COMPUTER AIDED PROCESS ENGINEERING

ASPEN PLUS TUTORIALS

Steady State Process Simulation Using ASPEN Plus

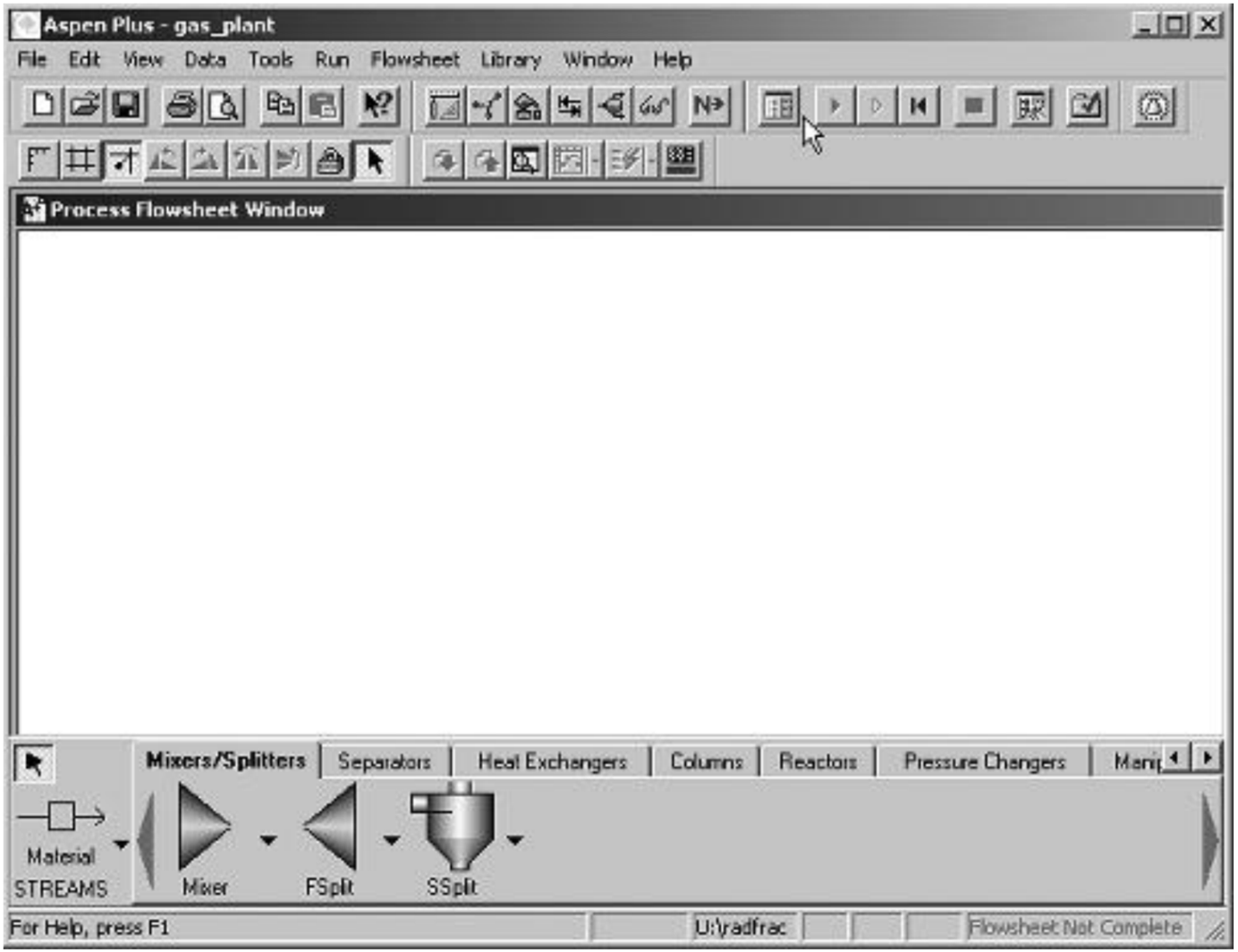
- It is based on steady state governing equations like conservation of mass, momentum and energy of various unit operations and unit processes.
- The governing equations results operating conditions of the process plant like, flowrate, enthalpy (temperature), pressure, compositions of each streams, amount of energy needed, overall yield, conversions etc.
- The steady state process simulation utilizes thermodynamic and transport properties of various species, equilibrium data of vapor-liquid, gas-liquid, liquid-liquid, solid-liquid, and chemical equilibrium data.
- It determines the size of equipment in a chemical plant.

Start

- Begin by opening Aspen Plus. A registration screen (connect to engine) comes up; click OK. Click ‘maximize’ to fill the screen. This step may differ depending upon installation.
- For a new problem, it is useful to choose a template that is similar to a problem;

Model Library

- Model library consists modules which are the replica of various units used in the flow sheeting of a chemical process plant.
- It can be viewed clicking on the icons at the bottom of the Aspen Plus screen. If the icons are not displayed, choose the View/Model Library from menu option. When the unit is clicked the words shown at the bottom of the screen give a brief description of the module.



Opening screen.

Selected Major Blocks Available in Aspen Plus

- **Mixers/splitters**
  a. Mixer – combine material
  b. Fsplit – split specifications for output
  c. Ssplit – splits using substreams
- **Separators**
  a. Flash2 – rigorous vapor–liquid split or vapor–liquid–liquid split
  b. Flash3 – rigorous vapor–liquid–liquid split
  c. Decanter – separate two liquid phases
  d. Sep – use split fractions
  e. Sep2 – separation based on flows and purities
- **Heat exchangers**
  a. Heater – heaters, coolers, condensers
  b. HeatX – co- and counter-current heat exchangers
  c. Hetran – shell and tube heat exchangers
  d. Aerotran – air-cooled heat exchangers

- **Columns**
  a. DSTWU – shortcut distillation using Winn–Underwood–Gilliland equations and correlations
  b. Distl – Edmister shortcut distillation
  c. RadFrac – rigorous two phase and three phase, absorber, stripper, distillation columns using stages
  d. Extract – liquid–liquid extraction
- **Reactors**
  a. RStoic – stoichiometric fractional conversion or extent of reaction
  b. RYield – nonstoichiometric – based on yield distribution
  c. REquil – rigorous equilibrium
  d. RGibbs – rigorous equilibrium and/or multiphase Gibbs free energy minimization
  e. RCSTR – continuous stirred-tank reactor, specify volume
  f. RPlug – plug flow reactor, specify length and diameter of tube
  g. RBatch – batch reactor, specify cycle times
  The RCSTR, Rplug, and RBatch reactors require the choice of a reaction set and the building up of a reaction rate expression

- **Pressure changes**
  a. Pump
  b. Compr – compressor
- **User model**

Aspen Plus Simulation

Vapor liquid equilibria in a flash chamber

Problem: For a mixture (100 mol) of propane, n-butane, n-pentene, and n-octane, phase equilibrium K-values and inlet compositions $\{z_i\}$ are given in the table below at ***180 ^oF*** and ***70 psi***. Estimate vapor ***$\{y_i\}$*** and liquid ***$\{x_i\}$*** phase compositions, vapor product ***V*** and liquid product ***L*** in a flash chamber using ***Aspen Plus simulator***.

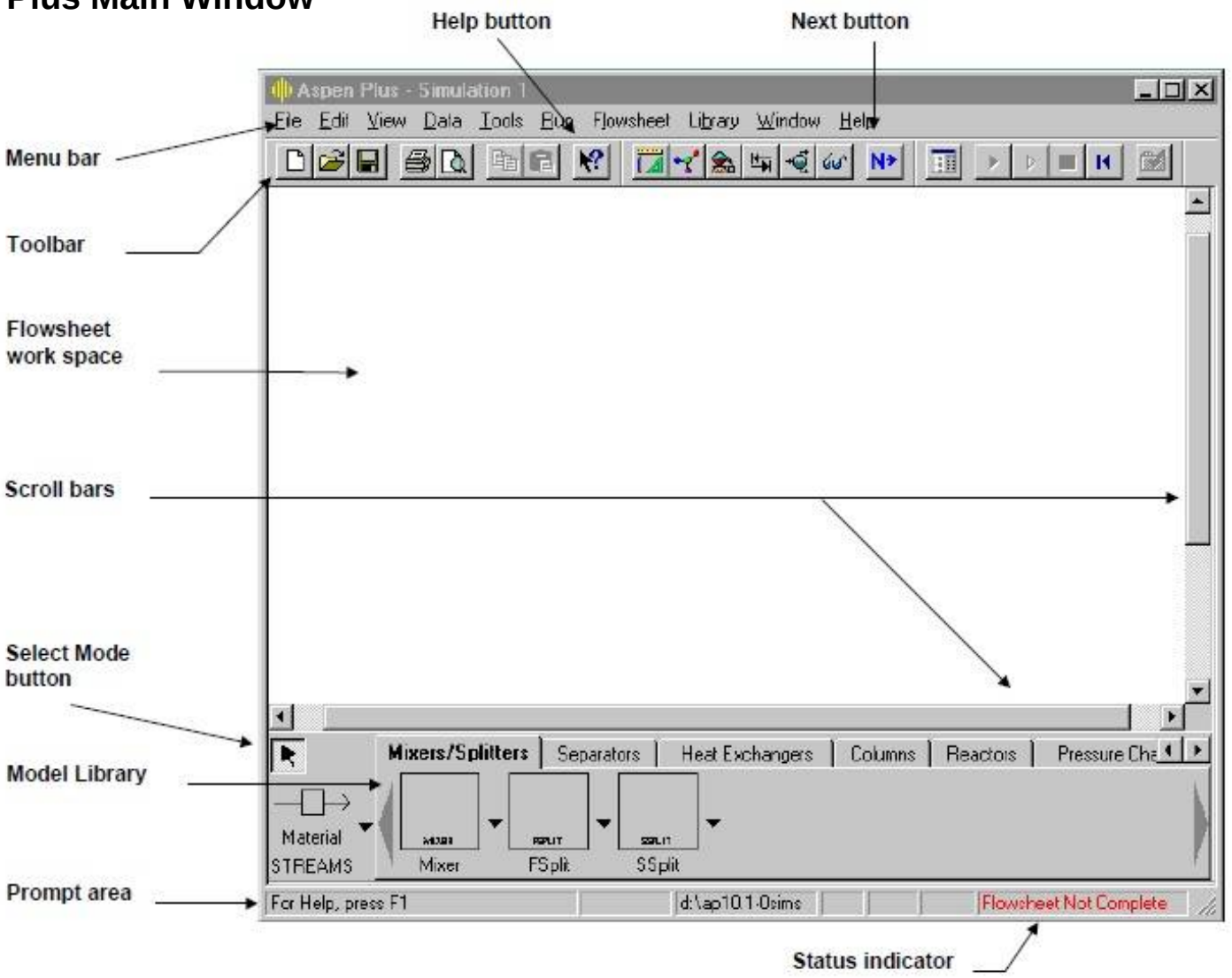
Components, i	$\{z_i\}$	*Phase Equilibrium K-value*
propane	0.1	6.8
n-butane	0.3	2.2
n-pentene	0.4	0.8
n-octane	0.2	0.052

- Start Aspen and ***choose Template***; ***OK***. When the window appears, choose General with ***English Units***. In the ***Run Type*** (lower right-hand corner), ***choose Flowsheet***. Click ***OK*** when the Aspen engine window appears. (This last step is specific to your installation.)

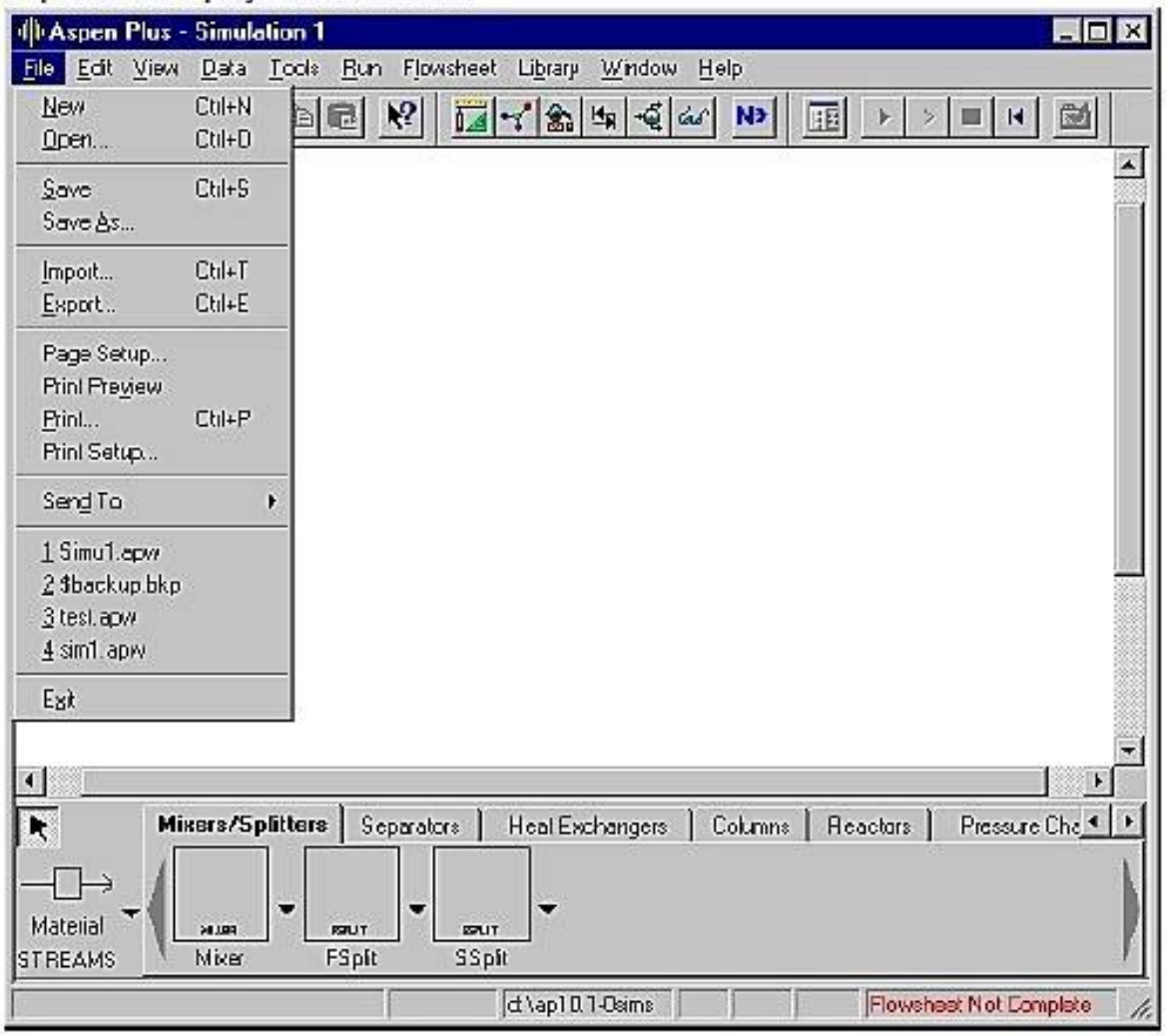
- ***Or***

- Click ***Aspen Tech***, select Aspen Plus 10.1-0, and click ***Aspen Plus User Interface***. The Aspen Plus ***Startup dialog box*** appears. You can use this dialog box to open an existing simulation or to create a new simulation using a ***template*** or a ***blank simulation***. Select the ***Blank Simulation*** option and click ***OK*** to start the new Aspen Plus simulation.

Aspen Plus Main Window

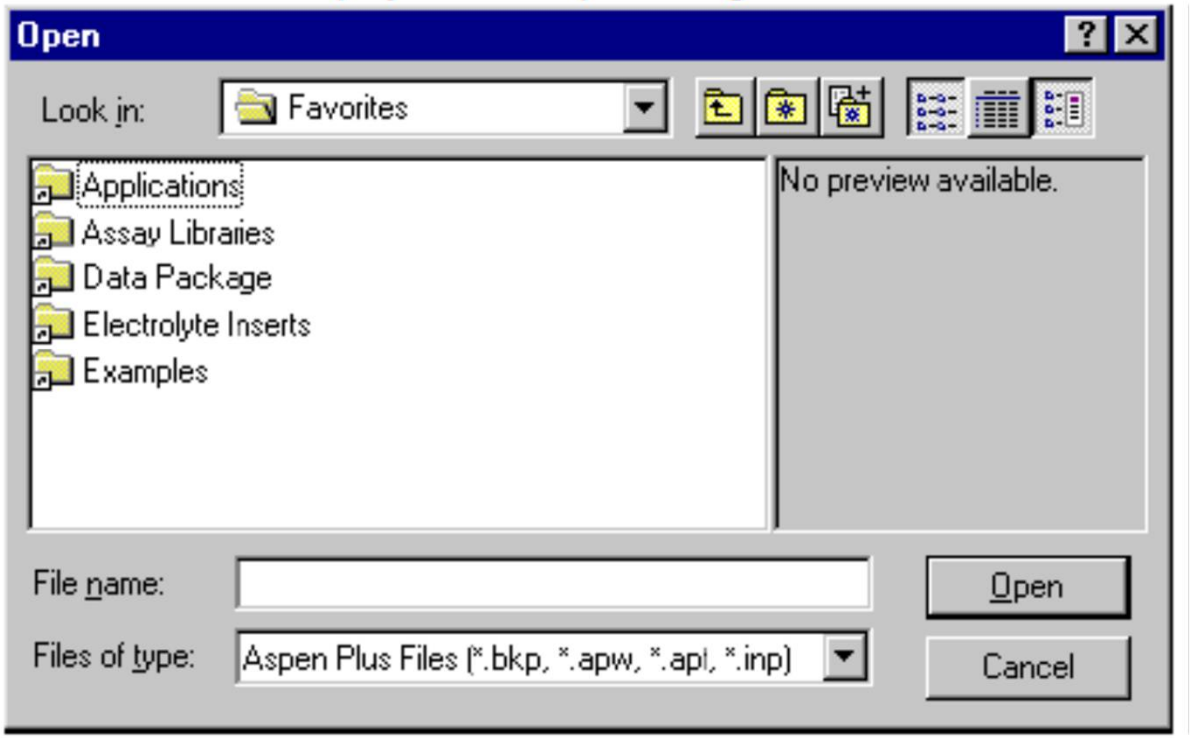


Aspen Plus displays the File menu:



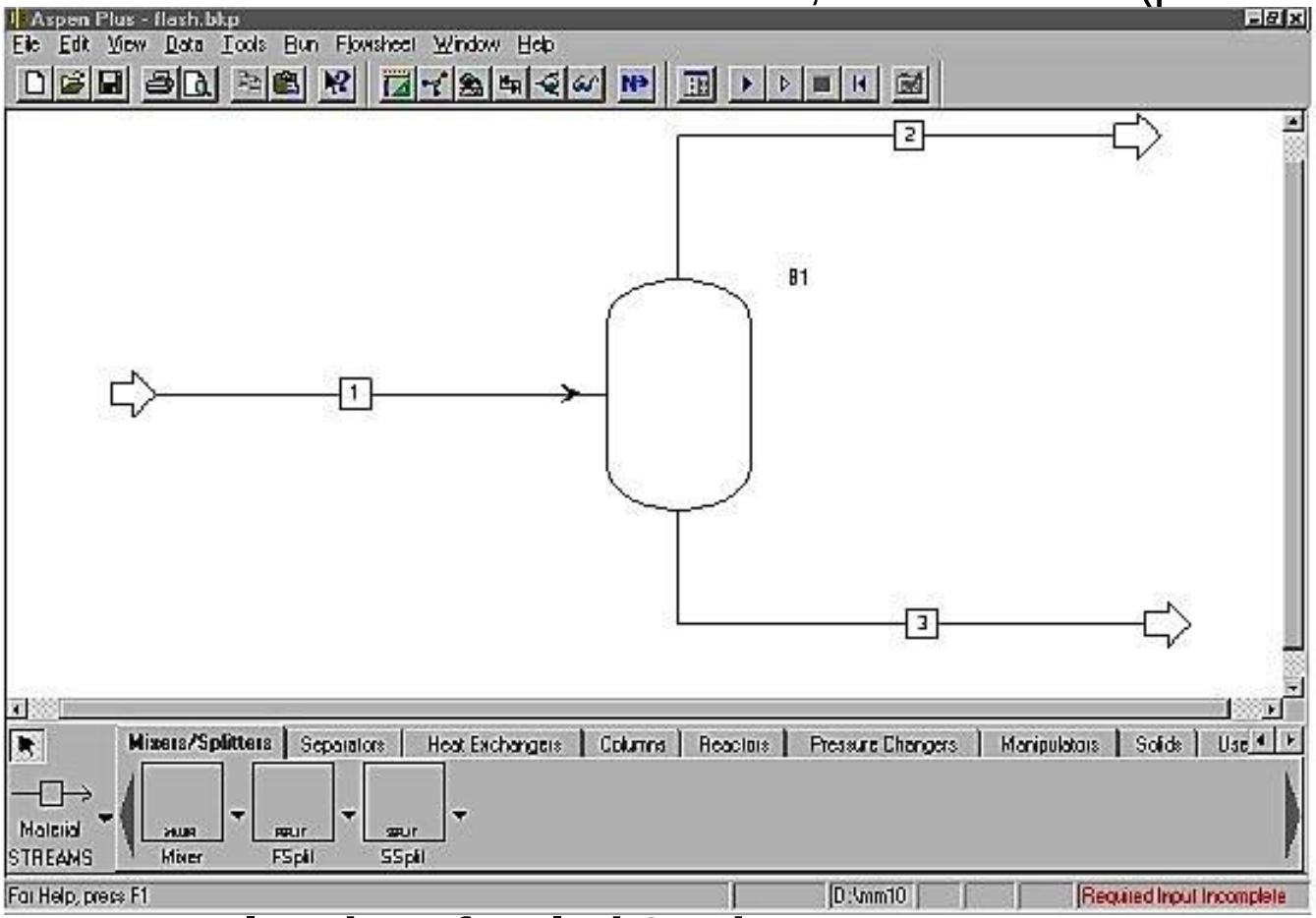
- From the File menu select Open.
- The Open dialog box appears. Your default working directory is displayed in the Look In box. You can navigate to the folder containing a file by using the Look In box or the Look In Favorites button
- Click the Look in Favorites button.

