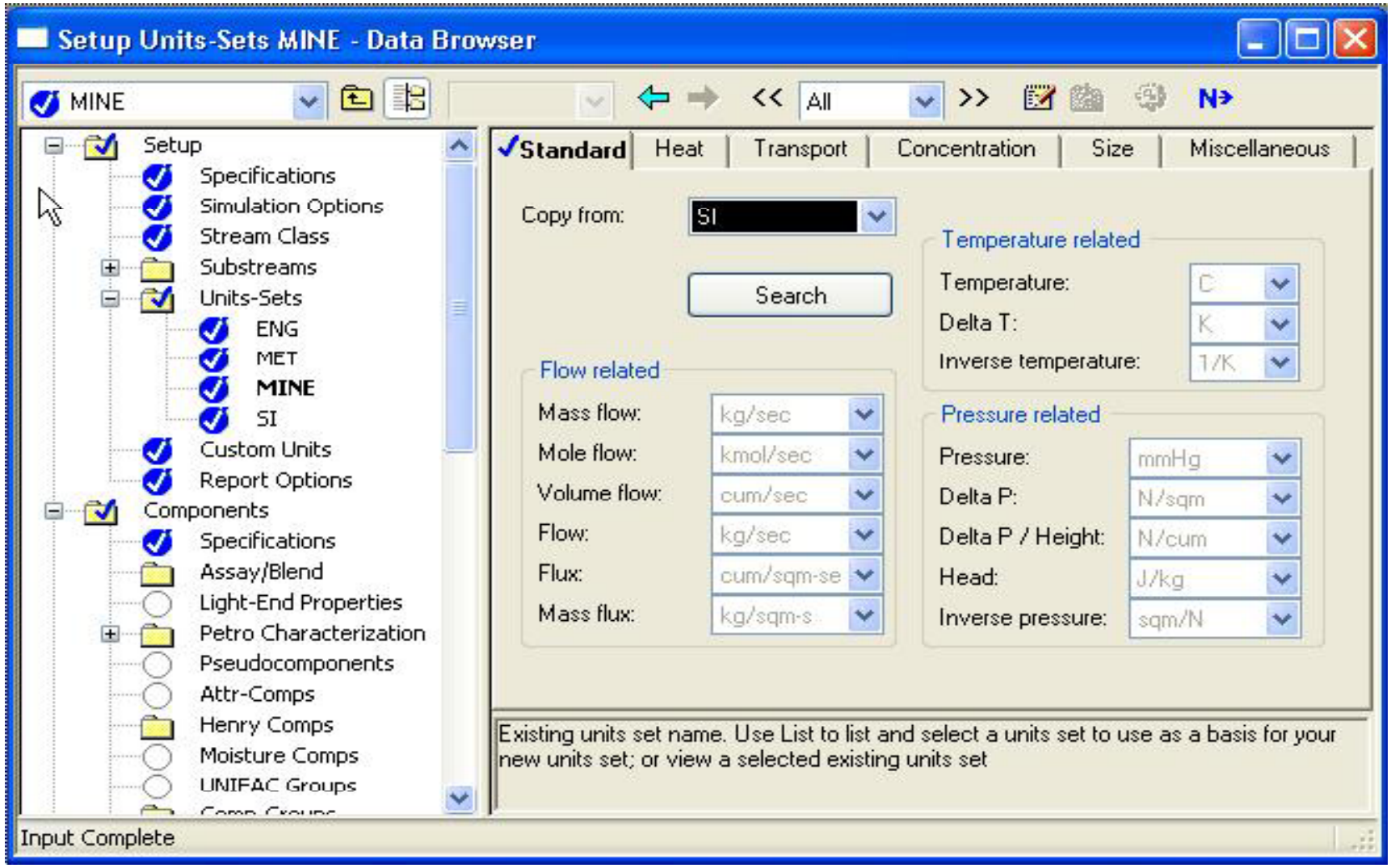
Configuring Units and Settings

- Now that you have defined the unit operations to be simulated and set up the streams into and out of the process, you must enter the rest of the information required to complete the simulation.
- Within Aspen Plus, the easiest way to find the next step is to use one of the following equivalent commands: (1) click the Next icon (blue N ->); (2) find 'Next' in the Tools menu; or (3) use keyboard shortcut F4. Any option will open the Data Browser.
- In the Data Browser, you are required to enter information at locations where there are red semicircles. When you have finished a section, a blue checkmark will appear. However, providing some 'Setup' settings is often desirable.
- You can change default units by opening the ‘Setup’ Folder as shown below.

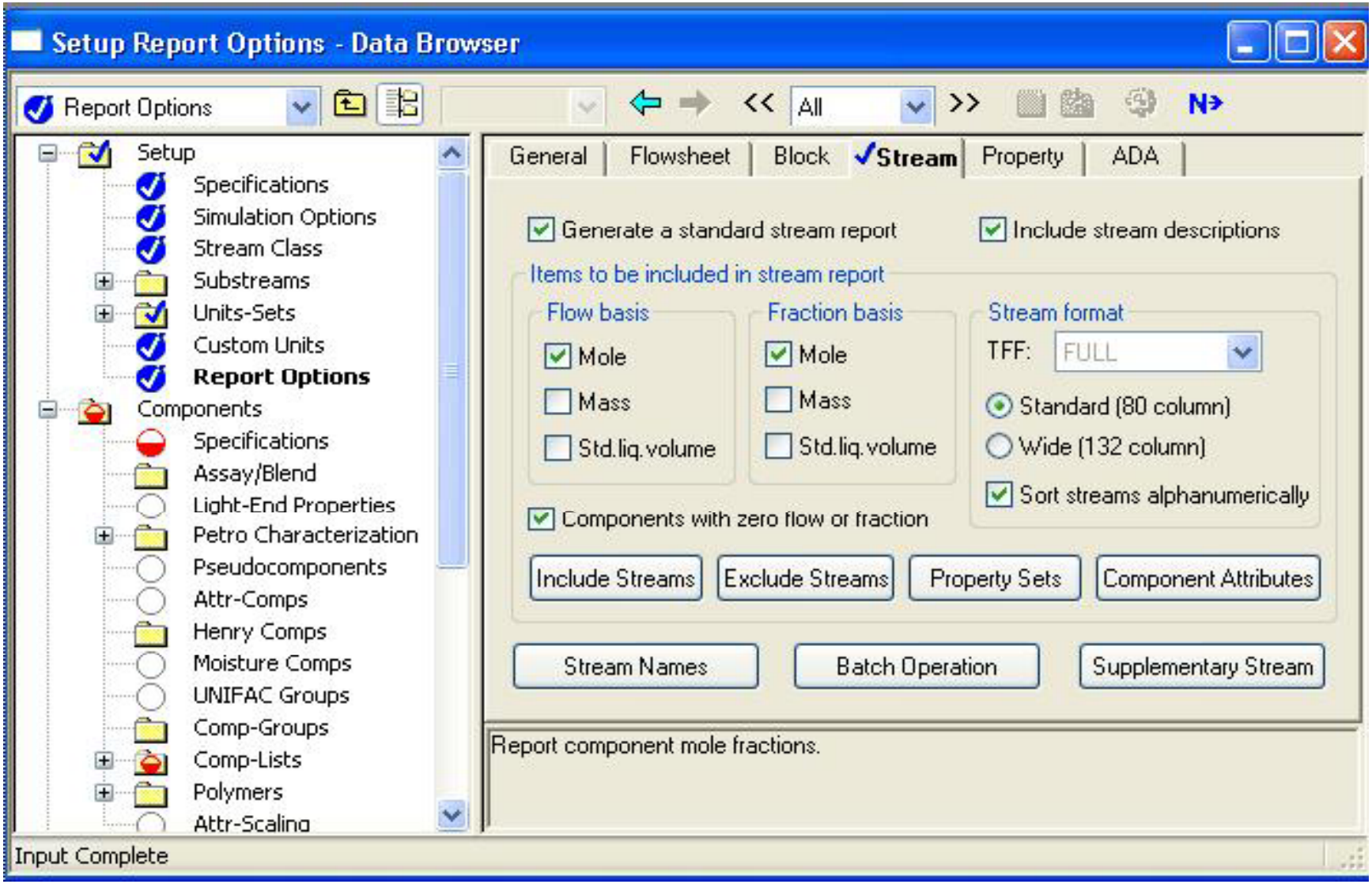
In the Data Browser, you are required to enter information at locations where there are red semicircles. When you have finished a section, a blue checkmark will appear. You can change default units by opening the 'Setup' Folder as shown below.



