Aspen Plus®

STEADY STATE SIMULATION

Version 10

Modeling Processes with Electrolytes

GETTING STARTED

AspenTech®

The flowsheet graphics and plot components of Aspen Plus were developed by MY-Tech, Inc.

Use of Aspen Plus and This Manual

This manual is intended as a guide to using Aspen Plus process modeling software. This documentation contains AspenTech proprietary and confidential information and may not be disclosed, used, or copied without the prior consent of AspenTech or as set forth in the applicable license agreement. Users are solely responsible for the proper use of Aspen Plus and the application of the results obtained.

Although AspenTech has tested the software and reviewed the documentation, the sole warranty for Aspen Plus may be found in the applicable license agreement between AspenTech and the user. **ASPENTECH MAKES NO WARRANTY OR REPRESENTATION, EITHER EXPRESS OR IMPLIED, WITH RESPECT TO THIS DOCUMENTATION, ITS QUALITY, PERFORMANCE, MERCHANTABILITY, OR FITNESS FOR A PARTICULAR PURPOSE.**

Contents

About *Getting Started Modeling Processes with Electrolytes*

You can easily model all types of electrolyte systems with Aspen Plus, including systems with strong electrolytes, weak electrolytes, salt precipitation, even mixed solvents.

The two sessions in this book – Modeling Electrolyte Chemistry and Modeling a Sour Water Stripper– introduce you to simulating electrolyte systems with Aspen Plus by guiding you through two simulations.

Getting Started Modeling Processes with Electrolytes assumes that you have an installed copy of the Aspen Plus and User Interface software.

Why Use Electrolyte Simulation?

A rigorous treatment of electrolytes is needed to model many industrial systems. With the Aspen Plus electrolyte capabilities, you can model:

Sour water solutions. Water containing dissolved H_2S, NH_3, CO_2, HCN, sometimes with additional solvents

Aqueous amines for gas sweetening. Water containing DGA, MEA, DEA, or MDEA for the removal of H_2S and CO_2

Aqueous acids or bases. HCl, HBr, H_2SO_4, H_3PO_4, HNO_3, HF, NaOH, KOH, and others, in aqueous solution, sometimes with additional solvents

Salt solutions. NaCL, KCl, Na_2SO_4, $CaSO_4$, $CaCO_3$ in solution, sometimes with participation

What is an Aspen Plus Electrolyte Model?

In Aspen Plus, an electrolyte system is defined as one in which some of the molecular species dissociate partially or completely into ions in a liquid solvent, and/or some of the molecular species precipitate as salts. These dissociation and precipitation reactions occur fast enough that the reactions can be considered to be at chemical equilibrium. The liquid phase equilibrium reactions that describe this behavior are referred to as the solution chemistry. In Aspen Plus, solution chemistry is often referred to simply as Chemistry.

Solution chemistry has a major impact on the simulation of electrolyte systems. For nonelectrolyte systems, chemical reactions generally occur only in reactors. In Aspen Plus, all unit operation models can handle electrolyte reactions.

Solution chemistry also impacts physical property calculations and phase equilibrium calculations. The presence of ions in the liquid phase causes highly nonideal thermodynamic behavior. Aspen Plus provides specialized thermodynamic models and built-in data to represent the nonideal behavior of liquid phase components in order to get accurate results.

Sessions in this Book

The two sessions in the book illustrate the following concepts:

- Types of electrolyte components
  - Solvents
  - Solutes
  - Ions
  - Salts
- Types of reactions in electrolyte solution chemistry
  - Complete dissociation
  - Partial dissociation (equilibrium reaction)
  - Salt precipitation (equilibrium reaction)
- Automatic Chemistry generation
- Recommended physical property methods for electrolytes
- Methods for calculating and reporting electrolyte systems
  - True component approach
  - Apparent component approach
- Use of stream properties (Property Sets) for electrolytes

Follow the steps in Chapter	To learn how to
1 Modeling Electrolyte Chemistry	Define electrolyte components. Use automatic chemistry generation. Examine Chemistry data. View electrolyte databank parameters. Use the true component modeling approach.
2 Modeling a Sour Water Stripper	Modify the generated Chemistry. Use the apparent component approach for electrolytes. Convert from apparent component approach to true component approach.

Using Backup Files

We recommend that you perform all sessions sequentially, because Chapter 2 assumes you are familiar with the concepts presented in Chapter 1.

Aspen Plus provides backup files containing all problem specifications and results for each tutorial session. You can use the backup files to check your results.

For More Information

Online Help Aspen Plus has a complete system of online help and context-sensitive prompts. The help system contains both context-sensitive help and reference information. For more information about using Aspen Plus help, see the *Aspen Plus User Guide*, Chapter 3.

Aspen Plus Getting Started Building and Running a Process Model This tutorial includes several hands-on sessions to familiarize you with Aspen Plus. The guide takes you step-by-step to learn the full power and scope of Aspen Plus.

Aspen Plus Getting Started Modeling Processes with Electrolytes This tutorial includes several hands-on sessions to familiarize you with simulating electrolyte systems with Aspen Plus.