A list of folders is displayed in the Open dialog box:



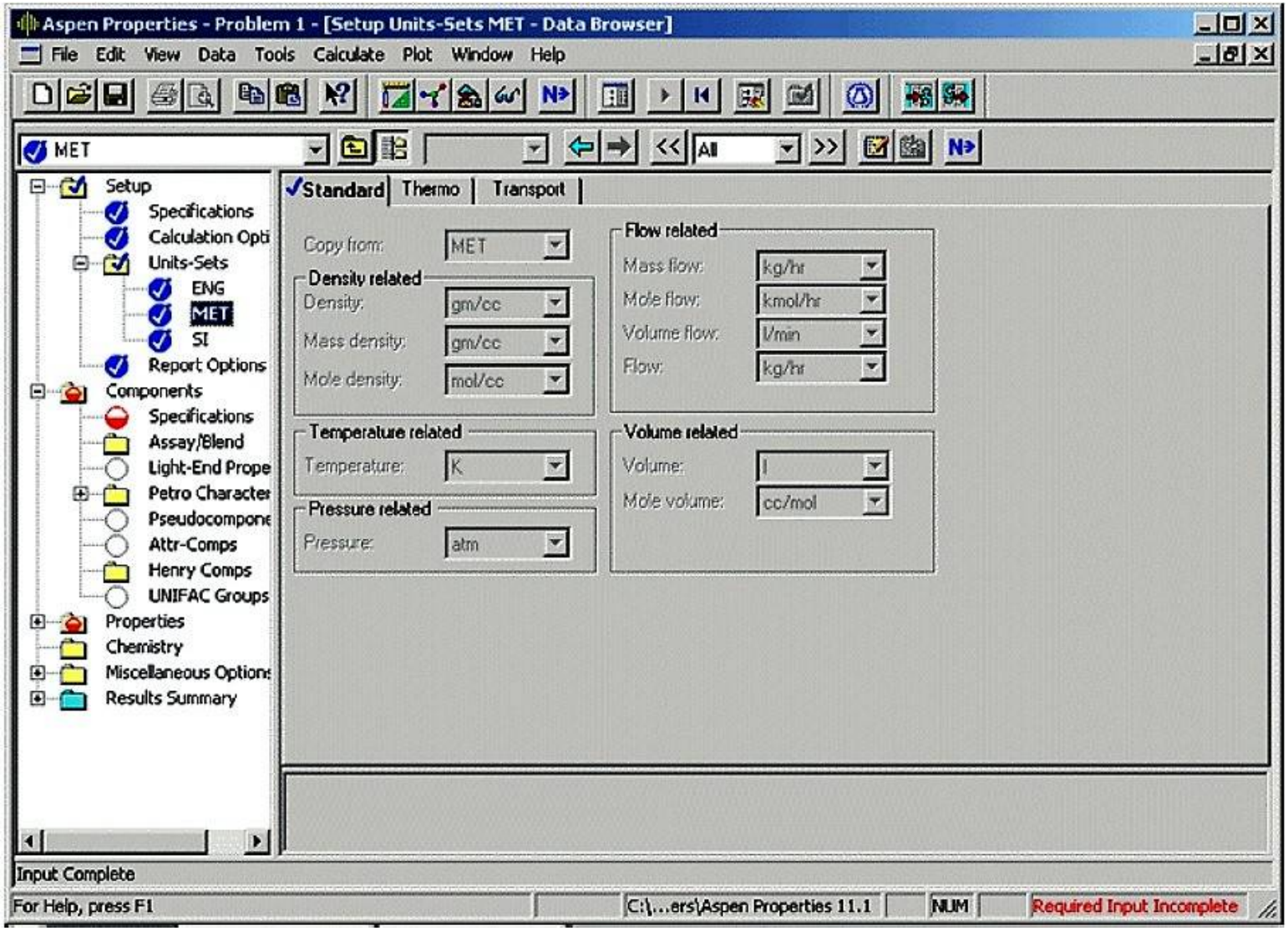
- Double-click the Examples folder.
- From the files list, select ***flash.bkp*** and click Open.
- Click Yes when Aspen Plus prompts "Do you want to close current run before opening new run?"
- Click No when Aspen Plus prompts "Save changes to Simulation 1?"

- If the bottom of the screen does not show the units, use the ***View/Model Library*** pull-down menu ***or press*** the ***F10 key***. In the units at the bottom, choose ***Separations***, then ***click*** on ***Flash2***. Click on the flow sheet, and the ***flash*** (phase separation) unit appears.



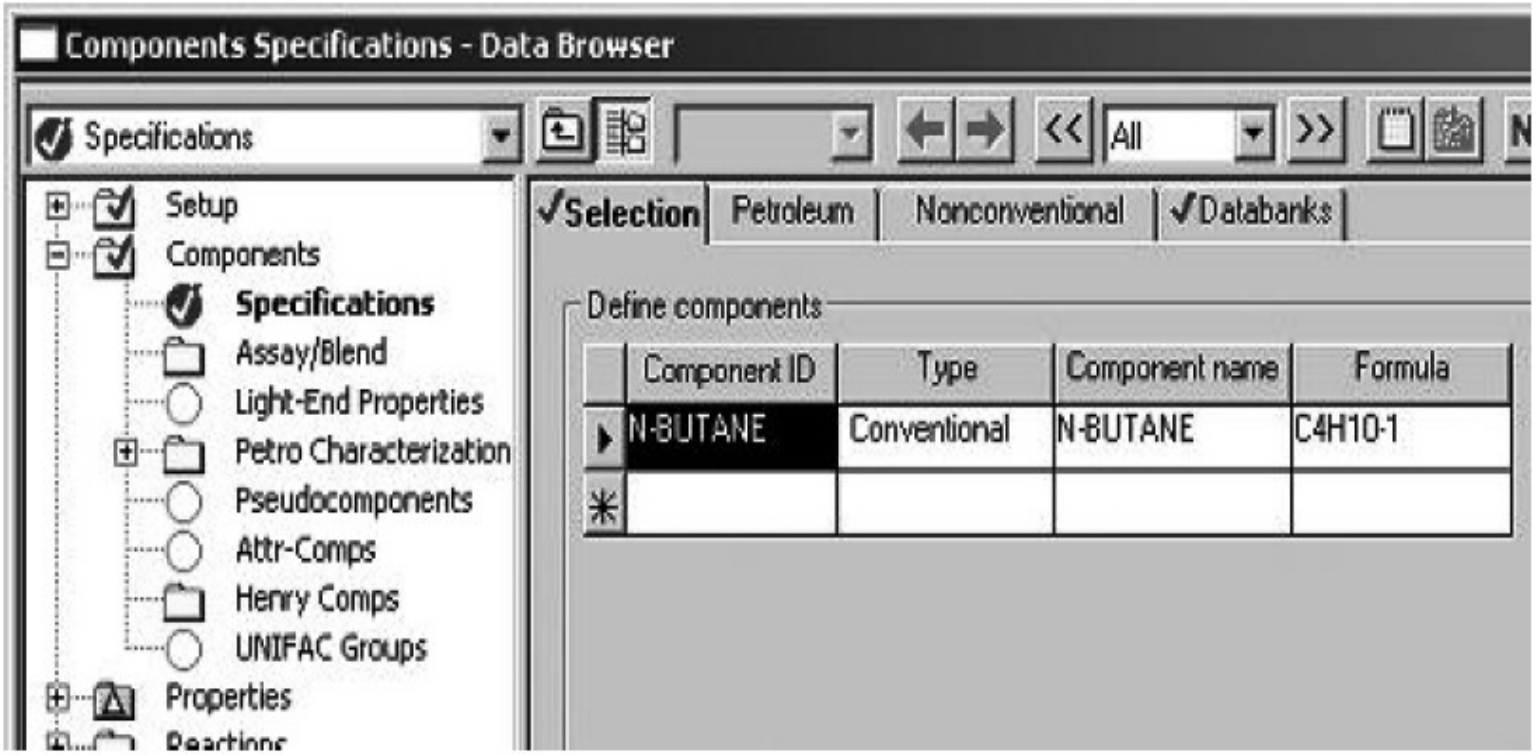
Flowsheet for Flash2 unit

- To add the input and output streams, ***click on Material Streams*** (lower left-hand corner), click on the flowsheet and drag a stream to the red arrow that is input to the flash unit. Click on the red arrows coming out and drag the stream away.
- If any red arrows show in the flowsheet, it means that the unit is not properly connected; it will ***message (Bottom right corner)*** in the ***status indicator*** '***Flowsheet not Complete***'.



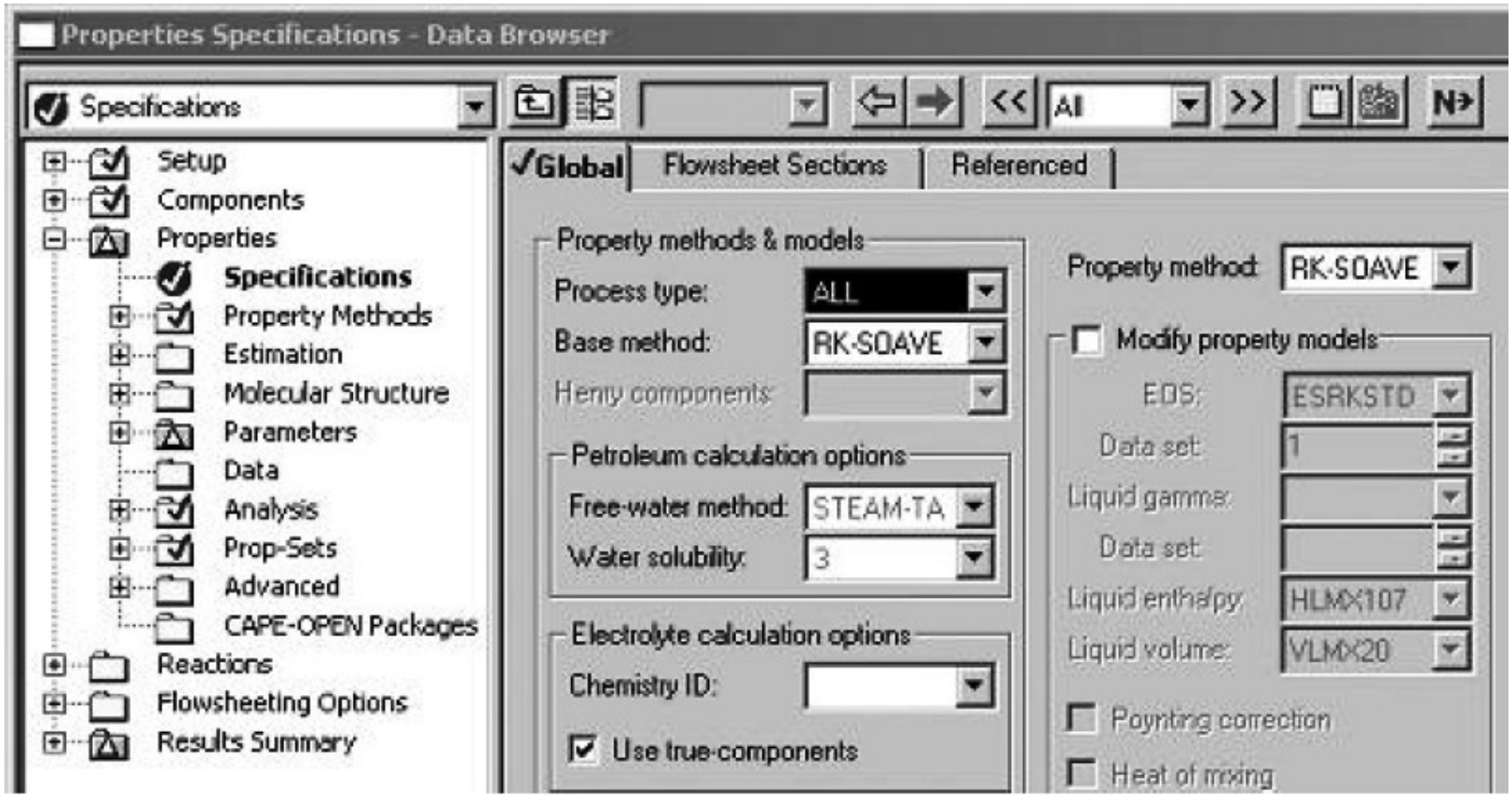
- If the flowsheet is complete, the ***status indicator*** message '***Required Input incomplete***'.
- Click on ***Next*** button or ***Data browser*** button in the in the toolbar.
- The data browser dialogue box will appear. This will bring a menu to the left of the screen.
- The boxes that are red indicate that you still need to supply information. Start at the top and work down, turning the red boxes into blue boxes by filling in the forms.

- Filling ***Component/Specifications*** in the ***data browser***

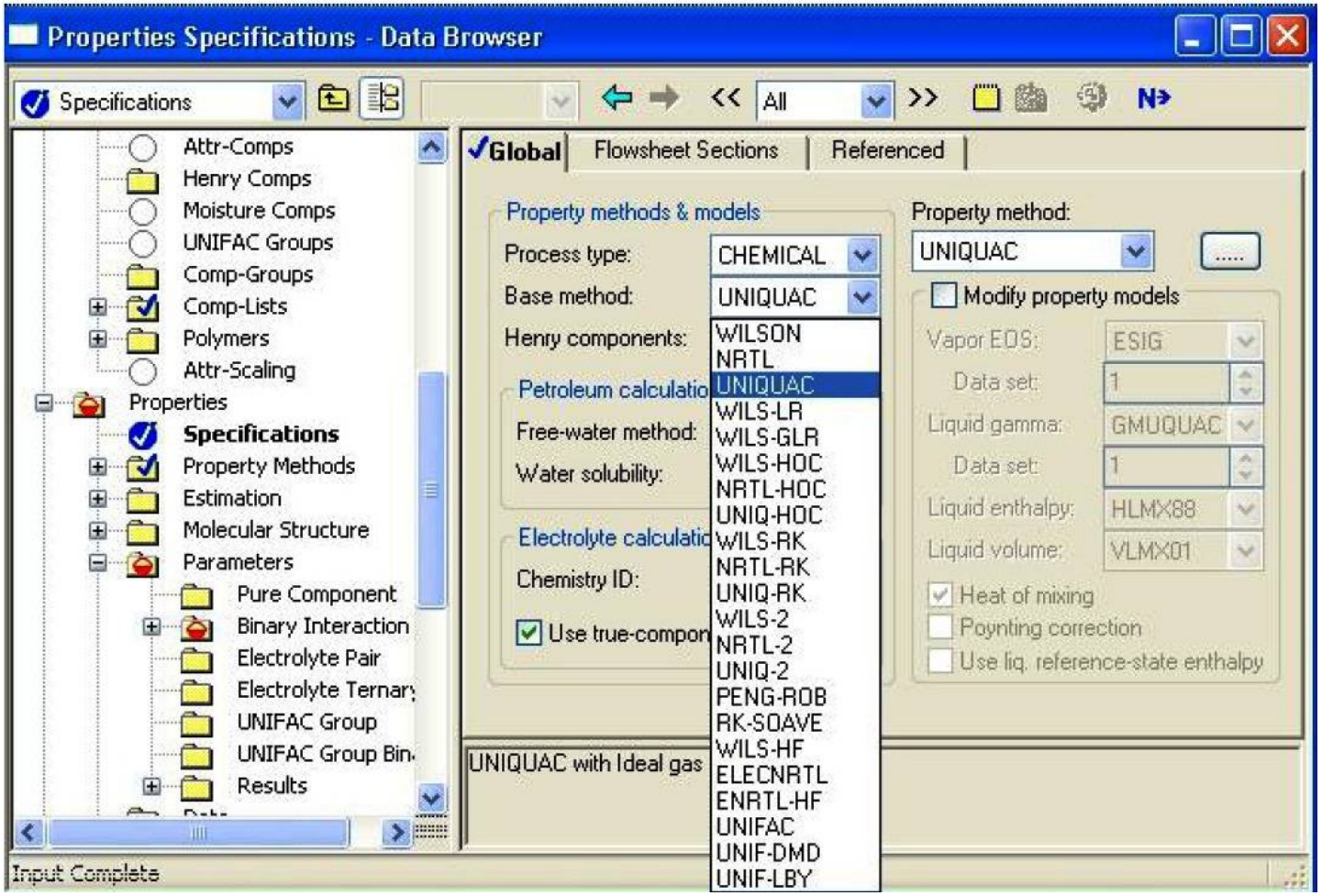


- Type the name or formula of the chemicals. If Aspen Plus does not recognize your chemical, a window appears that allows you to search again, and it will suggest a number of possibilities. When the components are completely specified, you should have an entry for every chemical in the column labeled Component name. The first column is what you are naming the chemicals, but the third column is what Aspen Plus uses when it obtains physical properties. If that column is blank, the program will not work.