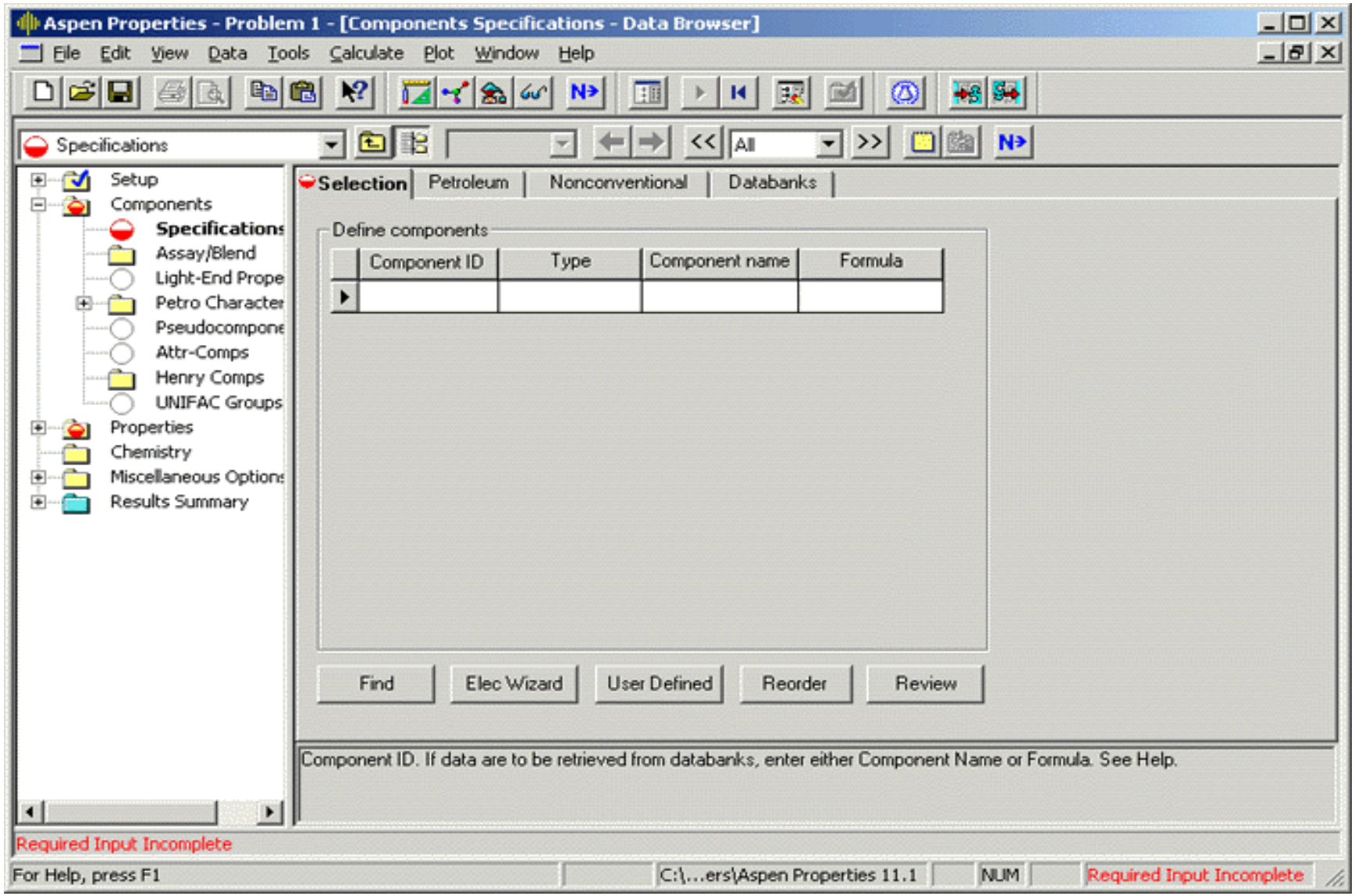
Unit option


Setup Units-Sets MINE - Data Browser
MINE
All
Setup
Specifications
Simulation Options
Stream Class
Substreams
Units-Sets
ENG
MET
MINE
SI
Custom Units
Report Options
Components
Specifications
Assay/Blend
Light-End Properties
Petro Characterization
Pseudocomponents
Attr-Comps
Henry Comps
Moisture Comps
UNIFAC Groups
Standard
Heat
Transport
Concentration
Size
Miscellaneous
Copy from:
SI
Search
Flow related
Mass flow:
kg/sec
Mole flow:
kmol/sec
Volume flow:
cum/sec
Flow:
kg/sec
Flux:
cum/sqm-se
Mass flux:
kg/sqm-s
Temperature related
Temperature:
C
Delta T:
K
Inverse temperature:
1/K
Pressure related
Pressure:
mmHg
Delta P:
N/sqm
Delta P / Height:
N/cum
Head:
J/kg
Inverse pressure:
sqm/N
Existing units set name. Use List to list and select a units set to use as a basis for your new units set; or view a selected existing units set
Input Complete