Aspen Plus Getting Started Modeling Petroleum Processes This tutorial includes several hands-on sessions to familiarize you with simulating petroleum processes with Aspen Plus.

Aspen Plus Getting Started Customizing Unit Operation Models This tutorial includes several hands-on sessions to familiarize you with the customization of unit operation models with Aspen Plus.

Aspen Plus User Guide The three-volume *Aspen Plus User Guide* provides step-by-step procedures for developing and using an Aspen Plus process simulation model. The guide is task-oriented to help you accomplish the engineering work you need to do, using the powerful capabilities of Aspen Plus.

Aspen Plus reference manual series Aspen Plus reference manuals provide detailed technical reference information. These manuals include background information about the unit operation models and the physical properties methods and models available in Aspen Plus, tables of Aspen Plus databank parameters, group contribution method functional groups, and a wide range of other reference information. The set comprises:

- *Unit Operation Models*
- *Physical Property Methods and Models*
- *Physical Property Data*
- *User Models*
- *System Management*
- *System Administration*
- *Summary File Toolkit*

Aspen Plus application examples A suite of sample online Aspen Plus simulations illustrating specific processes is delivered with Aspen Plus.

Aspen Plus Installation Guides These guides provide instructions on platform and network installation of Aspen Plus. The set comprises:

- *Aspen Plus Installation Guide* for Windows
- *Aspen Plus Installation Guide* for OpenVMS
- *Aspen Plus Installation Guide* for UNIX

The Aspen Plus manuals are delivered in Adobe portable document format (PDF) on the Aspen Plus Documentation CD.

Technical Support

World Wide Web For additional information about AspenTech products and services, check the AspenTech World Wide Web home page on the Internet at:

http://www.aspentech.com/

Technical resources To obtain in-depth technical support information on the Internet, visit the Technical Support homepage. Register at:

http://www.aspentech.com/ts/

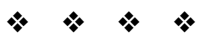
Approximately three days after registering, you will receive a confirmation e-mail and you will then be able to access this information.

The most current Hotline contact information is listed. Other information includes:

- Frequently asked questions
- Product training courses
- Technical tips

AspenTech Hotline If you need help from an AspenTech Customer Support engineer, contact our Hotline for any of the following locations:

If you are located in:	Phone Number	Fax Number	E-Mail Address
North America & the Caribbean	+1-617/949-1021 +1-888/996-7001 (toll free)	+1-617/949-1724	support@aspentech.com
South America			
(Argentina office)	+54-11/4393 5308	+54-11/4394-8621	tecnoba@aspentech.com
(Brazil office)	+55-11/5506-0756	+55-11/5506-0567	tecnosp@aspentech.com
Europe, Gulf Region, & Africa			atesupport@aspentech.com
(Brussels office)	+32-2/724-0100	+32-2/705-4034	
(UK office)	+44-1223/312220	+44-1223/366980	
Japan	+81-3/3262-1743	+81-3/3262-1744	atjsupport@aspentech.com
Asia & Australia			atasupport@aspentech.com
(Hong Kong office)	+85-2/2838-6077	+85-2/2833-5642	
(Korea office)	+82-2/761-5800	+82-2/761-5803	



1 Modeling Electrolyte Chemistry

In this session you will mix and flash two feed streams containing aqueous electrolytes.

You will:

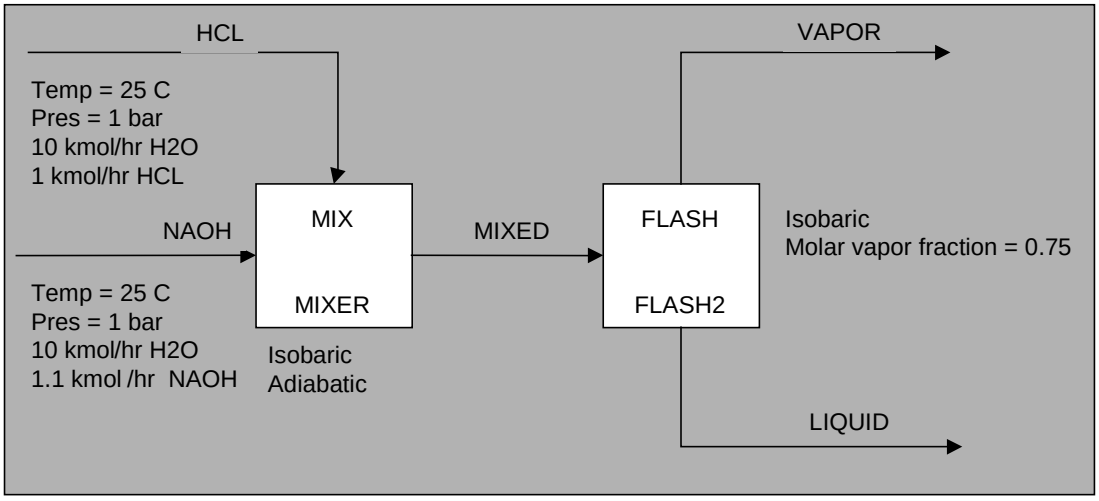
- Define electrolyte components
- Use the Electrolytes Expert System
- Examine Chemistry data
- View electrolytes databank parameters
- Use the true components modeling approach

Allow about 45 minutes to do this session.