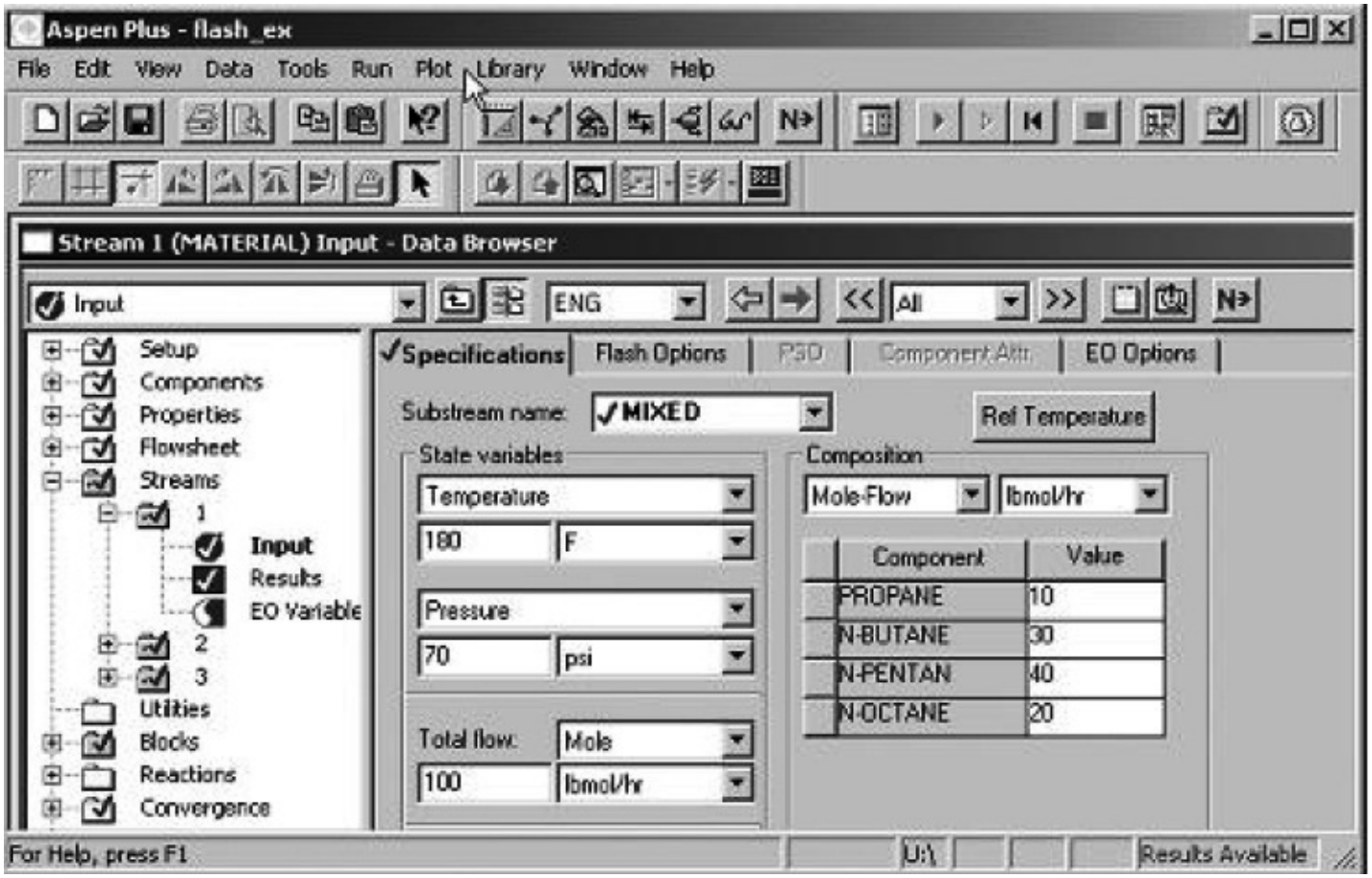
- Filling ***Property/Specifications***
- Choose the thermodynamic model
- Using Redlich–Kwong equation of state option in Aspen Plus



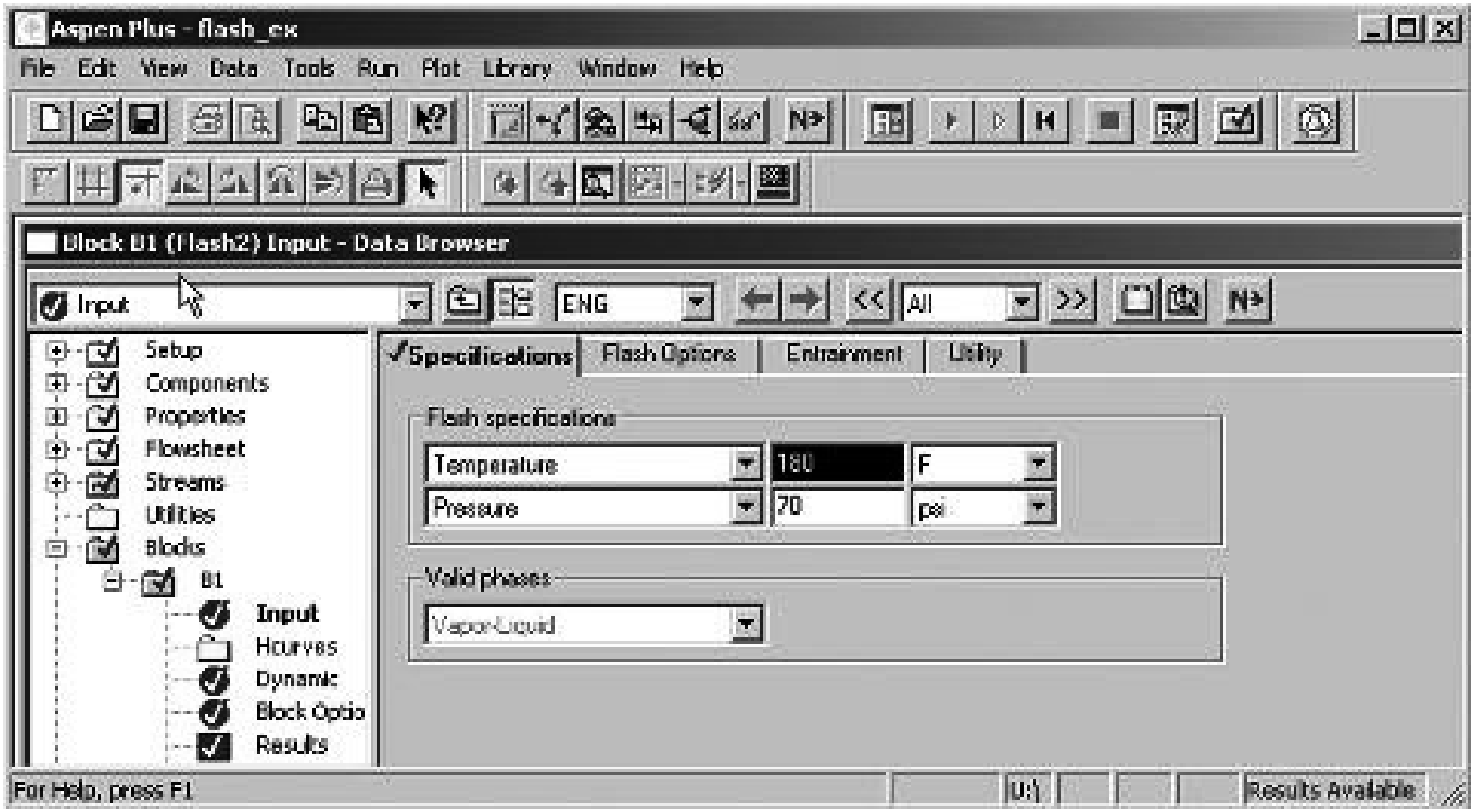
- Filling ***Property/Specifications***
- Choose the thermodynamic model



- Filling ***Streams***
- Choose the input stream, click on it, and insert the temperature, pressure, and flow rates of every chemical.



- Filling ***Block***
- In the list at the left, choose Blocks, then B1 (or whatever you have named your Flash2 unit), then Input. Choose Specifications, and insert the temperature and pressure of the unit.



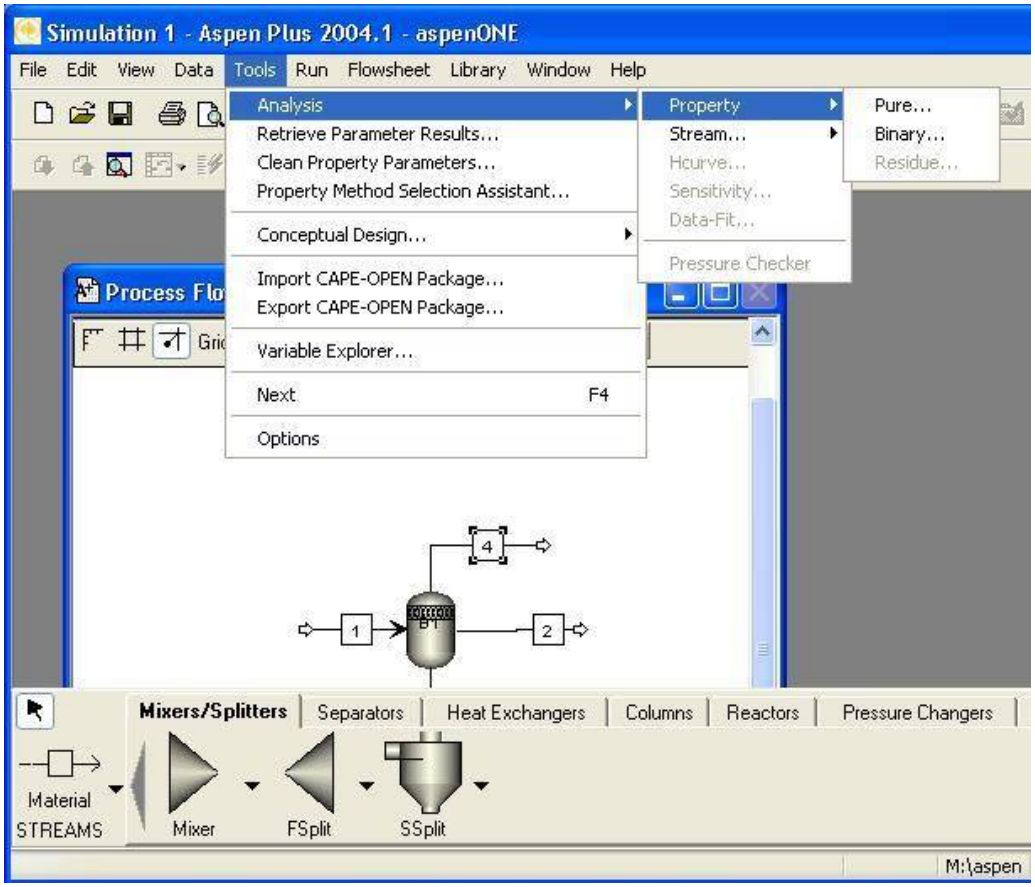
Flash2 Results

Temperature, °F	180	180	180
Pressure, psi	70	70	70
Vapor fraction	0.418979	1	0
Mole flow, lb mol/h	100	41.89795	58.10205
Mass flow, lb mol/h	7355.297	2587.239	4768.058
Volume flow, cubic ft/h	3865.909	3735.26	130.6492
Enthalpy, MMBtu/h	−6.767213	−2.262202	−4.505011
Mole flow, lb mol/h			
Propane	10	7.880996	2.119004
n-Butane	30	18.01565	11.98435
n-Pentane	40	15.09625	24.90375
n-Octane	20	0.90505	19.09495
Mole fraction			
Propane	0.1	0.1881	0.03647
n-Butane	0.3	0.429989	0.206264
n-Pentane	0.4	0.36031	0.428621
n-Octane	0.2	0.021601	0.328645

- Choose the next button at the top. If the input is incomplete, a window will appear to notify you and direct you to the missing data. If the input is complete, a window will appear to notify you of that, too. Click on the button to make it perform the calculation. This will cause the calculation of the process (here one unit) to proceed. Once the calculations finish (read the error messages, if any), click the Results box (lower one) to return to the regular menu. Then look at Results/Streams. The stream data will appear in tabular form, as shown in Table 3.3. If you click Stream Table, it will also be reproduced on your flowsheet.

Model the ***T–xy*** or ***p–xy*** diagram for the ***vapor–liquid of binary pairs*** using ***Property Analysis***

- Step 1: ***Start Aspen*** and choose ***Template***. A window appears; choose ***General*** with ***Metric Units***. From the ***Tools menu***, select ***Analysis***, then ***Property***, then ***Binary***. The Binary Analysis dialog box appears



Binary Analysis

Analysis type: Txy

Components
Component 1: ACETONE
Component 2: CHCL3

Compositions
Basis: Mole fraction
Component: ACETONE
Composition: Range
Lower: 0
Upper: 1
Points: 41
Increments:

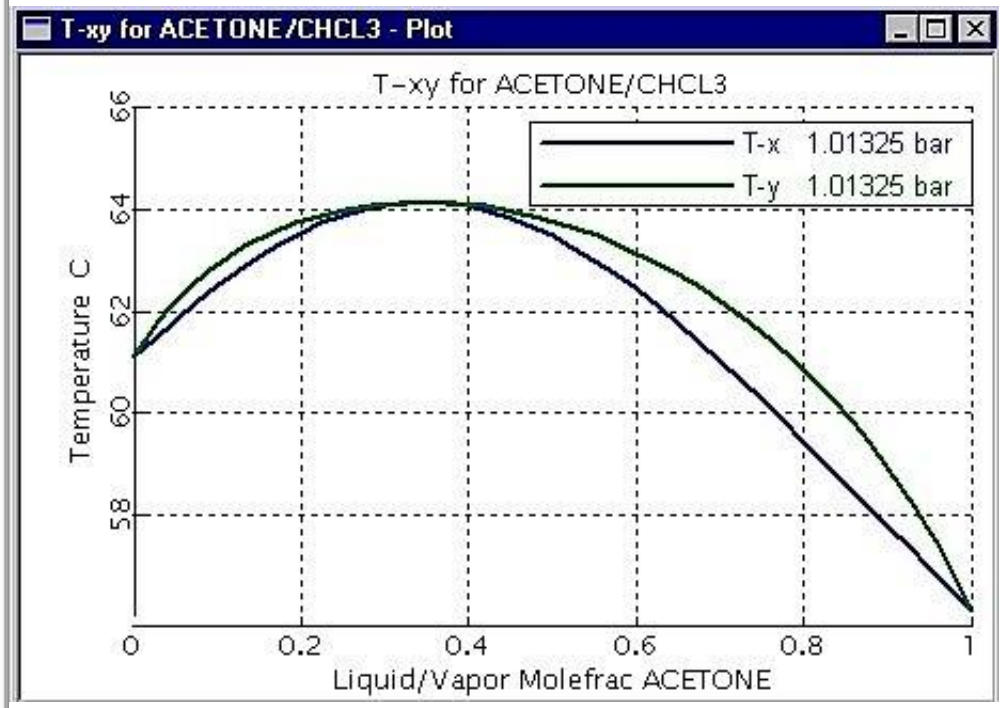
Valid phases
Vapor-Liquid

Pressure: List
Units: bar
1.01325

Property options
Property method: NRTL
Henry components:
Chemistry ID:

Save As Form | Go | Cancel

Analysis type.



- The options for the fugacity coefficient of the ***gaseous phase*** are: ***ideal gas***, ***Redlich–Kwong*** or ***Redlich–Kwong Soave***, ***Peng–Robinson***, plus a few specialized ones.
- In the liquid phase, the simplest option is an ***ideal liquid***, That choice leads to ***Raoult's law***. Other models include, ***NRTL***, ***Electrolyte NRTL***, ***UNIFAC***, ***UNIQUAC***, ***Van Laar***, and ***Wilson.***
- ***Oil and Gas Production (OIL GAS)*** – Peng–Robinson with Boston–Mathias a function (PR-BM) or Redlich–Kwong–Soave with Boston–Mathias a function (RKS-BM).
- ***Refinery, medium pressure (Refinery)*** – Chao–Seader, Grayson, Peng–Robinson, Redlich–Kwong–Soave.
- ***Refinery, hydrogen-rich applications (Refinery)*** – Grayson, Peng–Robinson, Redlich–Kwong–Soave.
- ***Gas processing, hydrocarbon separations (GASPROC)*** – Peng–Robinson with Boston–Mathias a function (PR-BM), Redlich–Kwong–Soave with Boston– Mathias a function (RKS-BM), Peng–Robinson, Redlich–Kwong–Soave.
- ***Gas Processing, acid gas absorption (Chemical and Electrol)*** – electrolyte NRTL.
- ***Petrochemicals, aromatics and ether production (Petchem)*** – Wilson, NRTL, UNIQUAC.

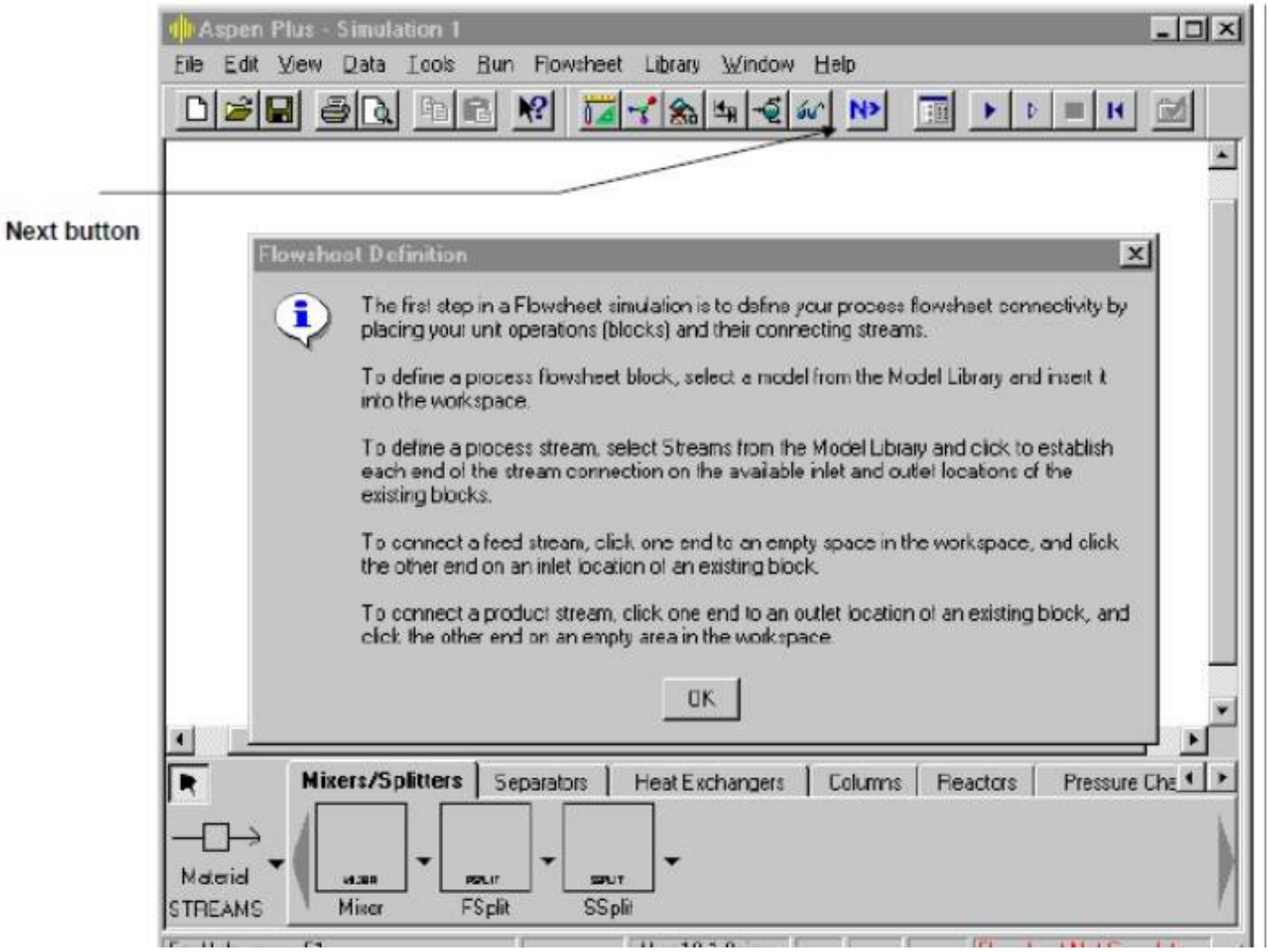
- ***Chemicals, phenol plants (Chemical)*** – Wilson, NRTL, UNIQUAC.
- ***Chemicals, ammonia plant (Chemical)*** – Peng–Robinson, Redlich–Kwong–Soave, SR-Polar (Schwartzentruber–Renon).
- ***Chemicals, inorganic chemicals (Chemical and Electrol)*** – electrolyte NRTL.
- ***Coal processing, combustion (Coalproc)*** – Peng–Robinson with Boston–Mathias a function (PR-BM), Redlich–Kwong–Soave with Boston–Mathias a function (RKS-BM), or the combustion databank.