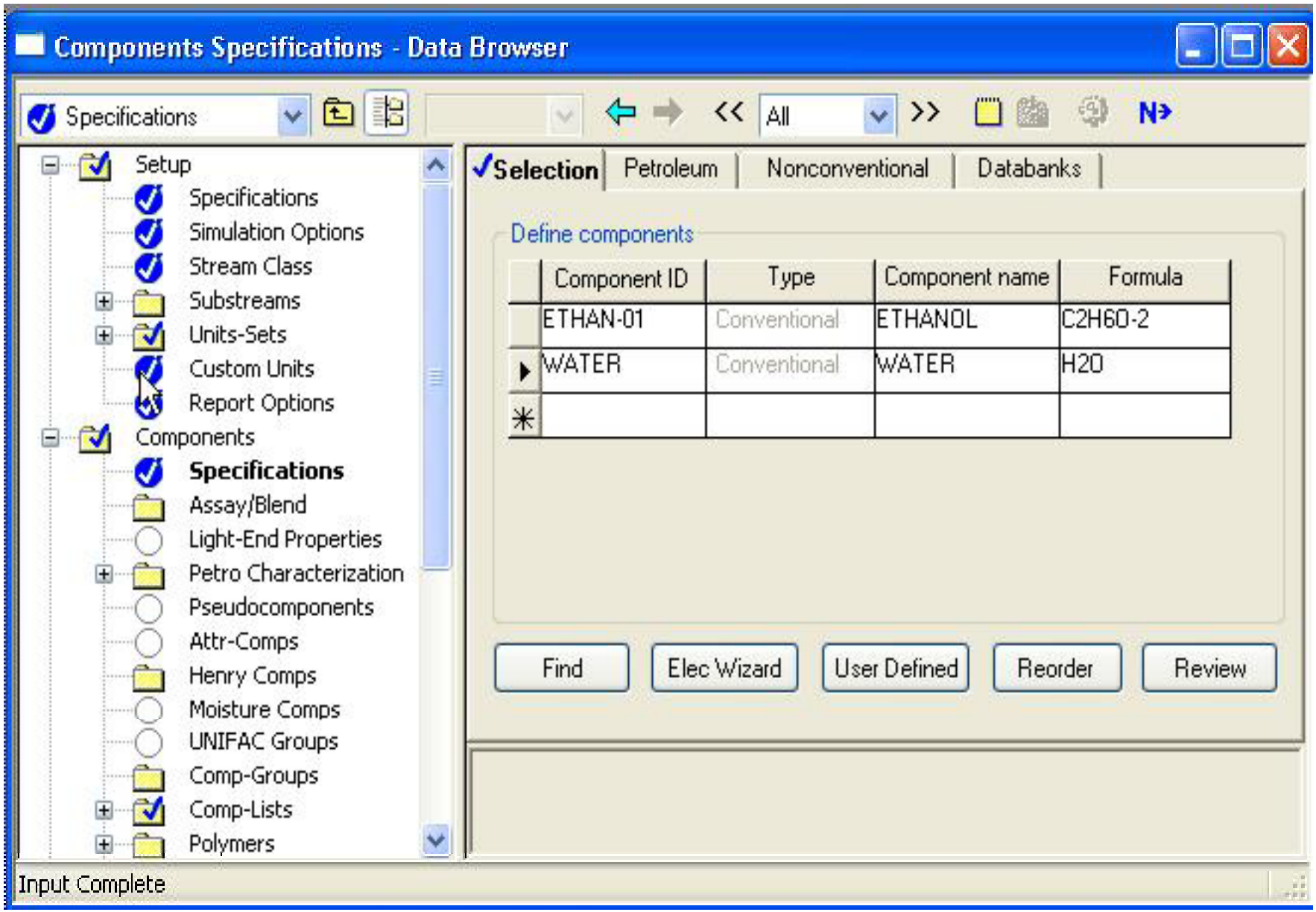
Report option



Enter all the components in the simulation.

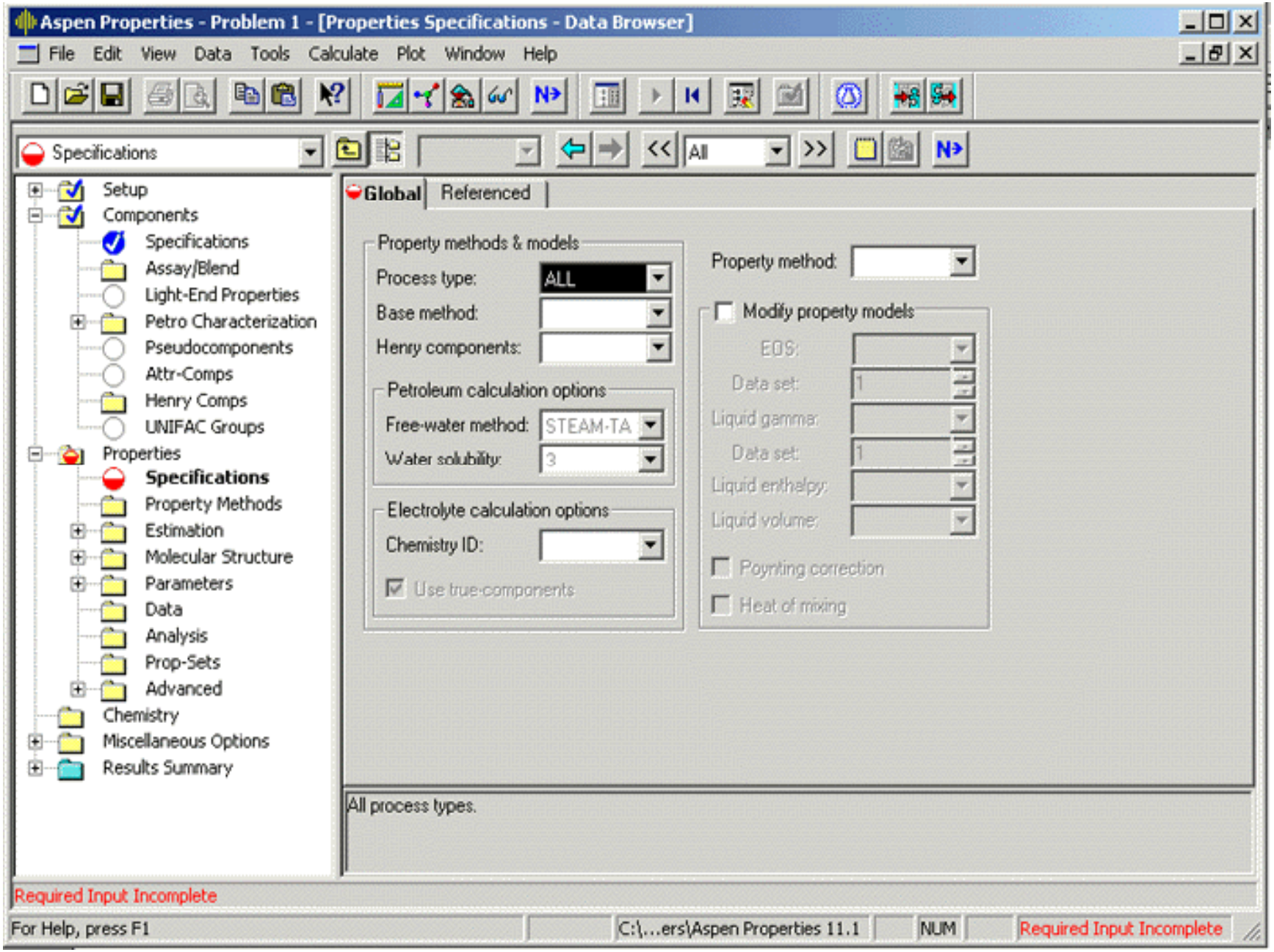


- The easiest way to enter component information is to click on the 'Find' button and enter the name of the component.
- Start by typing 'ethanol', and then select ETHANOL from the list of components that appears. Click the 'Add' button to add it to the components list.
- Repeat to add water to the components list. The ‘Component ID’ is an arbitrary name of your choice that will be used to label the component in your calculations.
- The ‘Type’ is a specification of how ASPEN will calculate thermodynamic properties. For processing of organic chemicals, it is usually appropriate to use ‘Conventional’ .


Components Specifications - Data Browser
Specifications
All
Setup
Specifications
Simulation Options
Stream Class
Substreams
Units-Sets
Custom Units
Report Options
Components
Specifications
Assay/Blend
Light-End Properties
Petro Characterization
Pseudocomponents
Attr-Comps
Henry Comps
Moisture Comps
UNIFAC Groups
Comp-Groups
Comp-Lists
Polymers
Selection
Petroleum
Nonconventional
Databanks
Define components
Component ID
Type
Component name
Formula
ETHAN-01
Conventional
ETHANOL
C2H6O-2
WATER
Conventional
WATER
H2O
Find
Elec Wizard
User Defined
Reorder
Review
Input Complete