Electrolyte Chemistry Flowsheet

The process flow diagram and operating conditions for this session are shown in the process diagram below: Electrolyte Chemistry. Two feed streams, one containing water and HCl, the other water and NaOH, are fed to a mixer. The mixer outlet is flashed to evaporate water and cause NaCl to precipitate. You will use the MIXER model for the mixer and the FLASH2 model for the flash.

Electrolyte Chemistry



Starting Aspen Plus

To start Aspen Plus:

➤ From your desktop, click Start and then select Programs.

➤ Select AspenTech, then Aspen Plus 10.1-0, then Aspen Plus User Interface.

The Aspen Plus Startup dialog box appears. Aspen Plus displays a dialog box whenever you must enter information or make a selection before proceeding. In this simulation, you will use an Aspen Plus template.

➤ To select the Template option, point the mouse to the Template radio button and click the left mouse button.

➤ Click OK to apply this option.

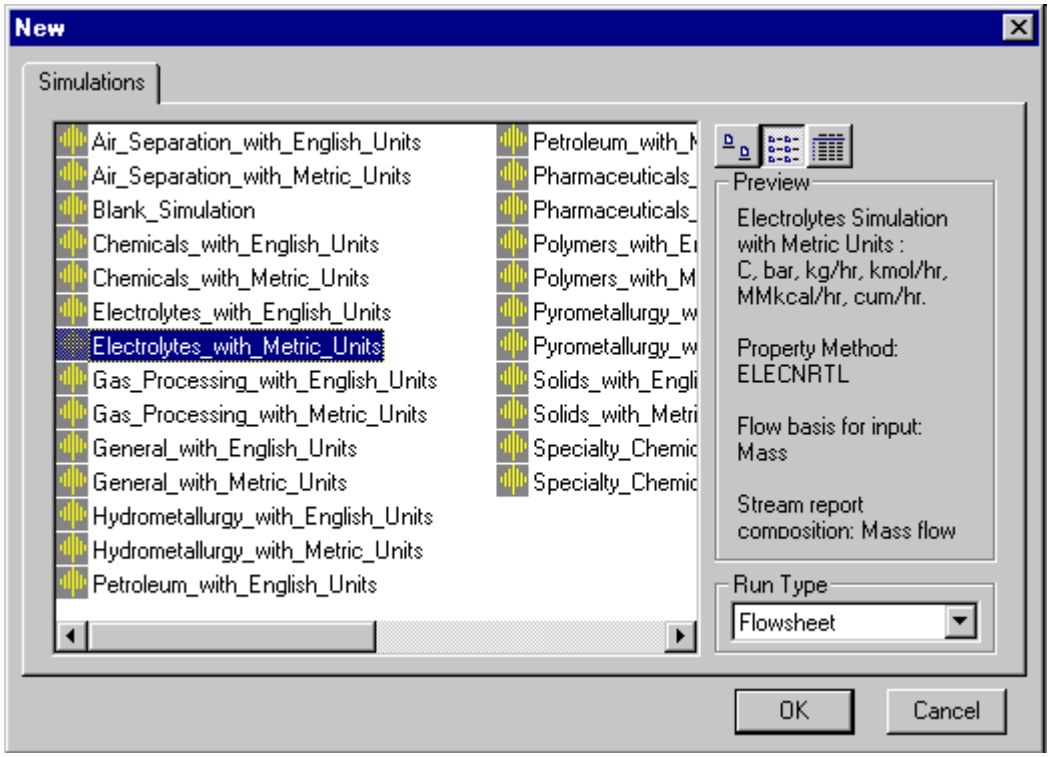
The New dialog box appears.

You use the New dialog box to specify the Application Type and the Run Type for the new run. Aspen Plus uses the Application Type you choose to automatically set various defaults appropriate to your application.

To specify the Application Type and Run Type for the new run:

➤ Select the Electrolytes with Metric Units template.

➤ The default Run Type, Flowsheet, is appropriate for this session. Click OK to apply these options.



It will take a few seconds for Aspen Plus to apply these options.

Note If the Connect Host dialog box appears, see Appendix A.

The Aspen Plus Main window is now active.