MULTICOMPONENT DISTILLATION WITH *RadFrac*

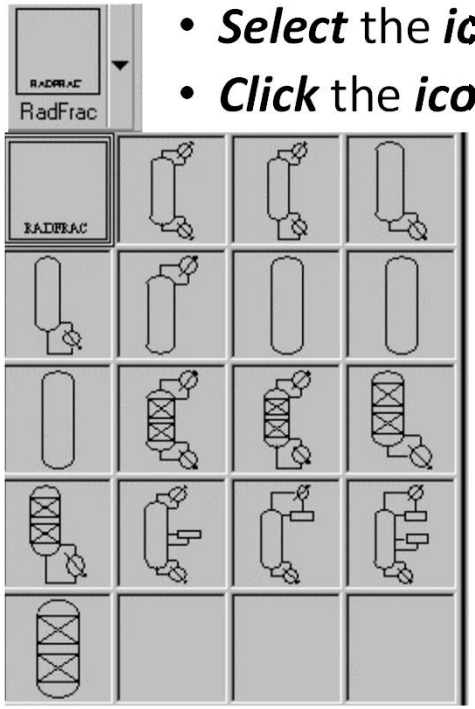
- **Problem:** The ***feed*** is ***100 lb mol/h propane***, ***300 lb mol/h i-butane***, and the other chemicals as listed in Table, at ***138 psia*** and ***75°F***. The column operates at ***138 psia*** with ***26 stages, reflux ratio 3.44*** and ***feed entrance*** on the ***19*** stage. The Refinery/Chao–Seader property method is used.

Chemical	Boiling Point (°C) at 1 atm
Propane	−42.1
i-Butane	−11.9
n-Butane	−0.5
i-Pentane	−27.9
n-Pentane	−36.1

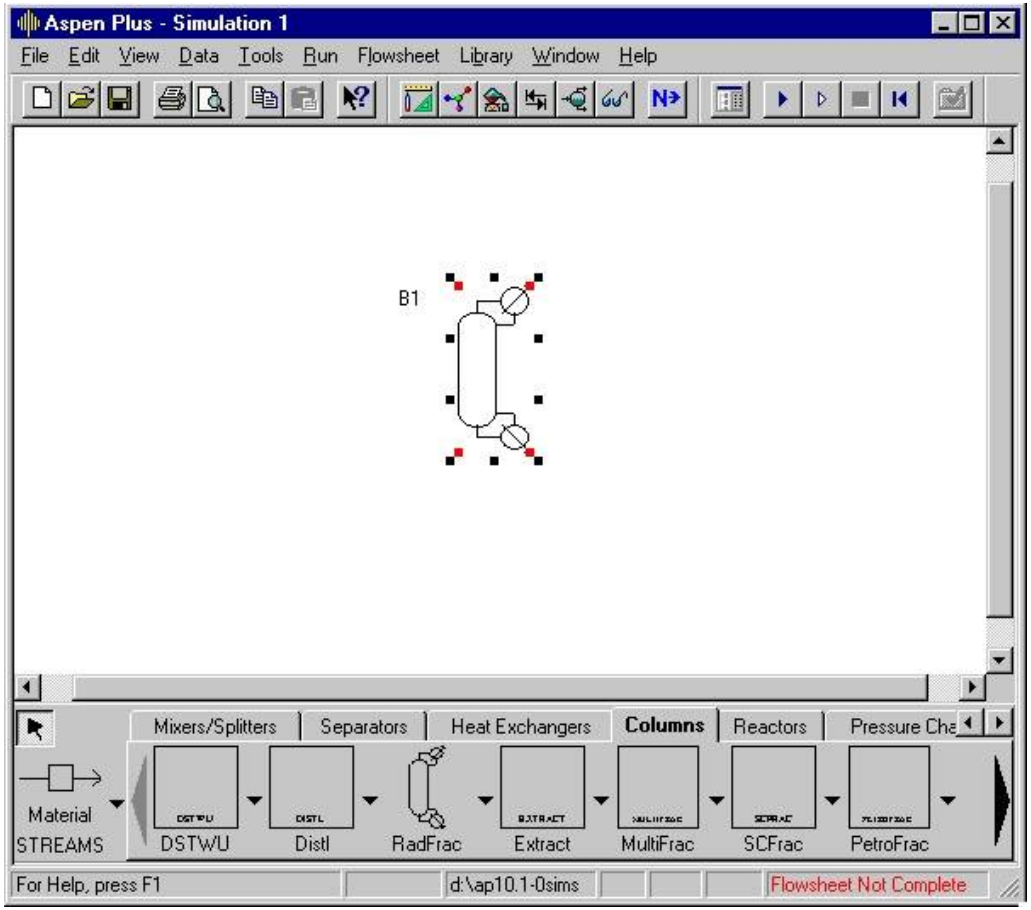
- On the Aspen Plus Startup ***dialog box***, select the ***Template*** option. Click ***OK*** to continue. The New ***dialog box*** appears.
- Select the General with ***English Units*** template for this session. The default Run Type, ***Flowsheet***, is appropriate for this session.
- Click ***OK*** to start the new Aspen Plus simulation.


Next button
Aspen Plus - Simulation 1
File Edit View Data Tools Run Flowsheet Library Window Help
Flowsheet Definition
The first step in a Flowsheet simulation is to define your process flowsheet connectivity by placing your unit operations (blocks) and their connecting streams.
To define a process flowsheet block, select a model from the Model Library and insert it into the workspace.
To define a process stream, select Streams from the Model Library and click to establish each end of the stream connection on the available inlet and outlet locations of the existing blocks.
To connect a feed stream, click one end to an empty space in the workspace, and click the other end on an inlet location of an existing block.
To connect a product stream, click one end to an outlet location of an existing block, and click the other end on an empty area in the workspace.
OK
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Material
STREAMS
Mixer
FSplit
SSplit

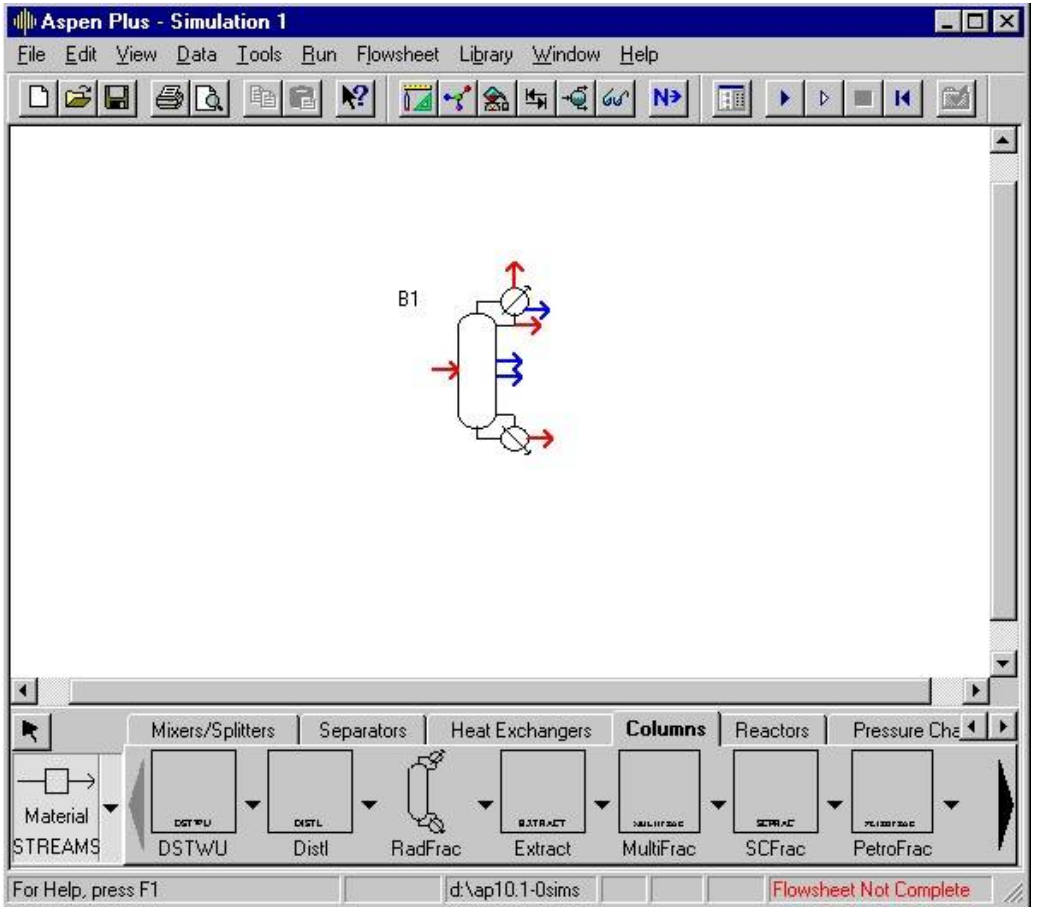
- From the Aspen Plus main window, ***click*** the ***Columns tab*** on the ***Model Library***.
- Move the mouse over the ***RadFrac*** block and read the ***prompt***. The prompt for RadFrac suggests this is the right model for this problem.
- Click ***RadFrac***, then ***press*** the Help key (***F1***).
- To ***choose*** a ***different icon*** for ***RadFrac***, click the down arrow to the right of RadFrac in the Model Library.



- ***Select*** the ***icon*** labeled ***FRACT1*** under the ***RadFrac*** block.
- ***Click*** the ***icon*** and ***drag*** it to the ***Process Flowsheet window***.
- ***Click*** the ***Material Stream*** icon on the left side of the ***Model Library***.

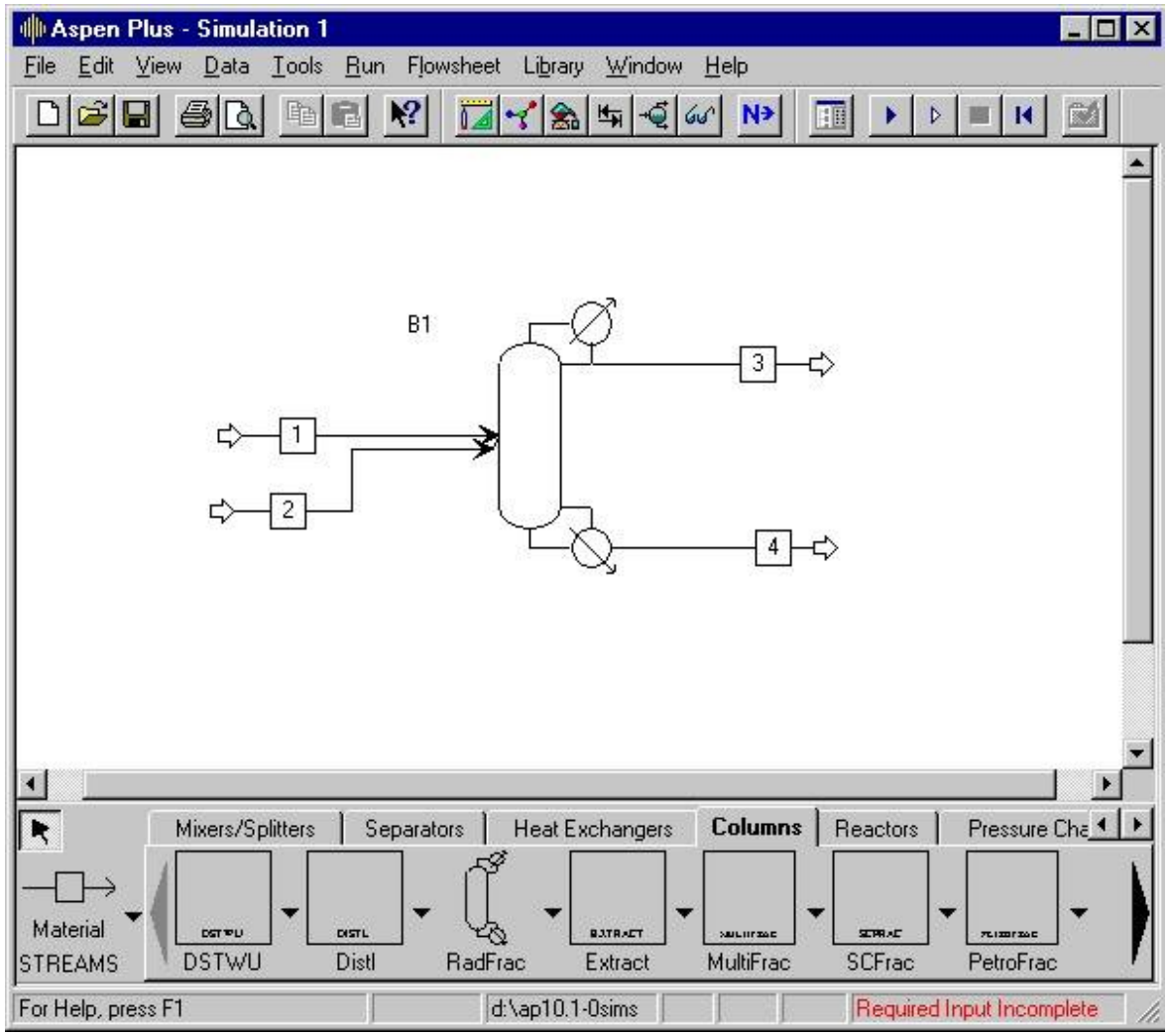


The inserted ***RadFrac*** block



Ports that must have at ***least one stream connected*** are shown in ***red***. ***Optional ports*** are shown in ***blue***. If you position the mouse pointer over a port for a few seconds, the arrow is highlighted and a description of the port appears.

To connect the feed streams



- Graphical simulation flowsheet is now complete. The ***status indicator*** in the bottom right of the main window says "***Required Input Incomplete***" indicating that further input specifications are required for the simulation.

Entering Components

- ***Click*** the ***Next button*** on the Data Browser window toolbar. ***Data browser*** window appears.
- In the first Component ID box, type PROPANE and press Enter.
- Click the next blank Component ID box, Type BUTANE and press Enter.

Selecting Thermodynamic Methods

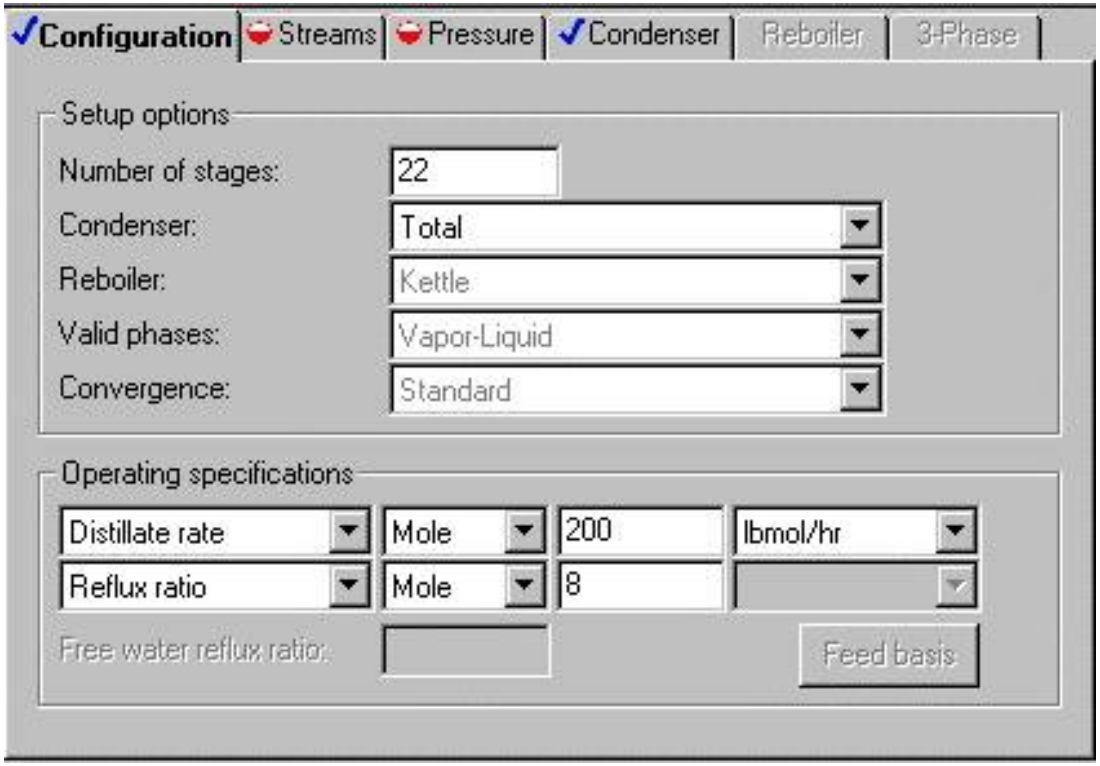
- Use the ***Properties Specifications*** Global sheet to select the thermodynamic methods used to calculate properties such as K-values, enthalpy, and density.
- In general, the ***UNIFAC*** property method for ***liquid phase nonideality*** is chosen.
- But for refinery product, ***Refinery/Chao–Seader*** property method is used.

Entering Stream Data

- Enter the following state variable and component flow specifications for the feed stream
- ***feed*** is ***100 lb mol/h propane***, ***300 lb mol/h i-butane***, ***500 lb mol/h n-butane, 400 lb mol/h i-pentane, 500 lb mol/h n-pentane.***
- *P*= ***138 psia*** and *T*= ***75^{o}F***

Entering Unit Operation Block Data

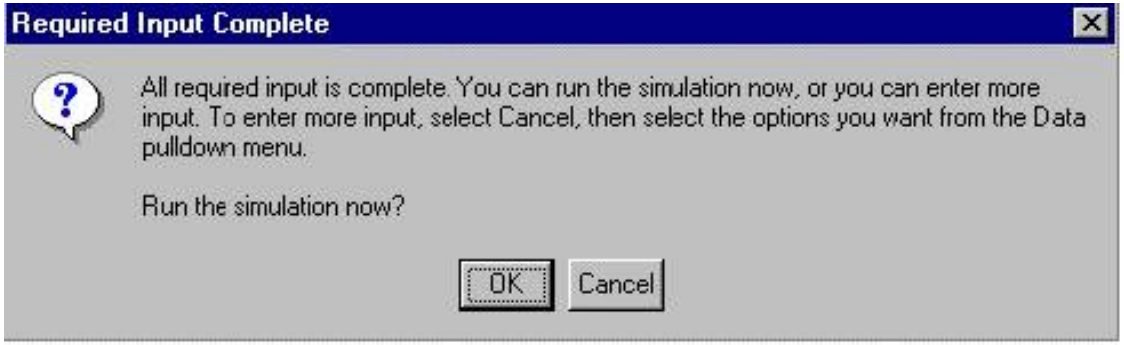
- ***Click*** the ***Next button*** on the Data Browser window title bar.
- The Aspen Plus expert system displays a Completion Status window, stating that you need to enter ***Number of stages***, ***Condenser type***, specifications, in order to complete this sheet:

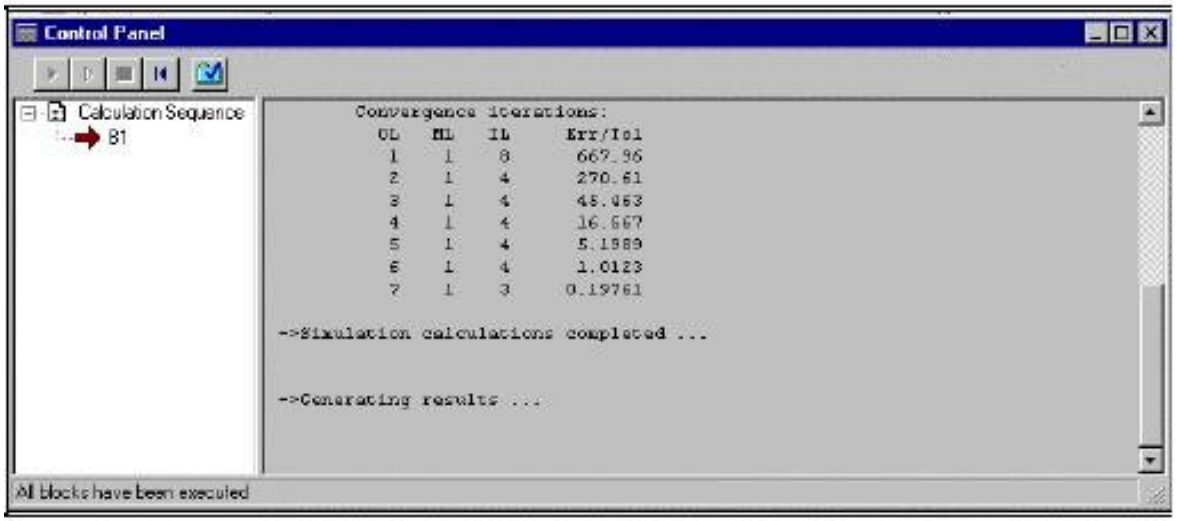


- Now enter the operating specifications for the column:
- ***26 stages***, Set the ***reflux ratio*** to ***3.44*** and enter the feed on the ***thirteenth stage***.