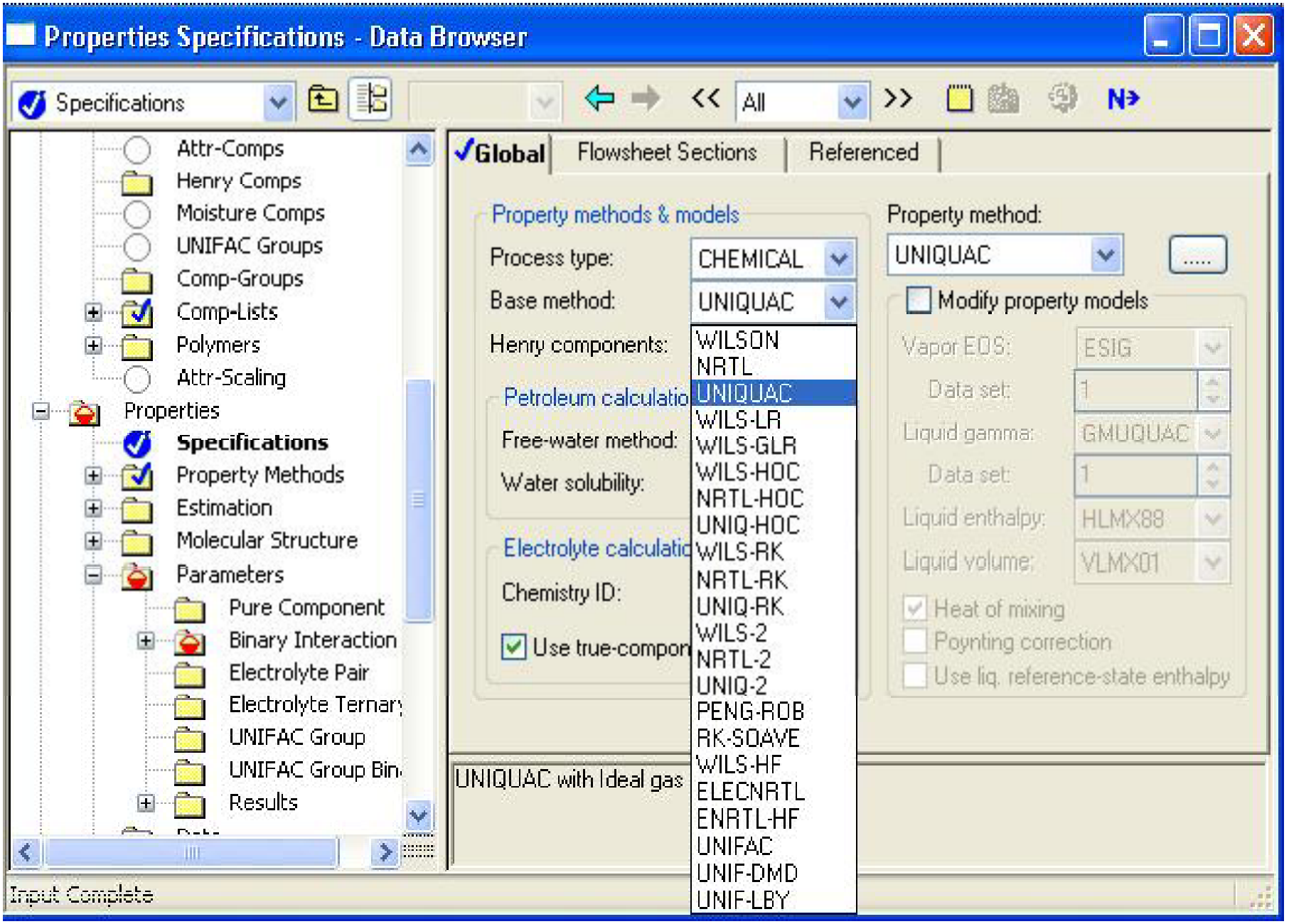
Property Method Selection Assistant.

- Aspen furnishes a "Property Method Selection Assistant" to assist in selection of a reasonable thermodynamic model, **Tools>Property Method Selection Assistant**.
- You need to be aware of the manner in which Aspen implements parameter values because Aspen offers temperature-dependent functions in place of parameters, and sometimes uses different signs on parameters than the same models in the literature.
- To find information on the property models, access the online help file, and on the page "Accessing other Help", use the link for "Aspen Properties Help". Then browse to "Aspen Properties Reference". Then, to find the model description and parameters implementation click in the help window, click on "Physical Property Methods and Models".
- The screen to select the property method is shown next.

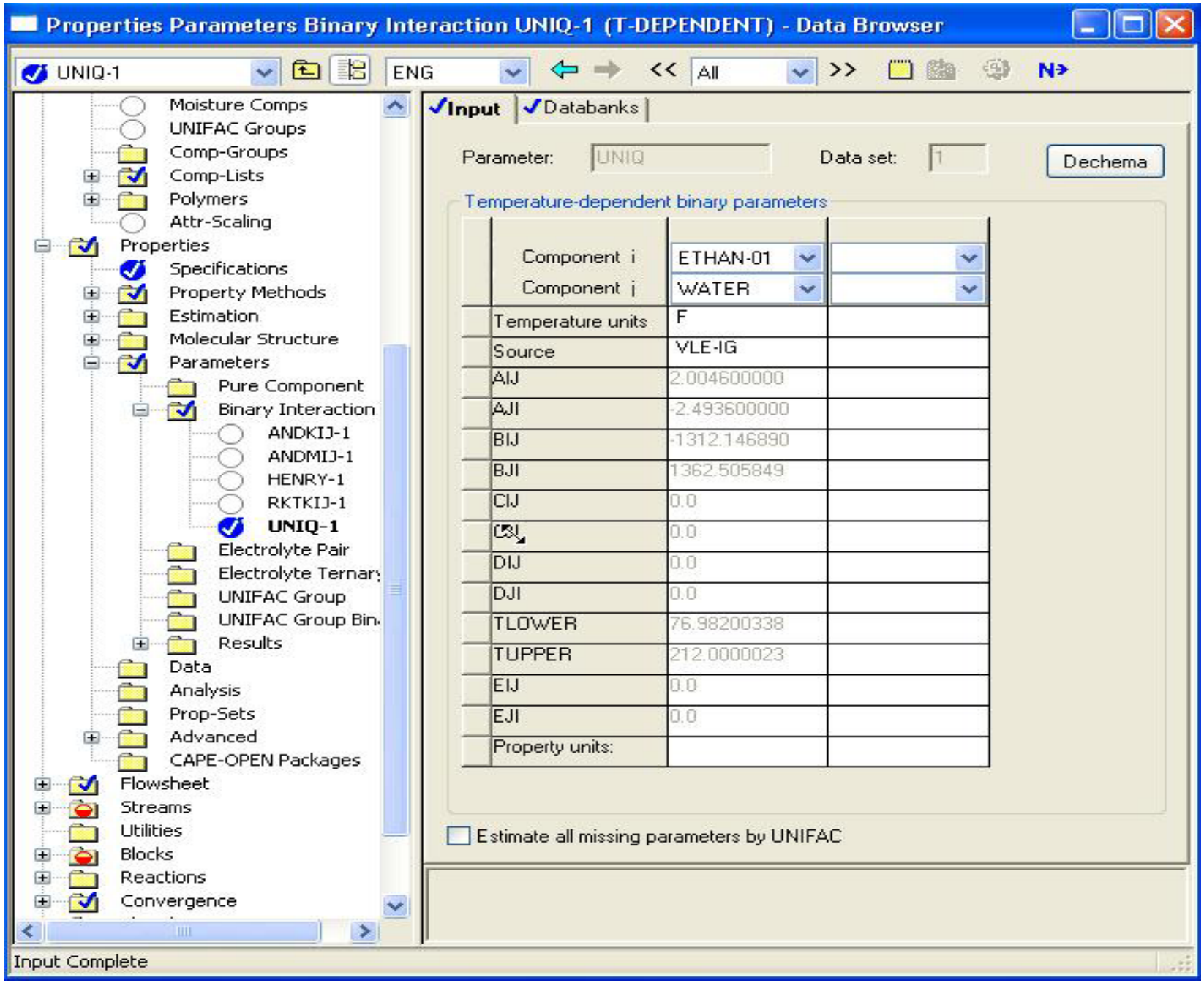

Aspen Properties - Problem 1 - [Properties Specifications - Data Browser]
File Edit View Data Tools Calculate Plot Window Help
Specifications
All
Setup
Components
Specifications
Assay/Blend
Light-End Properties
Petro Characterization
Pseudocomponents
Attr-Comps
Henry Comps
UNIFAC Groups
Properties
Specifications
Property Methods
Estimation
Molecular Structure
Parameters
Data
Analysis
Prop-Sets
Advanced
Chemistry
Miscellaneous Options
Results Summary
Global
Referenced
Property methods & models
Process type: ALL
Base method:
Henry components:
Petroleum calculation options
Free-water method: STEAM-TA
Water solubility: 3
Electrolyte calculation options
Chemistry ID:
Use true-components
Property method:
Modify property models
EOS:
Data set: 1
Liquid gamma:
Data set: 1
Liquid enthalpy:
Liquid volume:
Poynting correction
Heat of mixing
All process types.
Required Input Incomplete
For Help, press F1
C:\...ers\Aspen Properties 11.1
NUM
Required Input Incomplete