Drawing the Graphical Simulation Flowsheet

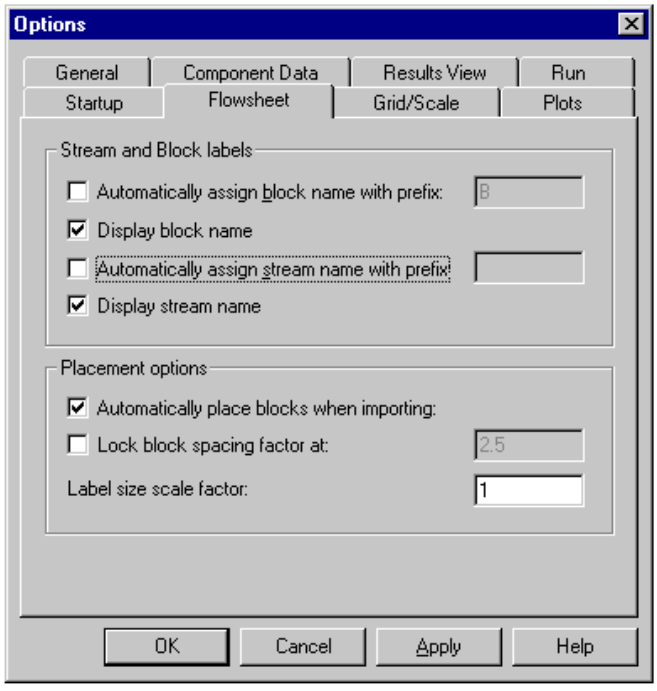
In this session you will begin to build the process flowsheet. Since you will enter your own block and stream IDs, you must turn off the default Create auto block ID and Create auto stream ID options, which provide these IDs automatically.

➤ From the Aspen Plus Tools menu, select Options.

The Options dialog box appears.

➤ Select the Flowsheet tab.

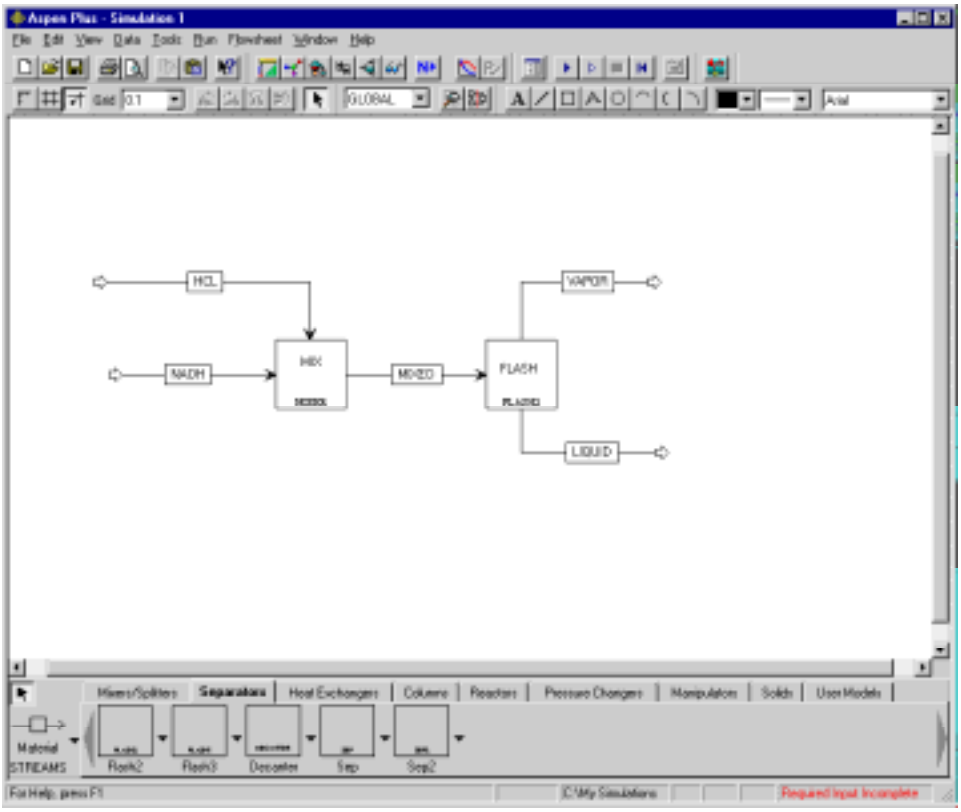
➤ Deselect the Automatically Assign Block Name with Prefix and the Automatically Assign Stream Name with Prefix options.



➤ Click OK to close the Options dialog box and apply the changes.

The process flow diagram and problem definition for this session are shown in the process diagram: Electrolyte Chemistry on page 1-2.

➤ Place the flowsheet blocks and streams to create the graphical simulation flowsheet shown below.



➤ Use Next (click the Next button  on the main window toolbar) to guide you to the next required input.

The Flowsheet Connectivity dialog box appears.

➤ Click OK, to continue.

Specifying Title, Stream Properties, and Global Options

The Data Browser window appears. The Setup Specifications Global sheet displays defaults Aspen Plus uses for other forms. You will use this form to give your simulation a title, and to review the stream properties and global options that were set when you selected the Electrolytes with Metric Units Application Type.

The Run Type box displays Flowsheet, which is appropriate for this session.

It is always good practice to describe your problem by entering a title for the simulation.

➤ Enter the title **Getting Started with Electrolytes – Session 1** in the Title box.