Running the Simulation

- ***Click*** the ***Next button*** on the Data Browser window toolbar.
- Click ***OK*** on the Required Input Complete dialog box.





- The ***Control Panel*** allows you to ***monitor and interact*** with the Aspen Plus ***simulation calculations***.
- The simulation calculations occur in three sequential steps:
  1) Processing input specifications
  2) Calculations begin
  3) Generating results

Examining Block Results

- ***Click*** The individua ***Block*** n the simulation flowsheet.
- Select ***Results*** from the ***menu***.
- ***Click*** the ***Profiles*** form in the ***menu tree*** on the left side of the Data Browser window.

Mole flow lb mol/h			
Propane	100	85.80379	14.19621
i-Butane	300	12.31199	287.688
n-Butane	500	1.883926	498.1161
i-Pentane	400	0.000257	399.9997
n-Pentane	500	4.61×10^{-5}	500
Mole fraction			
Propane	0.055556	0.858038	0.008351
i-Butane	0.166667	0.12312	0.169228
n-Butane	0.277778	0.018839	0.293009
i-Pentane	0.222222	2.57×10^{-6}	0.235294
n-Pentane	0.277778	4.61×10^{-7}	0.294118
Total flow, lb mol/h	1800	100	1700
Total flow, lb/h	115843.6	4608.785	111234.8
Total flow, cubic ft/h	3126.01	147.3943	3489.477
Temperature, °F	75	80	199.5242
Pressure, psi	138	138	138
Vapor fraction	0	0	0
Liquid fraction	1	1	1

TABLE. ***Stream*** data for Multicomponent Distillation with RadFrac, ***Reflux Ratio=3.44***

- ***86%*** of the ***propane*** goes out in the top stream; along with ***4%*** of the ***i-butane***. The ***condenser*** is at ***80°F*** and has a ***heat duty of –2.94 ×10⁶ Btu/h***, and the ***reboiler*** is at ***199.5°F*** and has a ***heat duty of 11.5 ×10⁶ Btu/h***. ***Above the feed***, the flow rate varies between ***283 and 344 lb mol/h***, and ***below it***, the flow rate varies between ***2998 and 3097 lb mol/h***.

Calculation with higher reflux ratio

- For ***reflux ratio 5***, ***94.2 lb mol/h*** of ***propane*** goes out in the ***top stream***. Increasing the reflux ratio to ***7.5*** gives ***98.2 lb mol/h*** of ***propane***, and a reflux ratio of ***10*** gives ***99.2 lb mol/h*** of ***propane***.

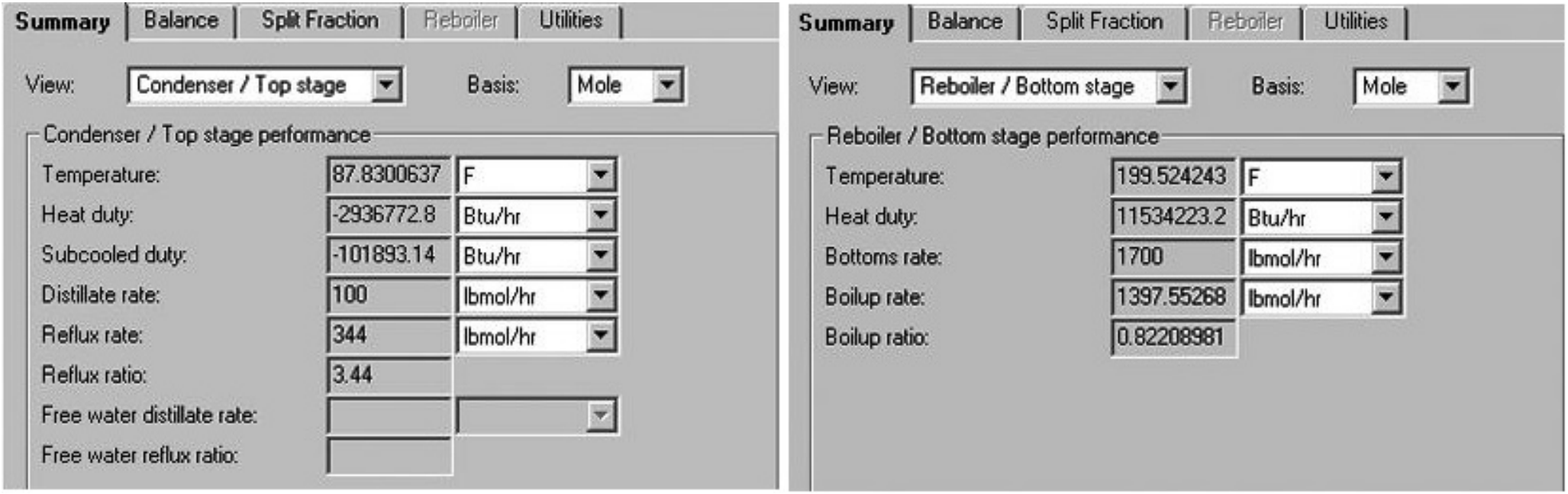


Fig. ***Condenser*** and ***reboiler*** calculations for Multicomponent distillation with ***RadFrac***, ***reflux ratio = 3.44.***

Reactors

- Chemical reactions occur under diverse conditions in many different types of equipment.
- ***RStoic***, ***RYield***, ***RGibbs***, and ***RCSTR*** can have ***any number*** of ***material feed streams***, which are ***mixed internally***. ***Heats of reaction*** are not required for any ***reactor model***. Aspen Plus calculates heats of reaction using ***heats of formation***.
- For ***RCSTR***, ***RPlug***, and ***Rbatch*** utilize ***reaction kinetics*** information using:
    1. The built-in ***power law*** model.
    2. The built-in generalized ***Langmuir-Hinschelwood-Hougen-Watson*** (LHHW) model.
    3. A user-written ***Fortran subroutine***.
- ***Rstoic***
    1. ***Reaction kinetics*** are ***unknown*** or ***unimportant***.
    2. ***Extent of reaction*** or ***conversion*** can be specified.
    3. ***Rstoic*** can handle reactions that occur independently in a ***series of reactors***.
    4. It can also perform ***product selectivity*** and ***heat of reaction calculations***.

- ***RYield***

  RYield models a reactor by specifying reaction yields of each component. This model is useful when:

  1. Reaction stoichiometry and kinetics are unknown.
  2. Yield distribution data or correlations are available.

- ***REquil***

  REquil models reactors when ***some or all*** reactions ***reach equilibrium***. REquil can calculate ***single-phase chemical equilibrium***, or ***simultaneous phase*** and chemical equilibria. REquil calculates equilibrium by solving ***stoichiometric chemical and phase equilibrium equations***.

- ***Rgibbs***

  1. RGibbs models ***single-phase chemical equilibrium***, or ***simultaneous phase*** and chemical equilibria.
  2. reactor ***temperature and pressure***, or ***pressure and enthalpy*** are specified***.***
  3. RGibbs ***minimizes Gibbs free energy***, subject to atom balance constraints. This model ***does not require reaction stoichiometry***.

4. Rgibbs can determine ***phase equilibrium*** without chemical reaction, ***particularly for multiple liquid phases***.
5. Assign components to be in particular phases in equilibrium.
6. Use different property models for each liquid or solid solution phase.
7. Chemical equilibria can be restricted by specifying
    I. Fixed moles of any product
    II. Percentage of a feed component that does not react
    III. Fixed extents of reaction
    IV. Temperature approach to equilibrium for the entire system
    V. Temperature approaches for individual reactions

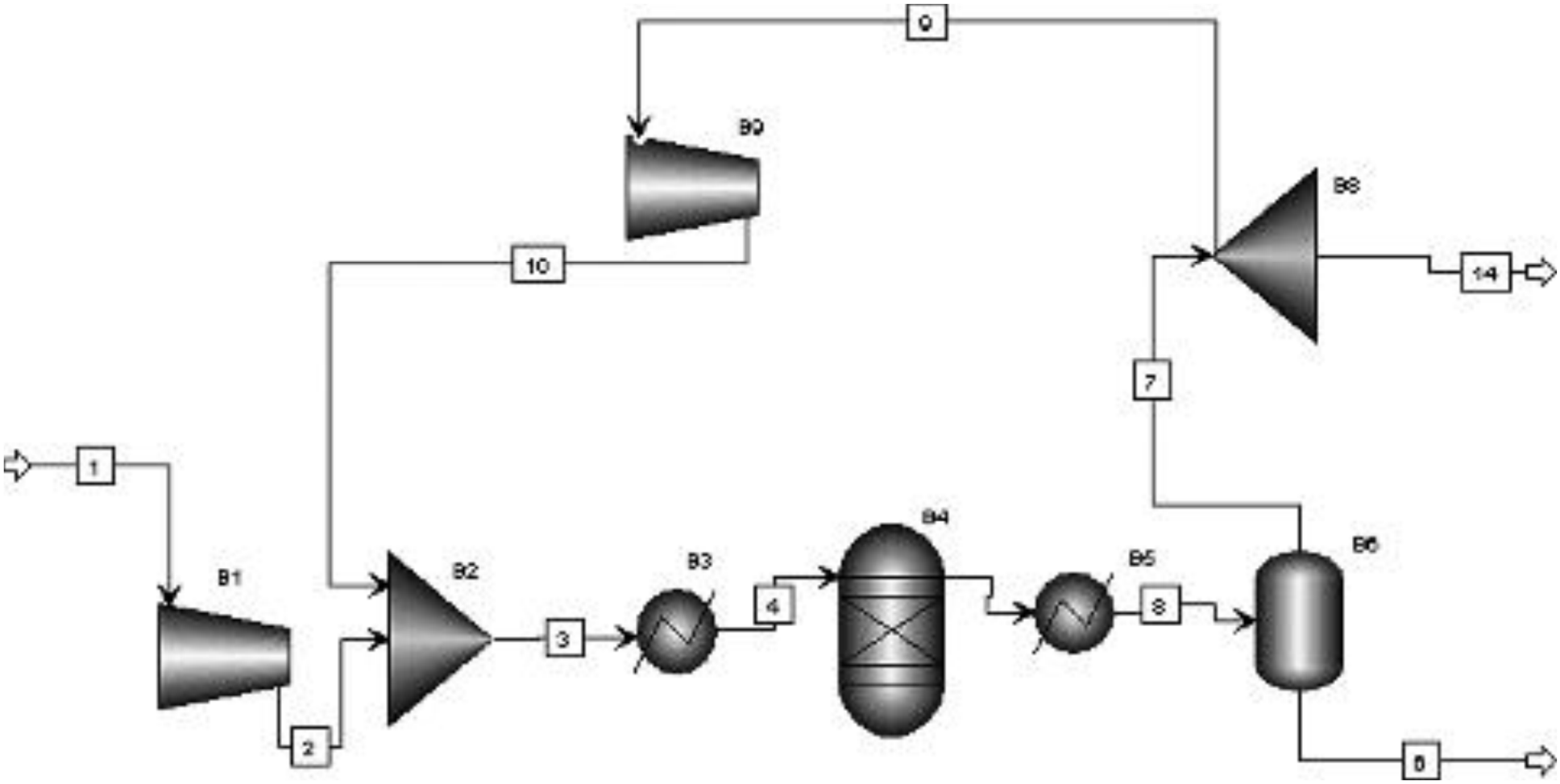
RCSTR

1. ***Reaction kinetics*** are ***known***.
2. The contents of the reactor have the same properties as the outlet stream.
3. RCSTR can model ***equilibrium reactions*** simultaneously with ***rate-based reactions***.
4. RCSTR computes ***heat duty*** given the ***temperature*** or ***temperature*** given the ***heat duty***.

- ***RPlug***
    1. RPlug rigorously models plug flow reactors.
    2. A ***cooling stream*** around the reactor is ***optional***.
    3. RPlug model reactors with ***cocurrent*** and ***countercurrent coolant streams***.
    4. RPlug handles ***rate-based kinetic reactions only***.
- Rbatch
    1. RBatch rigorously models ***batch or semi-batch*** reactors.
    2. For ***semi-batch*** reactors, a ***continuous vent*** and any number of ***continuous or delayed feeds*** can be specified.
    3. RBatch handles ***rate-based kinetic reactions only***.

Ammonia Process

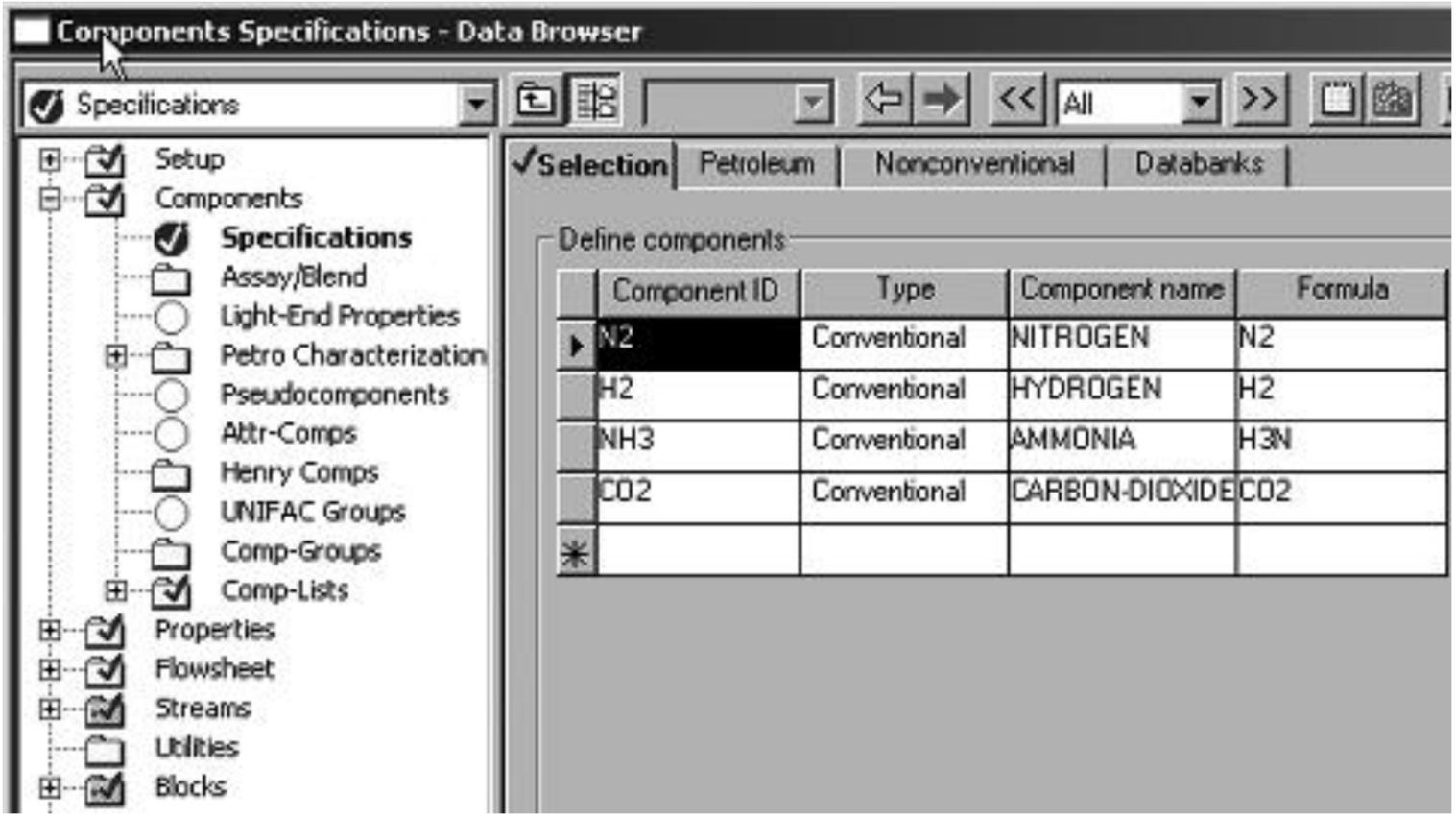
- The feed to the process is nitrogen, hydrogen, and a small amount of carbon dioxide (left over from the process to make the hydrogen).
- Input stream to the process (***at 80°F and 300 psia***): nitrogen, ***100 lb mol/h***; hydrogen, ***300 lb mol/h***; ammonia, ***0***; and carbon dioxide ***1 lbmol/h***. The inlet stream is ***compressed to 4000 psi*** with an isentropic compressor
- The ***process feed*** is ***mixed with a recycle stream*** and ***heated to 900°F***, the reactor temperature, and sent to the ***reactor***. The ***feed to the reactor is roughly a 3:1*** mixture of hydrogen and nitrogen, with some ammonia, too.
- In the reactor, there is a ***pressure drop of 30 psi***.
- The outlet is ***cooled to 80°F*** and the liquid and vapor phases are ***separated***.
- The vapor phase goes to ***recycle***, and ***0.01 percent*** of it is used as ***purge***.
- A ***recycle compressor*** then compresses the rest from ***3970 to 4000 psia***.
- A small part of the recycle stream is ***bled off as a purge*** stream to prevent the ***buildup of impurities***.