Process Type

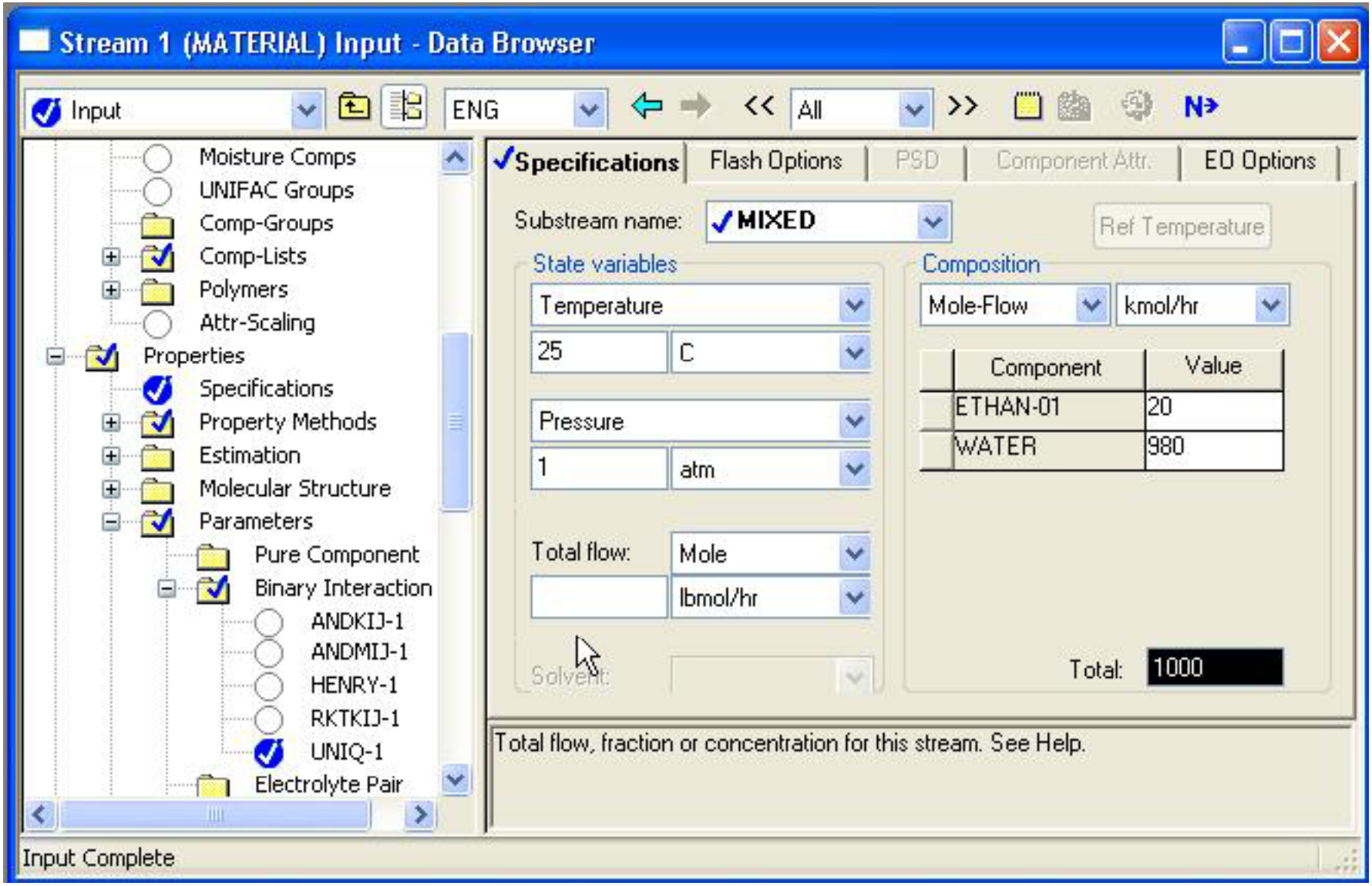
- The ‘Process Type’ will narrow down the choices for thermodynamic methods.
- Often for undergraduate design, ‘Chemical’ will provide a wide range of methods. However to access the van Laar model, you must select 'all'.
- The ‘Base method’ will specify the default calculation method for all blocks though you can control which method is used in individual blocks by editing the setup for the individual blocks.
- You will generally not use ‘Henry Components’ or ‘Free water’. For the example here, select UNIQUAC, a well-accepted model for non-ideal multicomponent liquid mixtures at low pressure.


Properties Specifications - Data Browser
Specifications
All
Attr-Comps
Henry Comps
Moisture Comps
UNIFAC Groups
Comp-Groups
Comp-Lists
Polymers
Attr-Scaling
Properties
Specifications
Property Methods
Estimation
Molecular Structure
Parameters
Pure Component
Binary Interaction
Electrolyte Pair
Electrolyte Ternary
UNIFAC Group
UNIFAC Group Bin
Results
Global
Flowsheet Sections
Referenced
Property methods & models
Process type:
CHEMICAL
Base method:
UNIQUAC
Henry components:
Petroleum calculatio
Free-water method:
Water solubility:
Electrolyte calculatic
Chemistry ID:
Use true-compon
WILSON
NRTL
UNIQUAC
WILS-LR
WILS-GLR
WILS-HOC
NRTL-HOC
UNIQ-HOC
WILS-RK
NRTL-RK
UNIQ-RK
WILS-2
NRTL-2
UNIQ-2
PENG-ROB
RK-SOAVE
WILS-HF
ELECNRTL
ENRTL-HF
UNIFAC
UNIF-DMD
UNIF-LBY
Property method:
UNIQUAC
.....
Modify property models
Vapor EOS:
ESIG
Data set:
1
Liquid gamma:
GMUQUAC
Data set:
1
Liquid enthalpy:
HLMX88
Liquid volume:
VLMX01
Heat of mixing
Poynting correction
Use liq. reference-state enthalpy
UNIQUAC with Ideal gas
Input Complete

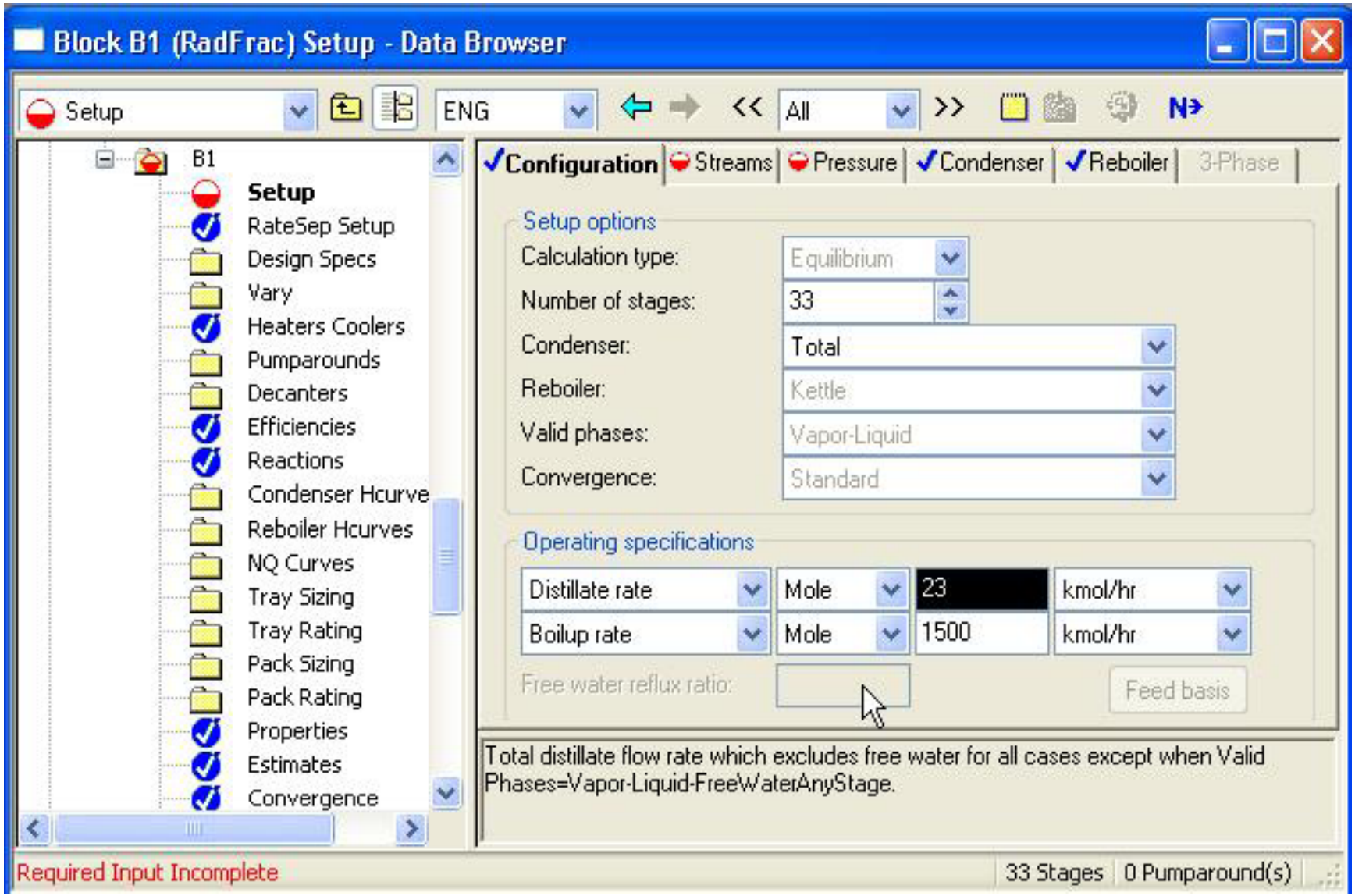
- By clicking the ‘N->’ button, you will be shown the binary parameters as shown in the screenshot.
- When you close the window or click Next, you have provided ***approval*** of the values,and you will receive no further prompting for parameter values.
- **If parameters are blank, zeros will be used. This does not imply that the ideal mixture assumption will be used because many models predict non-ideal behavior with parameter values of zero.**