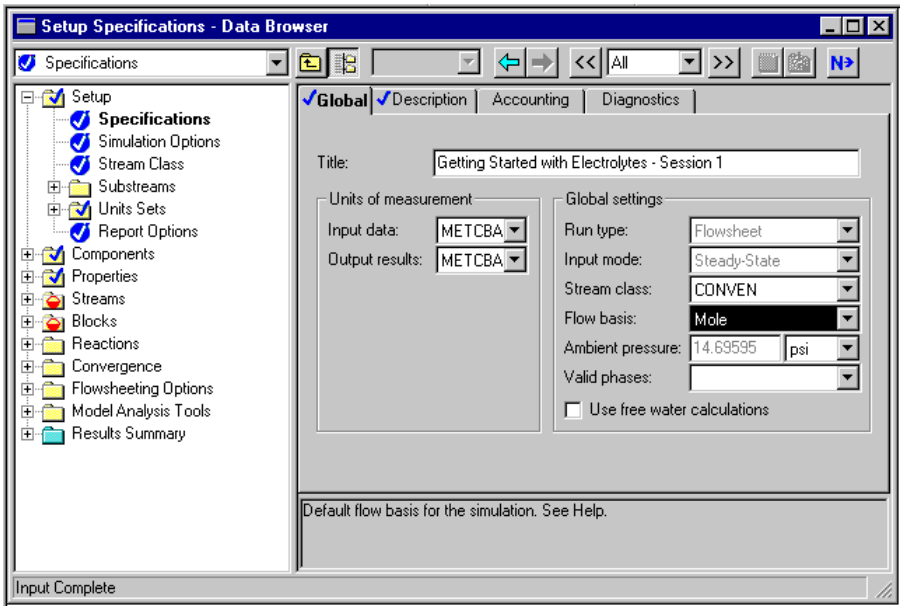
The Electrolytes with Metric Units Application Type sets the following global defaults for electrolytes applications:

- METCBAR units (Metric units with temperature in degrees Centigrade and pressure in bars)
- Mass Flow Basis for all flow inputs

To specify flows on a mole basis for this session:

➤ Move to the Flow basis box and click the Down arrow to display the available list for the simulation.

➤ Select Mole.



Since you chose the Electrolytes with Metric Units Application Type when you started this session, Aspen Plus has set the following defaults for calculating and reporting stream properties:

- Flow and Fraction Basis of Mass: Aspen Plus will report the component flow rates on a mass flow basis
- ELEC_E Stream Format: Aspen Plus formats the Stream Summary form for electrolytes.

To review the report options specified in the selected Template:

➤ In the menu tree of the Data Browser window, click the Report Options form in the Setup folder.

➤ Click on the Stream tab to view the Stream sheet.

You will return to this form and specify stream properties later in this session.

To move to the next required input:

➤ Click Components on the Data Browser menu tree, then Specifications.

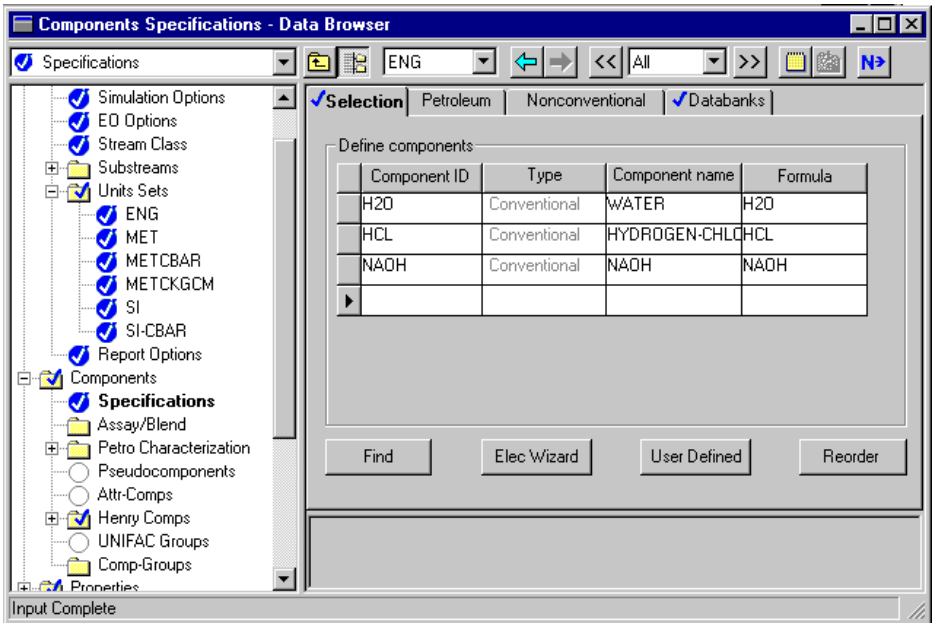
Specifying Components

The Components Specifications Selection sheet appears.

The apparent (or base) components for this session are H_2O, HCl, and NaOH.

Because you chose an electrolytes Application Type, water already appears on the form.

➤ Enter the remaining components as shown below:



➤ You can rename H20 to Water, by selecting H20 in the Component ID box, and typing Water. When the Aspen Plus dialog box appears, click the Rename button.