ASPEN Flow Sheet of Ammonia Process

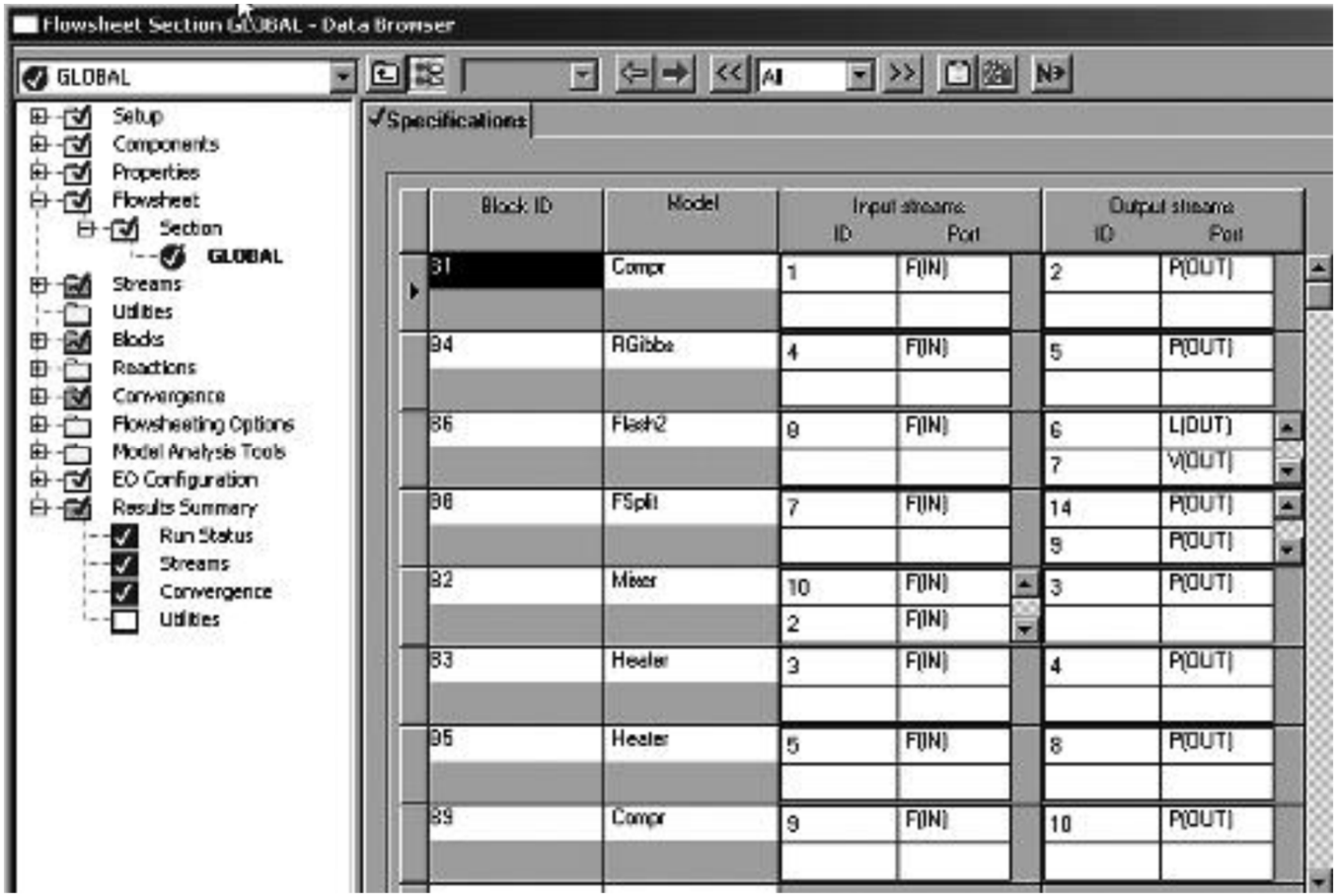
The identification of components

- It is useful to ***check the connections*** between the ***units*** using the ***Flowsheet option/Section//GLOBAL***



Components of the process

- After selecting ***Flowsheet option/Section//GLOBAL***, the data browser screen is shown in the following figure:

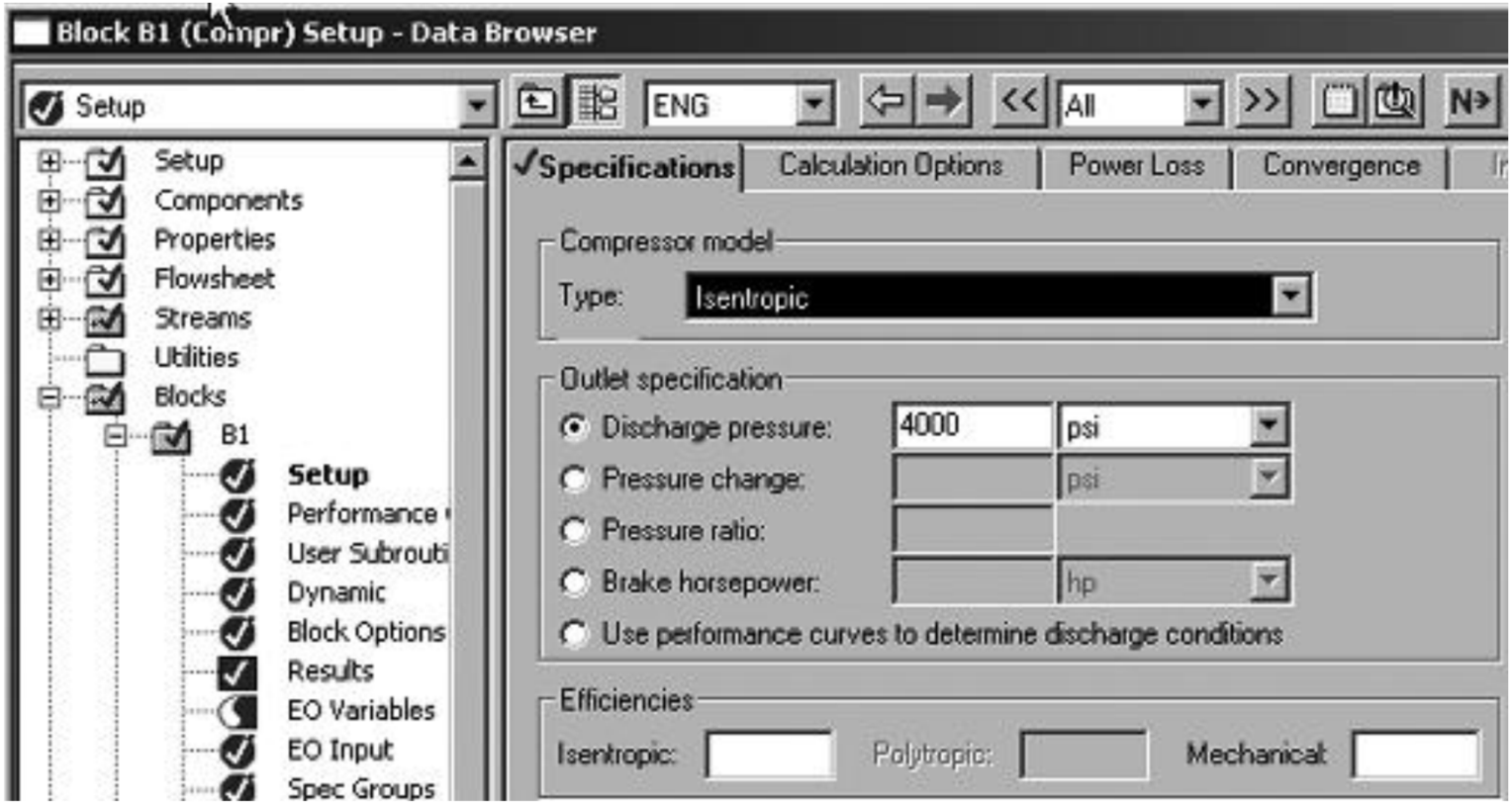


Flowsheet in brief

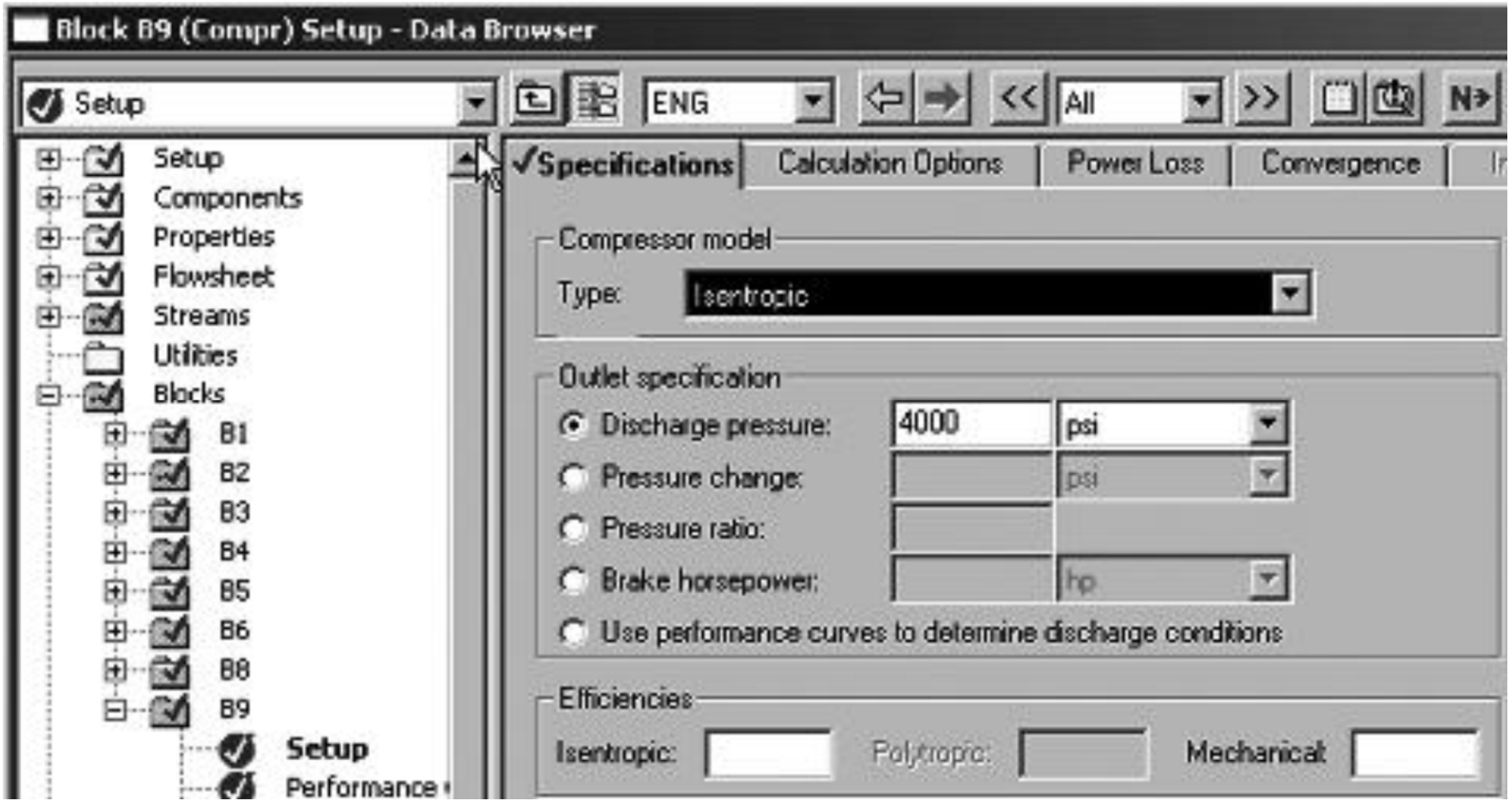
Any ***disconnected stream*** will not show its numbers that is shown by input ***stream ID and Port***.

The operating parameters for the compressors

- An ***isentropic compressor (B1)*** in the ***feed*** stream to ***compress feed gases***.
- Discharge pressure ***4000 psi***.

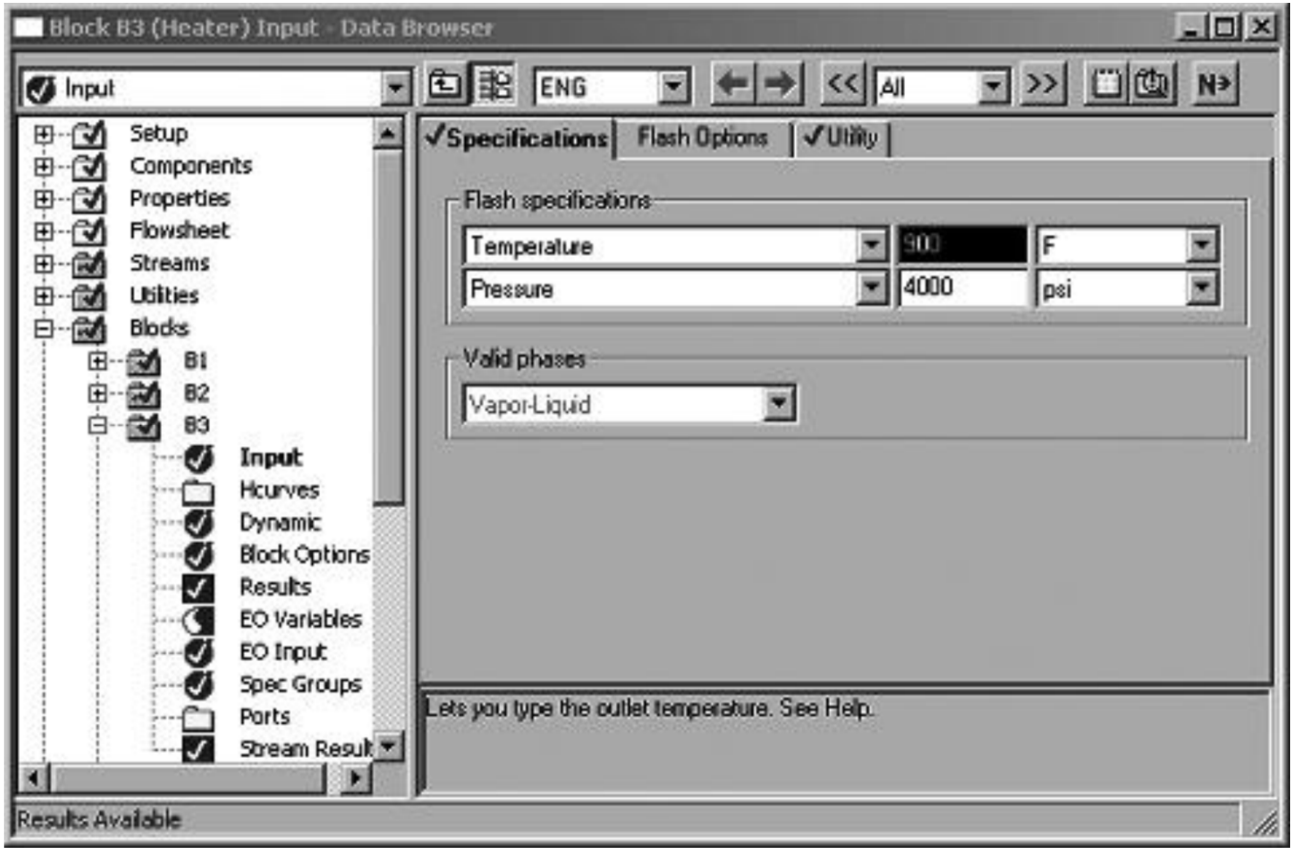


- An ***isentropic compressor (B9)*** in the ***recycle*** stream to ***compress recycle gases***.
- Discharge pressure ***4000 psi***.

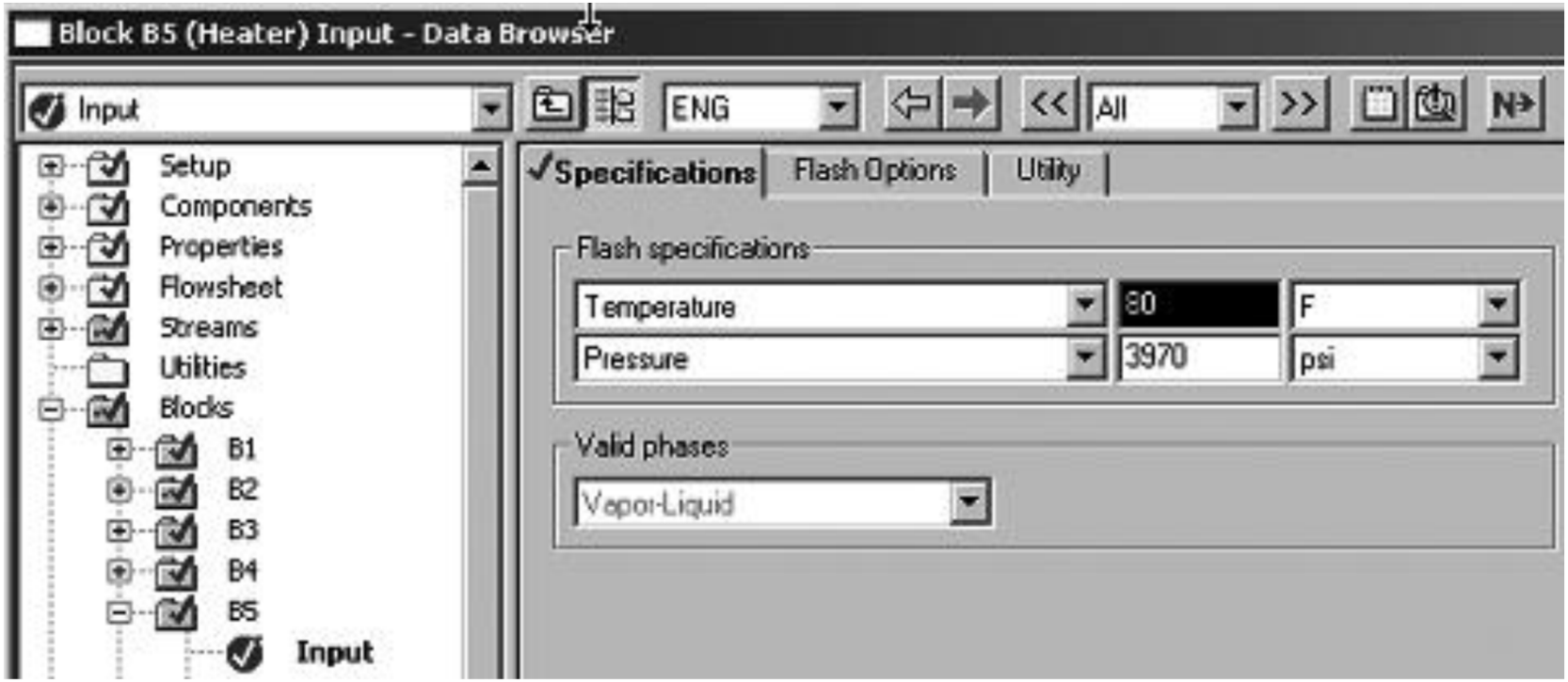


The operating parameters for the heaters

- A ***heater (B3)*** in the ***reactor inlet*** to ***heat*** the reactor feed to ***900 ºF***, and at a pressure of ***4000 psi***.

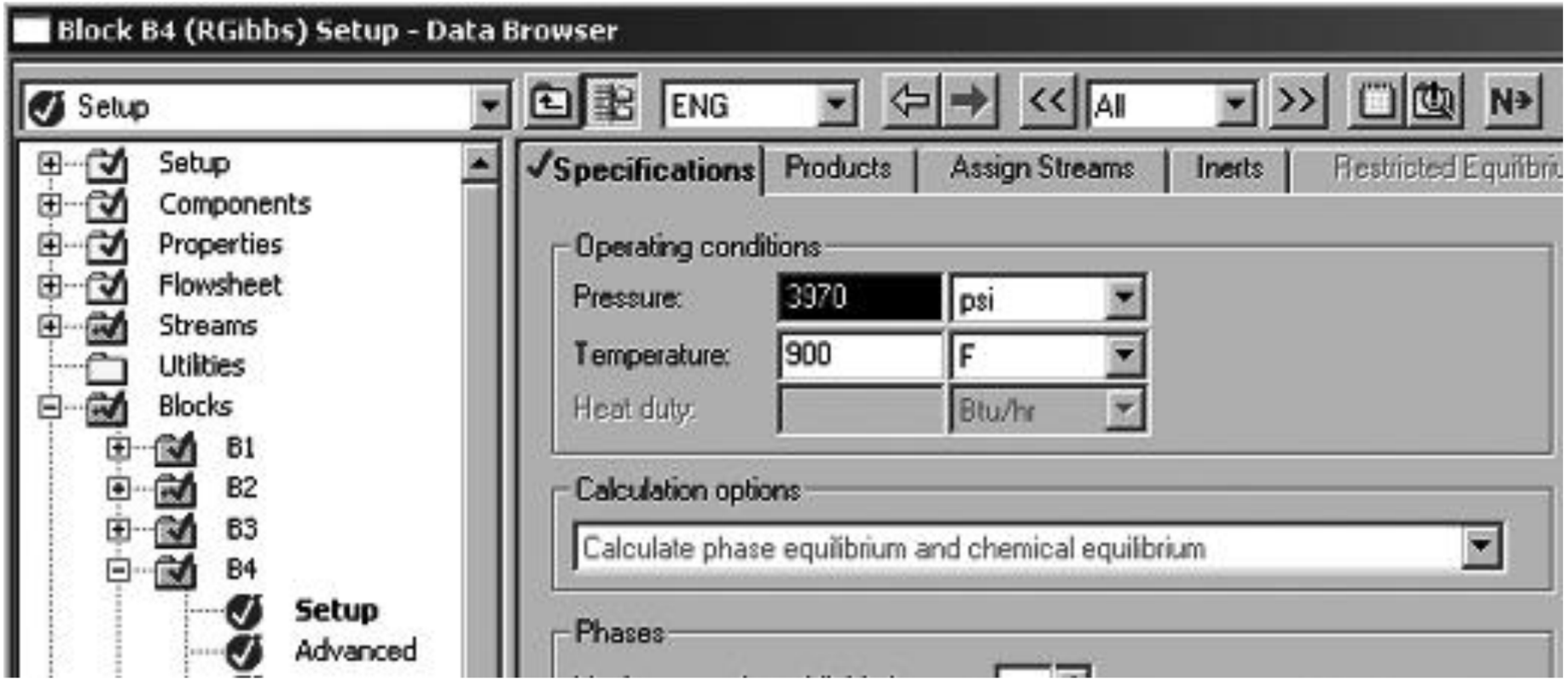


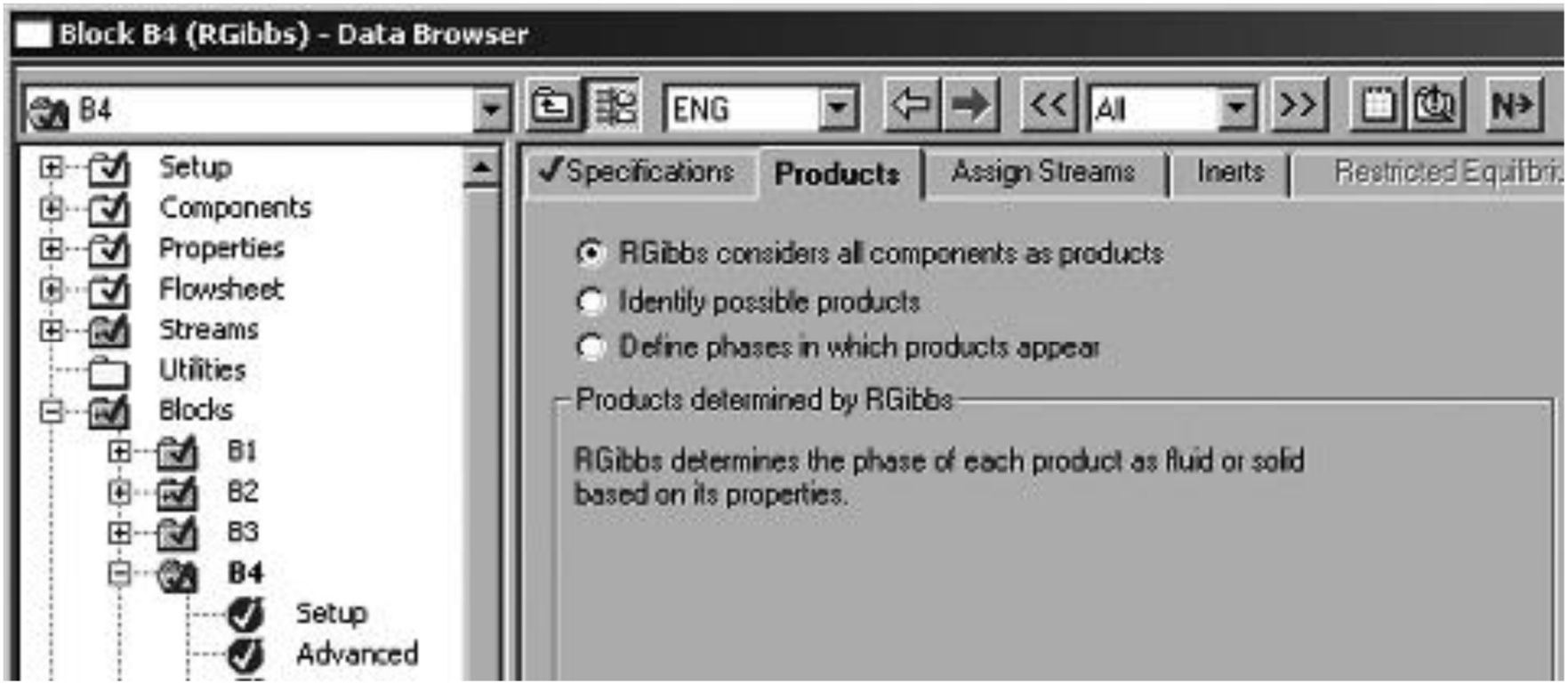
- A ***cooler (B5)*** in the ***reactor outlet*** to ***cool*** the reactor product to ***80 ºF***, and at a pressure of ***3970 psi***.