Properties Parameters Binary Interaction UNIQ-1 (T-DEPENDENT) - Data Browser
UNIQ-1
ENG
All
Moisture Comps
UNIFAC Groups
Comp-Groups
Comp-Lists
Polymers
Attr-Scaling
Properties
Specifications
Property Methods
Estimation
Molecular Structure
Parameters
Pure Component
Binary Interaction
ANDKIJ-1
ANDMIJ-1
HENRY-1
RKTKIJ-1
UNIQ-1
Electrolyte Pair
Electrolyte Ternary
UNIFAC Group
UNIFAC Group Bin
Results
Data
Analysis
Prop-Sets
Advanced
CAPE-OPEN Packages
Flowsheet
Streams
Utilities
Blocks
Reactions
Convergence
Input
Databanks
Parameter: UNIQ
Data set: 1
Dechema
Temperature-dependent binary parameters
Component i ETHAN-01
Component j WATER
Temperature units F
Source VLE-IG
AIJ 2.004600000
AJI -2.493600000
BIJ -1312.146890
BJI 1362.505849
CIJ 0.0
CJI 0.0
DIJ 0.0
DJI 0.0
TLOWER 76.98200338
TUPPER 212.0000023
EIJ 0.0
EJI 0.0
Property units:
Estimate all missing parameters by UNIFAC
Input Complete