➤ Click the Elec Wizard button.

The Electrolytes Wizard dialog box, for defining automatic chemistry generation, appears.

The Electrolytes Wizard

You use the Electrolytes Wizard to define the ionic species and salts that can be generated from the base components entered on the Components Specifications Selection sheet, and to generate the reactions that occur among these components in the liquid phase.

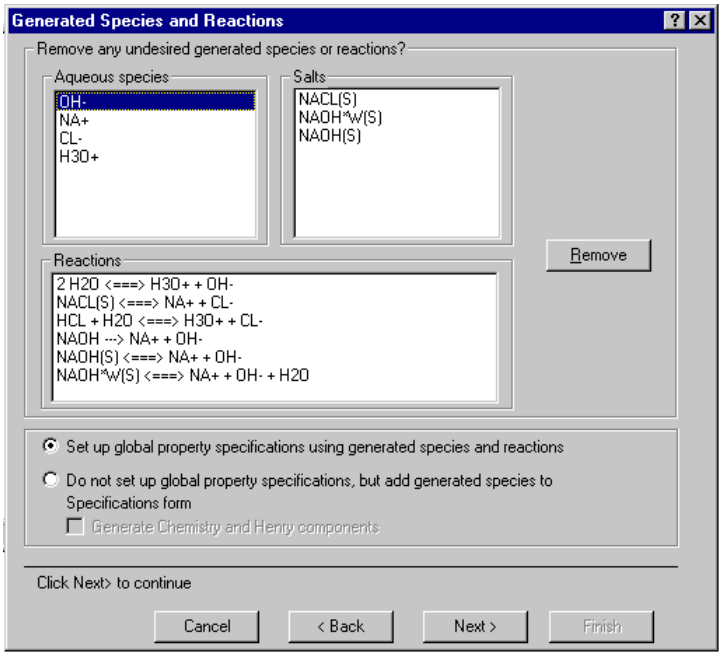
➤ Click the Next > button on the Electrolytes Wizard dialog box.

The Base Components and Reactions Generation Option dialog box appears. In this dialog box, there is an option (turned off) labeled Hydrogen Ion type Hydronium ion H+. Aspen Plus can treat acidic species as either H+ or H3O+. However, use of H3O+ is strongly recommended, because the presence of H3O+ in the solution chemistry is better able to represent the phase and chemical equilibrium of almost all electrolyte systems.

➤ Move all components to the Selected components area using Move All button >>.

➤ Click the Next > button to continue.

The Generated Species and Reactions dialog box appears:



Aspen Plus generates all possible ionic and salt species, and reactions for the H2O-NAOH-HCL system.

In the Reactions section in the Generated Species and Reactions dialog box, different style arrows denote the type of reaction:

<<===>> Denotes ionic equilibrium or salt precipitation

--->> Denotes complete dissociation

In this example, three types of reactions are generated: ionic equilibrium, complete dissociation, and salt precipitation.

The dissociation of water and the dissociation of HCL are equilibrium reactions. NACL precipitation/dissolution is also an equilibrium reaction. In contrast, NAOH dissociates completely and irreversibly into NA^+ and OH^-.

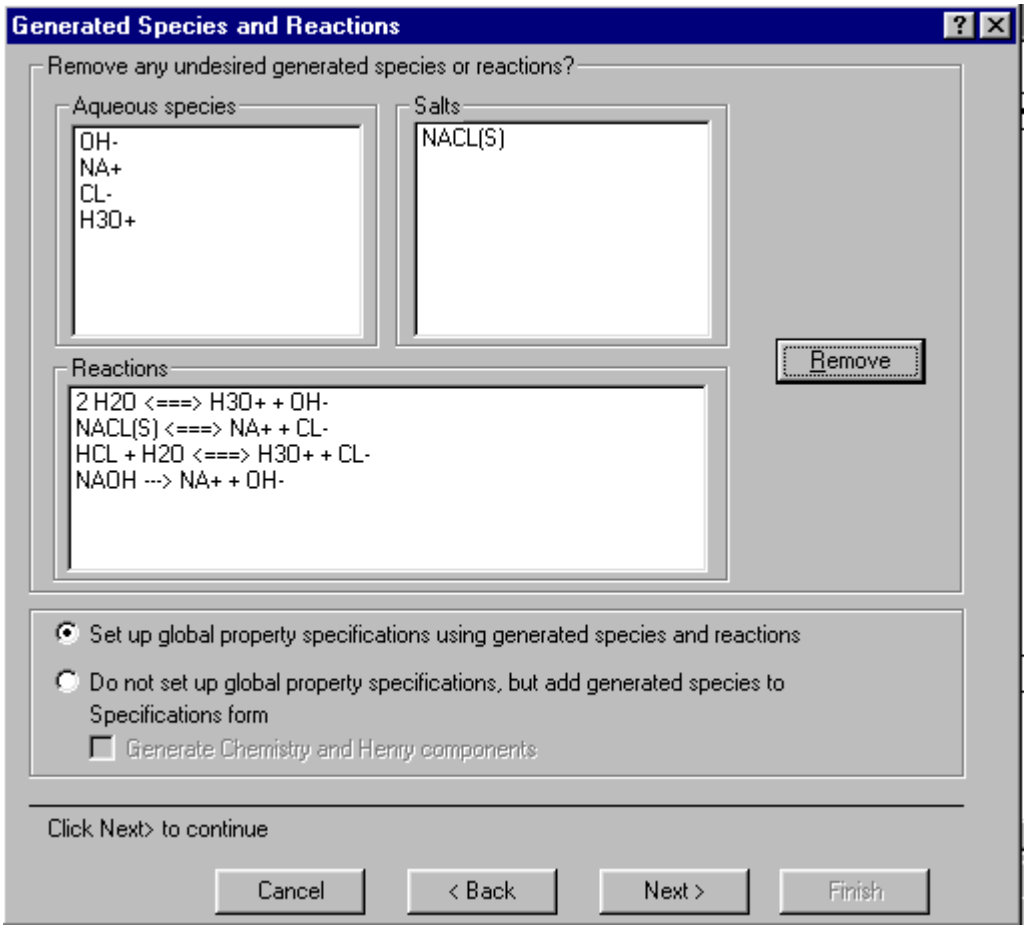
You can use the Remove button to eliminate any of the generated species and reactions. In this session, the NaOH and the NaOH*W salts are not relevant