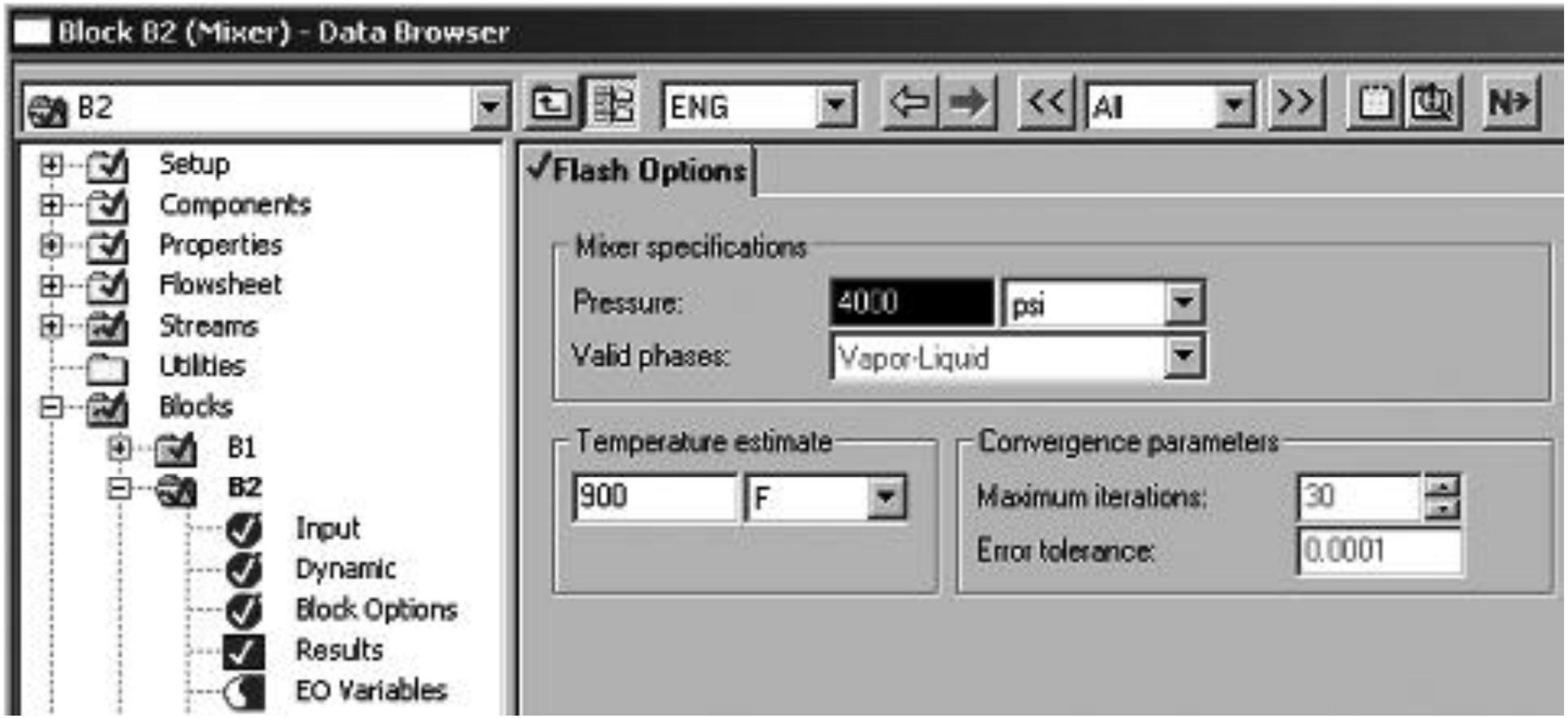
The operating parameters for the reactor

- A ***Gibbs reactor (B4, RGibbs)*** operated at a pressure of ***3970 psi*** and at a temperature of ***900 ^{o}F***.

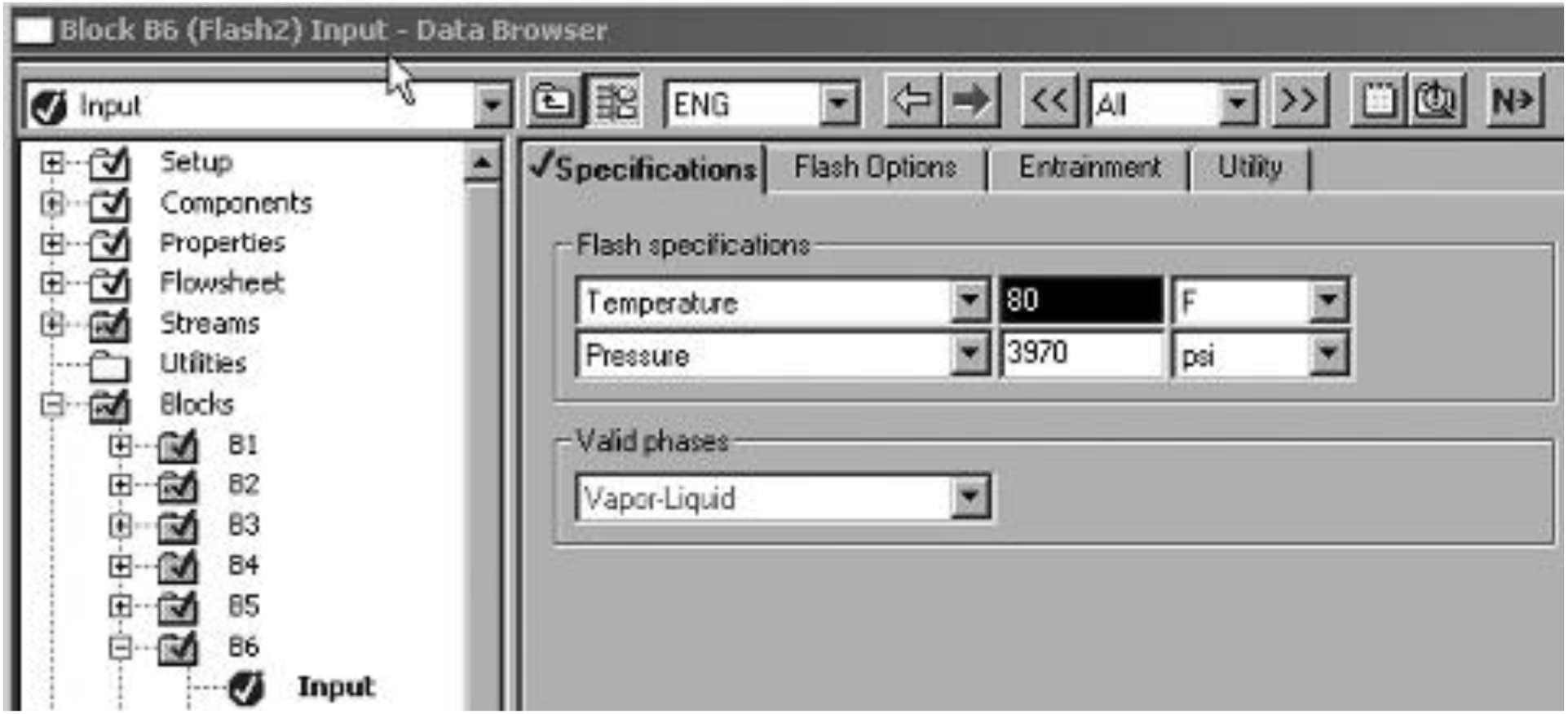



Block B4 (RGibbs) - Data Browser
B4
ENG
All
Setup
Components
Properties
Flowsheet
Streams
Utilities
Blocks
B1
B2
B3
B4
Setup
Advanced
Specifications
Products
Assign Streams
Inerts
Restricted Equilibri
RGibbs considers all components as products
Identify possible products
Define phases in which products appear
Products determined by RGibbs
RGibbs determines the phase of each product as fluid or solid based on its properties.

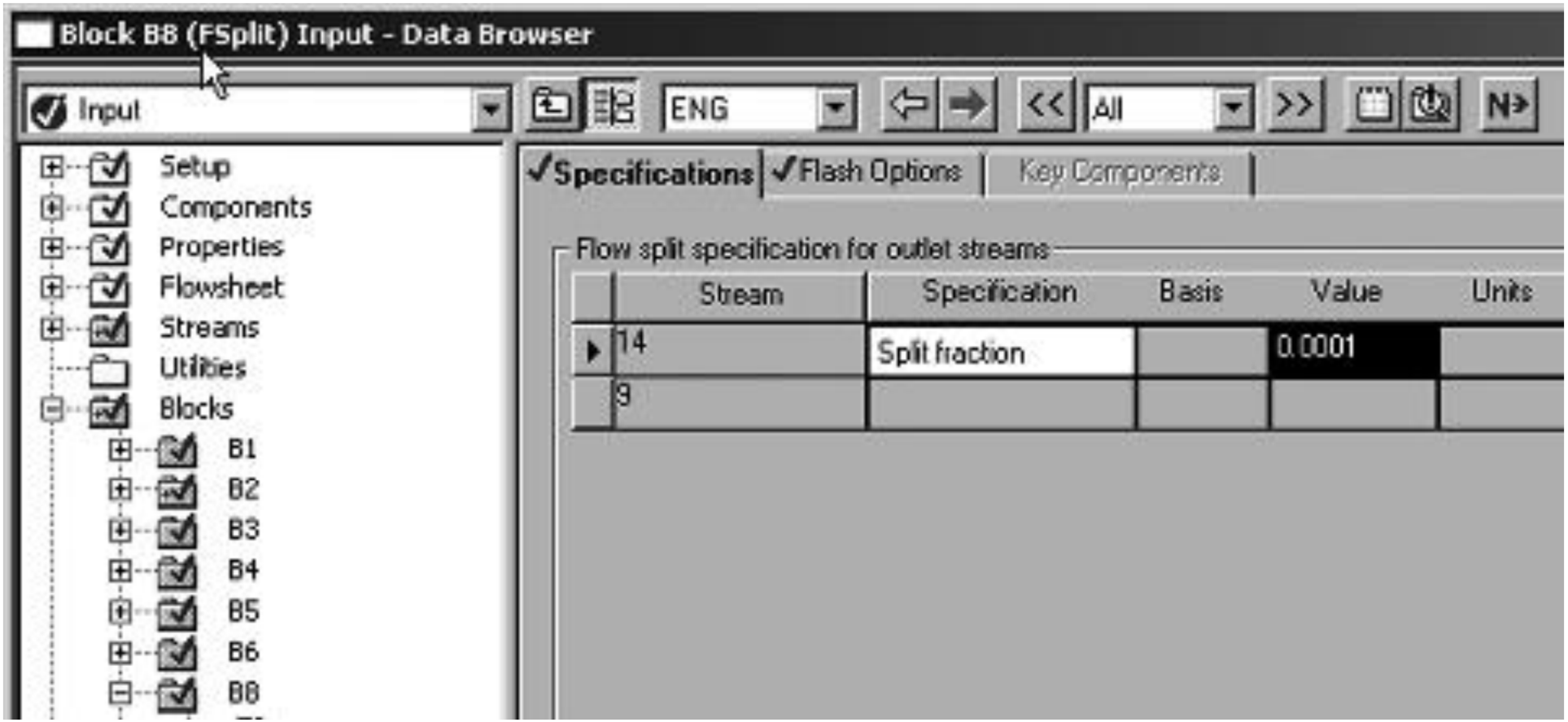
The specifications for the mixer (B2)



- **The specifications for the separator/flash chamber (B6, flash2)**

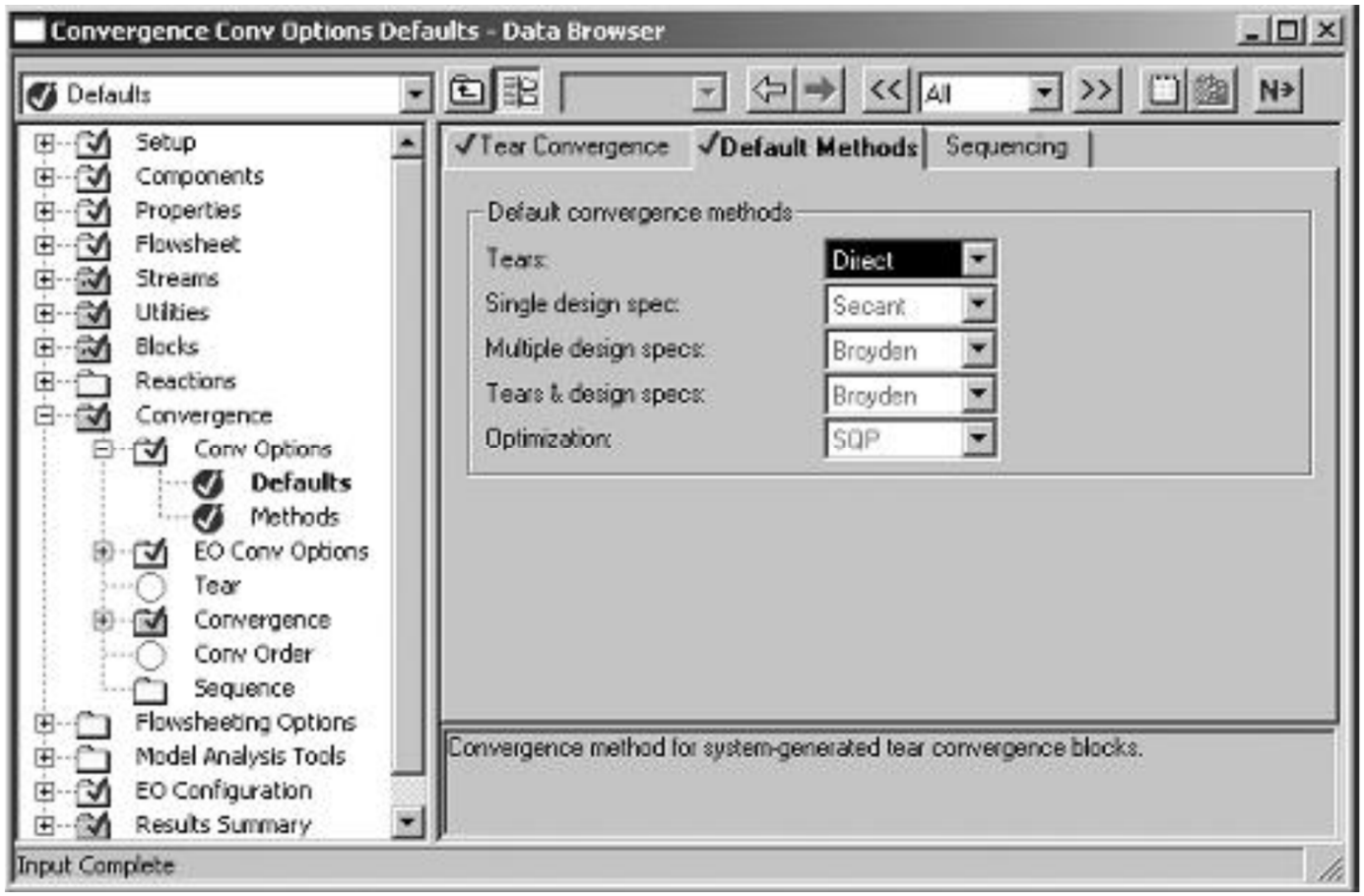


Specifications for the simple splitter (B8, FSplit)



- In Aspen Plus streams and units different operating conditions like, T, P etc can be specified.

Aspen Plus convergence



Sequential module for iteration

- Unit B1 is calculated only once, since the exact input to that unit is known.
- Then units B2–B9 are calculated.
- Since B9 is the last unit, Aspen Plus compares the output from unit B9 on this iteration to the output from unit B9 one iteration before. If they are the same, convergence has been achieved.
- If not, it iterates more.

- This simulation used the ***Wegstein method*** of accelerating convergence.
- The solutions have not fully converged after ***30 iterations***; the ***mass balance error*** is in block B9 (the recycle compressor); discrepancy as 0.5805 vs 0.5801, for a relative difference of 0.07 percent.
- The small difference is acceptable.
- The ***Broyden method*** does not converge much better.
- ***Direct method*** of iteration did converge
- It calculates all the equations simultaneously around the loop over and over again.