Stream specifications



RadFrac Block

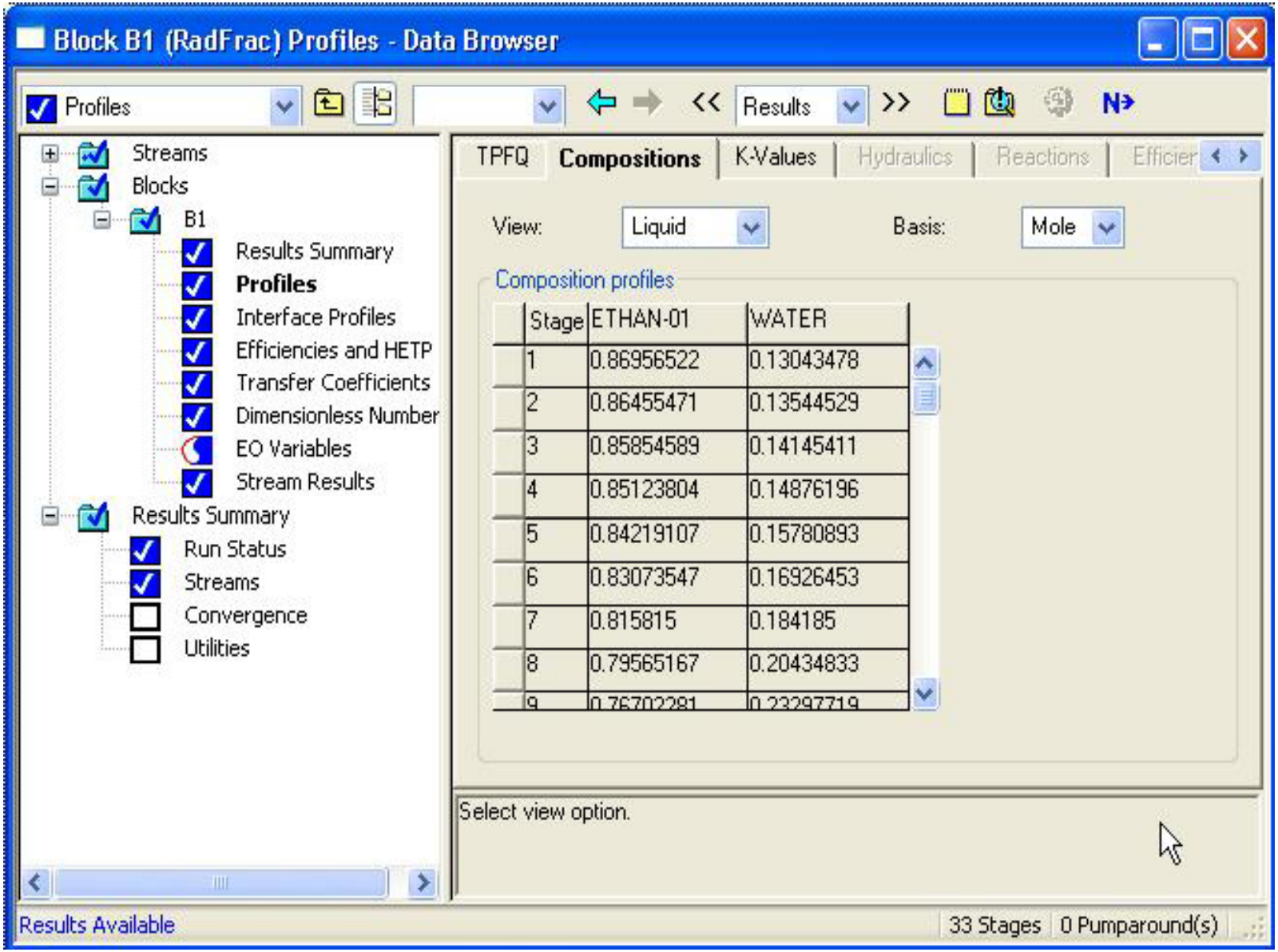


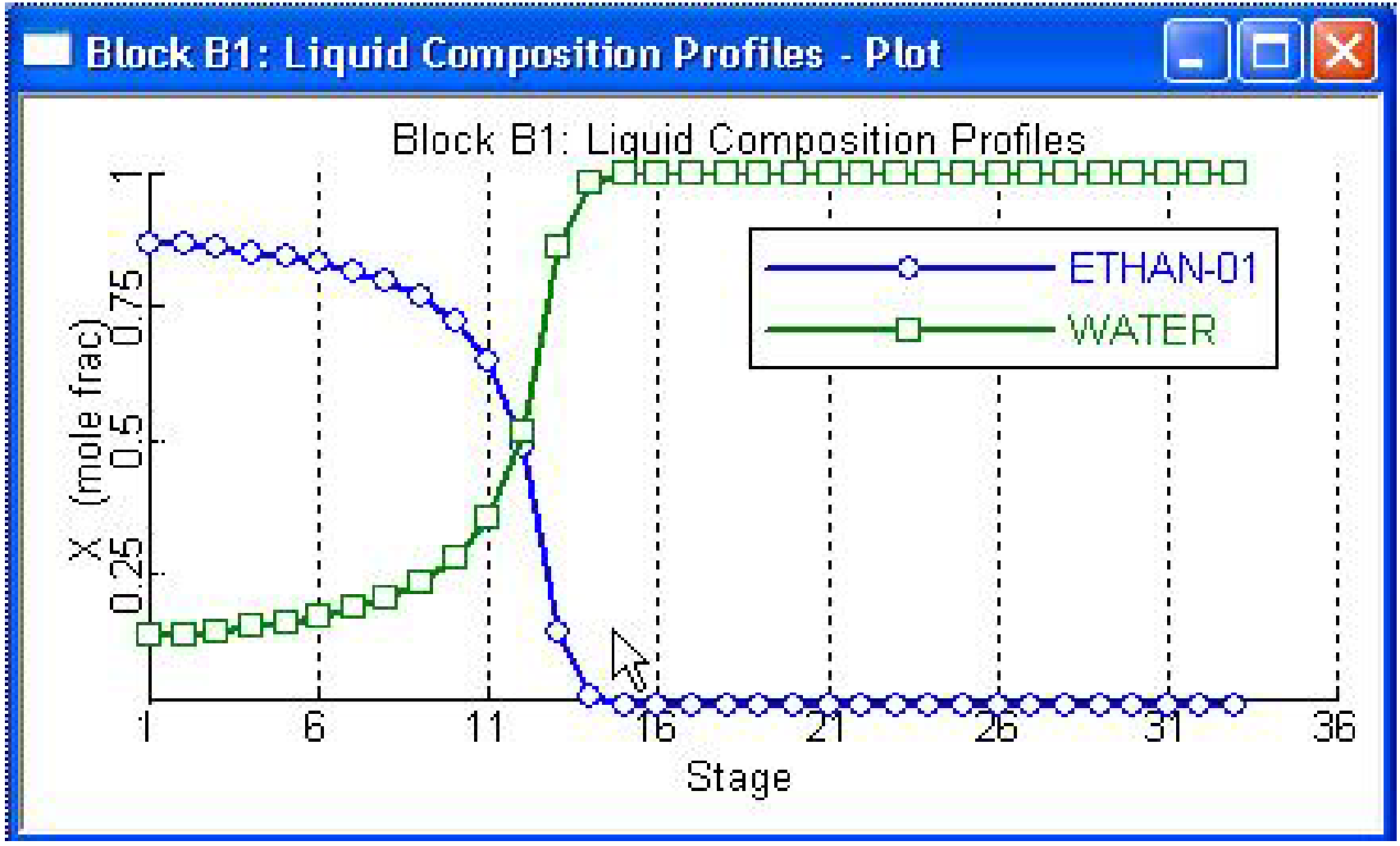
- Hit 'Next' and the 'Stream' page appears. Locate the feed stream (1) on stage 17. Hit 'Next' to get to the 'Pressure' page. Specify the 'Stage 1/Condenser' pressure as 1 atm. By leaving the other sections of the pressure page alone, pressure drop through the column will be ignored in this calculation.

Running the simulation

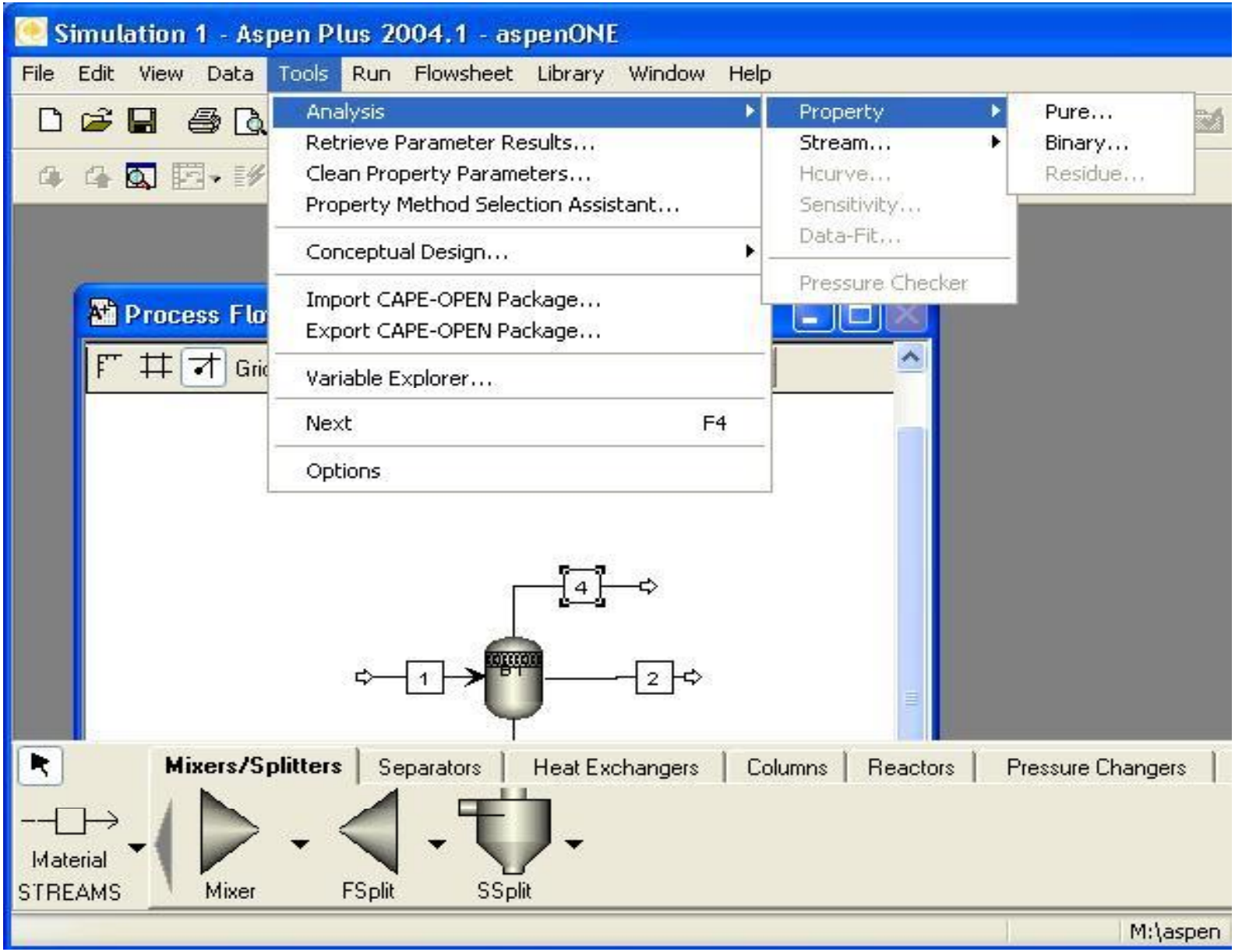
- All required information should now be complete. Click 'Next'. You should now get a message that all required information has been entered.
- If you don't, complete the required form or look at the menu on the left for any red semicircles. To run the simulation, click OK on the message.

To view results, click on the blue folder in the toolbar. Choose 'Stream ' to view stream properties, or 'Block' to view column properties.