To remove these salts from the solution chemistry:

➤ Select NaOH(S) and NaOH*W(S) from the Salts list.

➤ Click the Remove button to the right of the Generated Reactions list.

Now that you have removed these salts from the Generated Aqueous Species list, Aspen Plus automatically removes all reactions involving NaOH(S) and NaOH*W(S) from the Reactions list.



Note Any time you know that a reaction can be neglected because of expected process conditions, you should remove it from the solution chemistry, to decrease the execution time required for your simulation.

➤ Click Next > on the Generated Species and Reactions dialog box to accept the generated species and reactions. The Simulation Approach dialog box appears, allowing you to choose between the true component approach and the apparent component approach. For this problem, you use the true component approach.

When you use the true component approach, Aspen Plus solves the equations describing solution chemistry simultaneously with the unit operation equations. The unit operations deal directly with the ions and salts formed by solution chemistry. In addition, the true component approach defines how Aspen Plus reports the simulation results. Results are reported in terms of the ions, salts, and molecular components that are actually present, not in terms of the original base components.

For example, the generated chemistry for this system specifies that NAOH fully dissociates into NA^+ and OH^-. If you choose the true component approach, Aspen Plus will report NAOH flow in terms of NA^+ flow and OH^- flow, not in terms of the NAOH base component flow. You can request that composition and flows also be reported in terms of the apparent (base) components. You will do this later in this session.

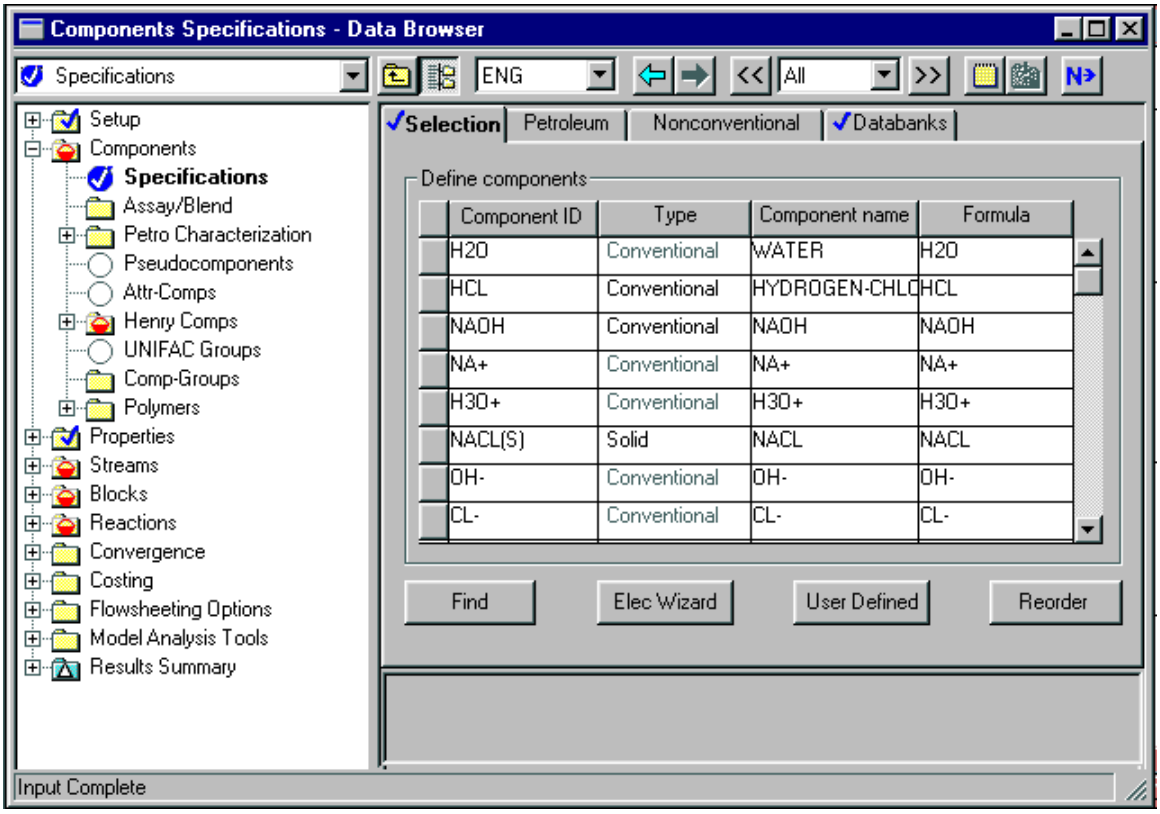
➤ Select True component approach.