Mass balance for ammonia process

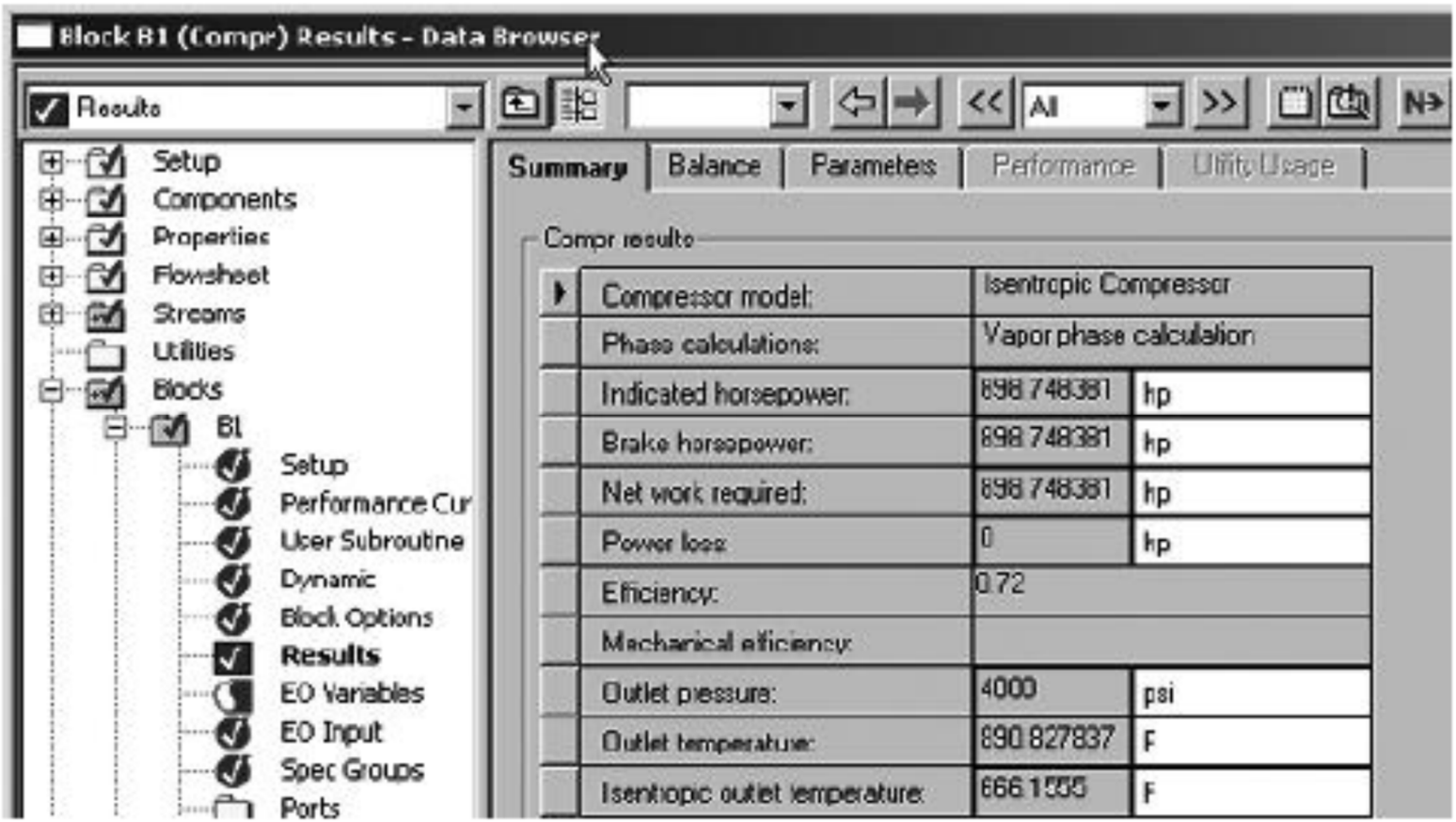
Molar flow, lb mol/h	1	2	3	4	5	6	7	8	9	10	14
N_2	100.00	100.00	135.25	135.25	36.49	1.24	35.25	36.49	35.25	35.25	0.00
H_2	300.00	300.00	1789.98	1789.98	1493.70	3.62	1490.08	1493.70	1489.93	1489.98	0.15
NH_3	0.00	0.00	59.21	59.21	256.73	197.51	59.21	256.73	59.21	59.21	0.01
CO_2	1.00	1.00	2.91	2.91	2.91	1.00	1.91	2.91	1.91	1.91	0.00
Total flow, lb mol/h	401.00	401.00	1987.34	1987.34	1789.83	203.38	1586.45	1789.83	1586.29	1586.34	0.16
Total flow, lb/h	3450.12	3450.12	8533.52	8533.52	8533.52	3449.73	5083.80	8533.52	5083.29	5083.40	0.51
Total flow, cubic ft/h	7741.20	1452.90	3761.47	7249.42	6578.25	95.66	2314.31	2409.97	2314.08	2303.65	0.23

- Discrepancy between ***streams 9 and 10***; hydrogen flow rate is ***off by 0.05 lb mol/h***, compared with a total flow of 1490 lb mol/h.
- Conversion is $\frac{(135.25-36.49)100}{135.25}$ = ***73%***of N_2 which is a ***limiting reactant***.
- Most of the carbon dioxide ***1 lb mol/h*** goes out in the product ammonia stream and remaining ***1.91 lb mol/h*** in the recycle stream; the purge stream was no carbon dioxide so it is not necessary.

Energy balance for ammonia process

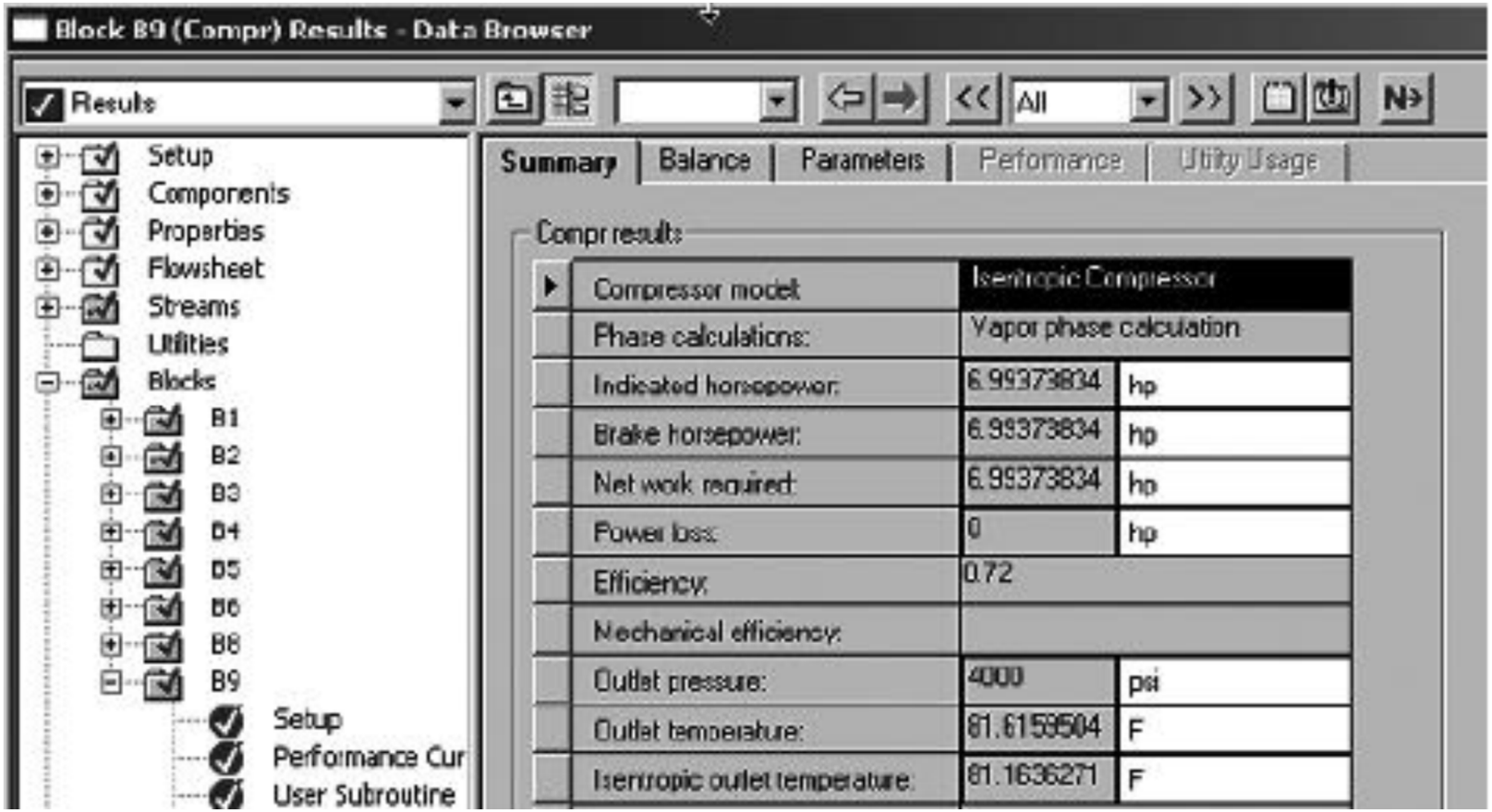
Temperature, °F	80.00	890.83	245.82	900.00	900.00	80.00	80.00	80.00	80.00	81.62	80.00
Pressure, psi	300	4000	4000	4000	3970	3970	3970	3970	3970	4000	3970
Vapor fraction	1	1	1	1	1	0	1	0.8864	1	1	1
Liquid fraction	0	0	0	0	0	1	0	0.1136	0	0	0
Solid fraction	0	0	0	0	0	0	0	0	0	0	0
Enthalpy, Btu/lb mol	−401.19	5301.56	344.96	5009.06	3038.18	−28222.34	−919.19	−4021.60	−919.19	−907.98	−919.19
Enthalpy, Btu/lb	−46.63	616.19	80.34	1166.54	637.23	−1663.82	−286.84	−843.49	−286.84	−283.35	−286.84
Enthalpy, Btu/h	−160878	2125927	685562	9954720	5437816	−5739722	−1458248	−7197970	−1458102	−1440365	−146
Entropy, Btu/lb mol-R	−4.8010	−3.5080	−9.1477	−4.4755	−6.5801	−42.8532	−11.4165	−14.9886	−11.4165	−11.4105	−11.4165
Entropy, Btu/lb-R	−0.5580	−0.4077	−2.1304	−1.0423	−1.3801	−2.5264	−3.5626	−3.1437	−3.5626	−3.5608	−3.5626
Density, lb mol/cubic ft	0.0518	0.2760	0.5283	0.2741	0.2721	2.1261	0.6855	0.7427	0.6855	0.6886	0.6855
Density, lb/cubic ft	0.4457	2.3746	2.2687	1.1771	1.2972	36.0634	2.1967	3.5409	2.1967	2.2067	2.1967
Average MW	8.6038	8.6038	4.2939	4.2939	4.7678	16.9624	3.2045	4.7678	3.2045	3.2045	3.2045
Liquid volume 60°F, cubic ft/h	344.02	344.02	1704.97	1704.97	1535.52	174.48	1361.04	1535.52	1360.90	1360.95	0.14

Feed compressor variables, unit B1.

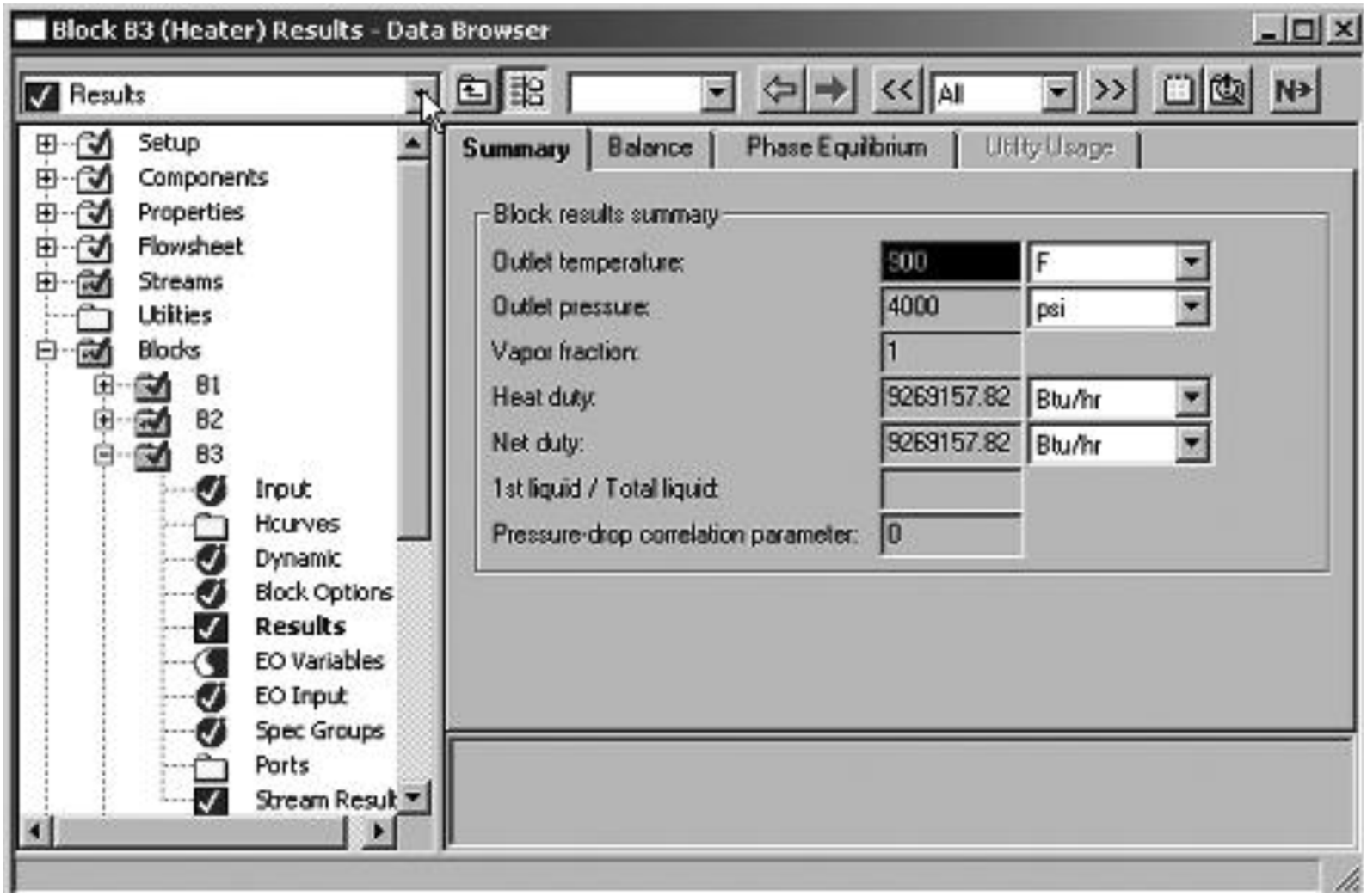


- The compressor is very large ~ 900 HP with compression ratio 4000/300=13.3.
- Instead, two stage compressors each of compression ratio $\sqrt{13.3}$ = 3.65 can be used to maximize work efficiency.
- From the thermodynamics point of view, optimal configuration has equal compression ratios with inter-stage cooling back to the inlet temperature.

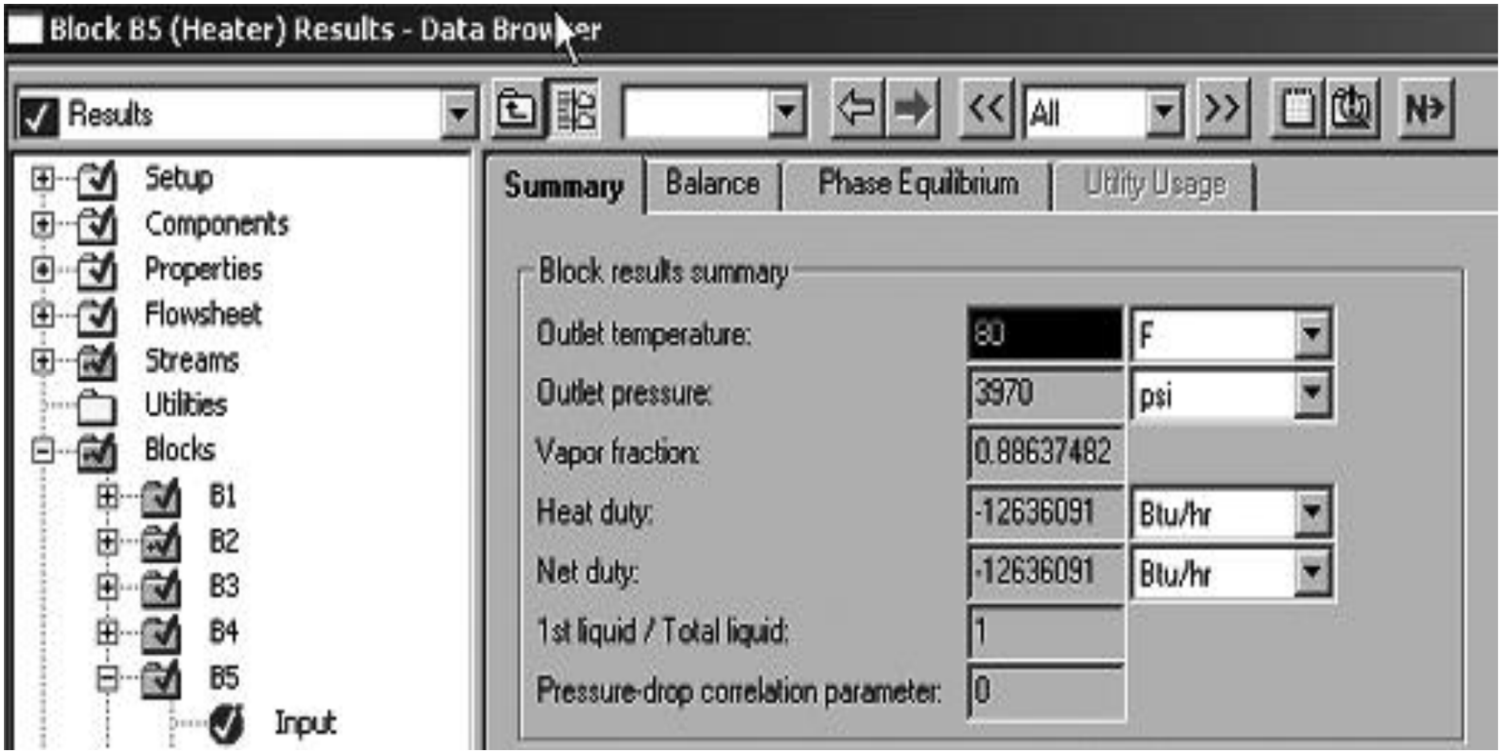
Recycle compressor variables, unit B9.



Heat exchanger (upstream to the reactor) variables, unit B3.



Heat exchanger (downstream to the reactor)variables, unit B5.



- From given heat duty capital cost can be estimated.
- Enthalpies of the process streams from energy balance table can be integrated over the process combined with the heat duty that verifies the overall energy balance.

Mass balance for ammonia process (repeated figure)

Molar flow, lb mol/h	1	2	3	4	5	6	7	8	9	10	14
N_2	100.00	100.00	135.25	135.25	36.49	1.24	35.25	36.49	35.25	35.25	0.00
H_2	300.00	300.00	1789.98	1789.98	1493.70	3.62	1490.08	1493.70	1489.93	1489.98	0.15
NH_3	0.00	0.00	59.21	59.21	256.73	197.51	59.21	256.73	59.21	59.21	0.01
CO_2	1.00	1.00	2.91	2.91	2.91	1.00	1.91	2.91	1.91	1.91	0.00
Total flow, lb mol/h	401.00	401.00	1987.34	1987.34	1789.83	203.38	1586.45	1789.83	1586.29	1586.34	0.16
Total flow, lb/h	3450.12	3450.12	8533.52	8533.52	8533.52	3449.73	5083.80	8533.52	5083.29	5083.40	0.51
Total flow, cubic ft/h	7741.20	1452.90	3761.47	7249.42	6578.25	95.66	2314.31	2409.97	2314.08	2303.65	0.23

- ***Equilibrium*** persists in the ***reactor effluent***.
- From the thermodynamic of ***chemical equilibria, K-values*** can be calculated from the mole fraction of the ***scream 5***.
- y_{N_2} = 0.0204; y_{H_2} = 0.8346; y_{NH_3} = 0.1434; $\boldsymbol{K = 0.00488}$
- It is close to the value of ***0.00473*** measured by ***Stephenson (1966).***
- The reactor utilizes the ***NRTL thermodynamic model*** for ***chemical reaction equilibrium***.

Testing vapor-liquid equilibria in streams 6 and 7

- ***Solubility*** of ***nitrogen*** is ***27.6 cm^3/g ammonia*** when the pressure is 270 atm(~4000 psia) and at 25^oC (~80 ^oF). It corresponds ***0.021 mole fraction*** of ***nitrogen*** in the liquid phase that is interpolated from values measured by Stephen and Stephen.
- Using the values for ***stream 6*** from the mass balance table gives a mole fraction of ***0.0061*** that is smaller than literature but there is carbon dioxide (ternary equilibrium) in the stream 6.