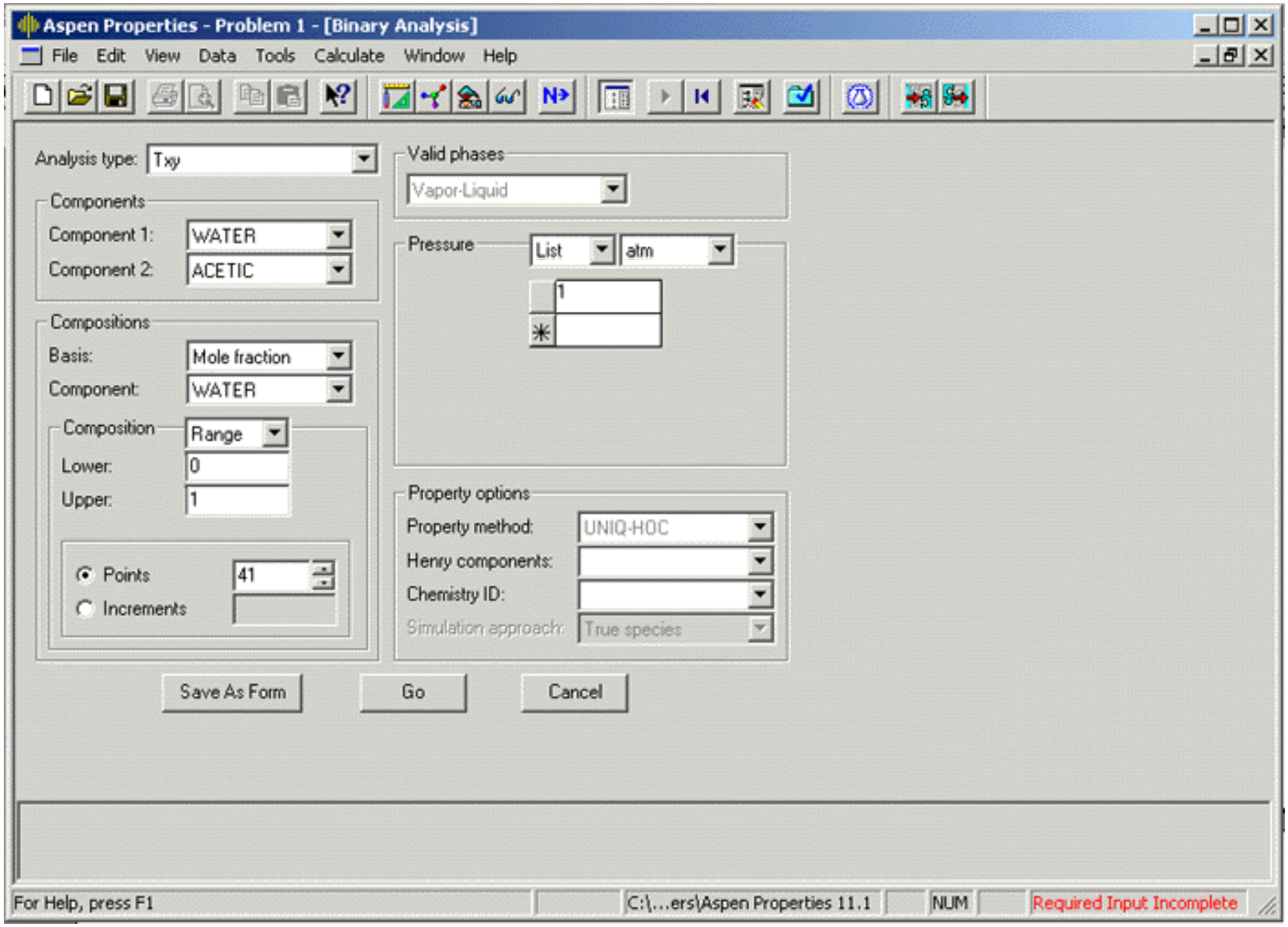


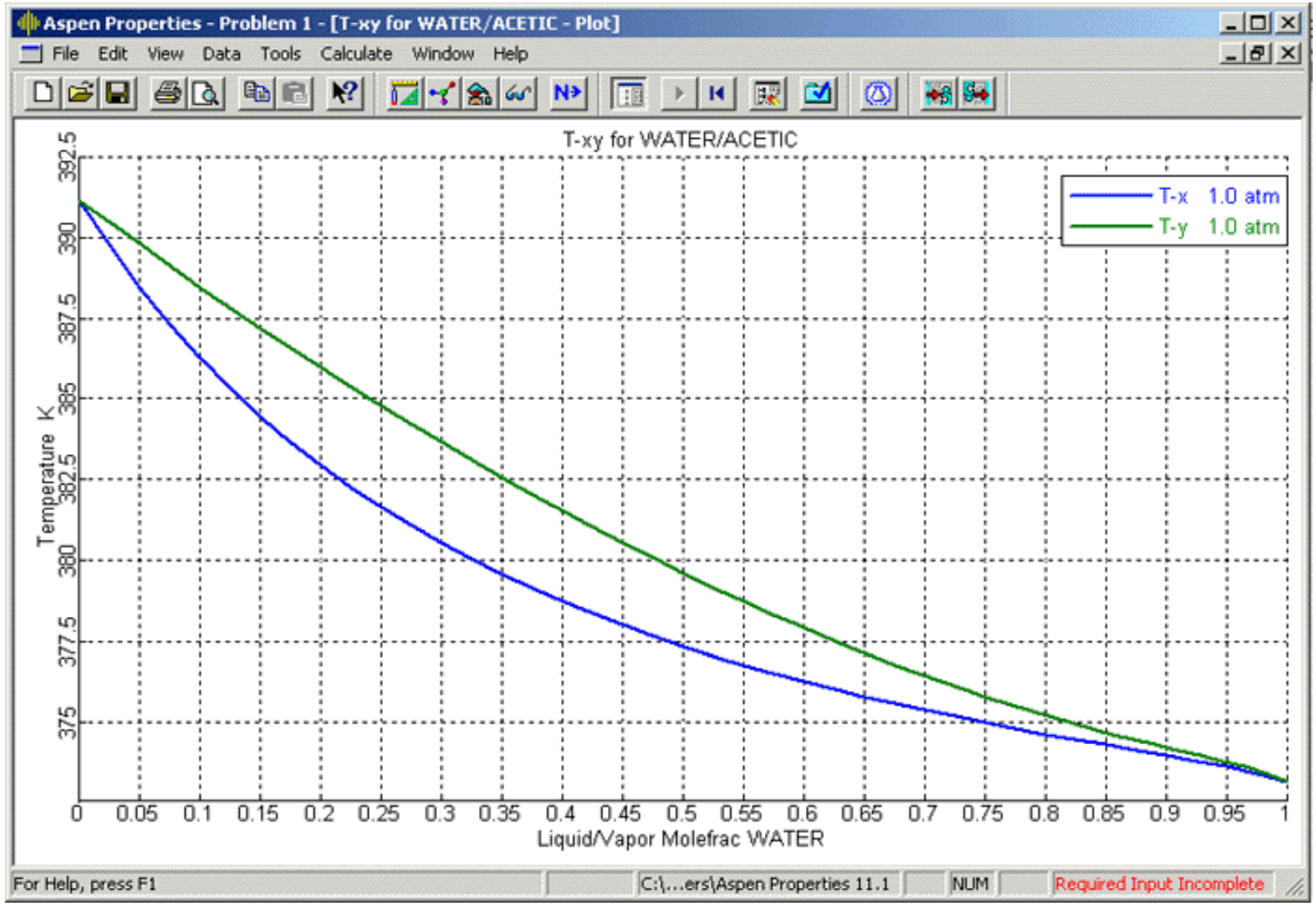

Block B1: Liquid Composition Profiles - Plot
Block B1: Liquid Composition Profiles
X (mole frac)
0.25
0.5
0.75
1
1
6
11
16
21
26
31
36
Stage
ETHAN-01
WATER

Analysis report



Water-Acetic acid system




Aspen Properties - Problem 1 - [T-xy for WATER/ACETIC - Plot]
File Edit View Data Tools Calculate Window Help
T-xy for WATER/ACETIC
T-x 1.0 atm
T-y 1.0 atm
Temperature K
392.5
390
387.5
385
382.5
380
377.5
375
0 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5 0.55 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95 1
Liquid/Vapor Molefrac WATER
For Help, press F1
C:\...ers\Aspen Properties 11.1
NUM
Required Input Incomplete