➤ Click Next > to move to the next dialog box.

The Summary dialog box appears, telling you what the Aspen Plus electrolytes expert system has done.

➤ Click Finish to close the dialog box.

On the Components Specifications Selection sheet, Aspen Plus has now added the generated electrolyte components. Since all components are databank components, Aspen Plus will automatically retrieve all relevant physical property parameters. Note that the salt NACL(S) is identified as type SOLID.



➤ Click the Next button  on the Data Browser window toolbar to continue.

The Components Henry Comps Global sheet appears, which was defined by the Electrolytes Wizard. The Next function takes you to this form so you can see which components have been declared as Henry's Law components by the Electrolytes Wizard. If you had additional Henry's Law components in your simulation (such as nitrogen and oxygen), you would add them to the list on this form.

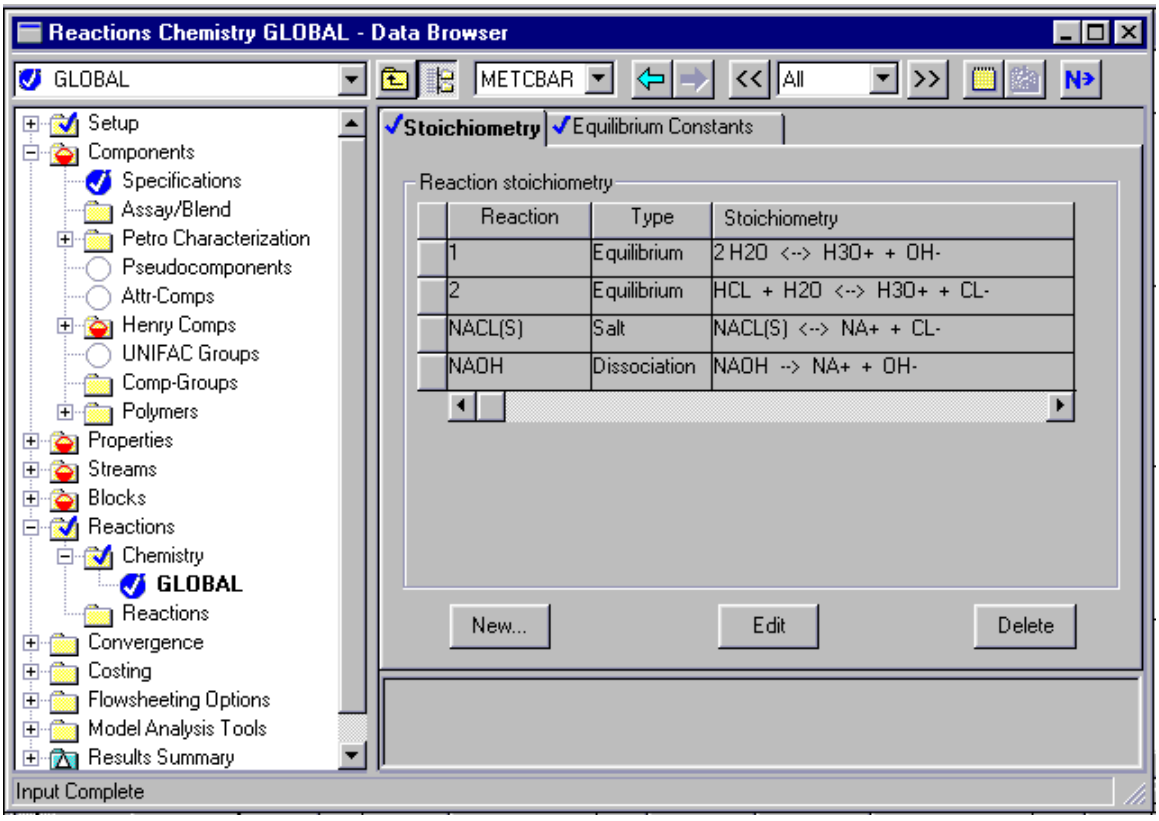
Examining Generated Chemistry

In the previous step, the Aspen Plus Electrolyte Expert System automatically generated the chemistry definition for your problem and named it GLOBAL.

To examine the generated Chemistry:

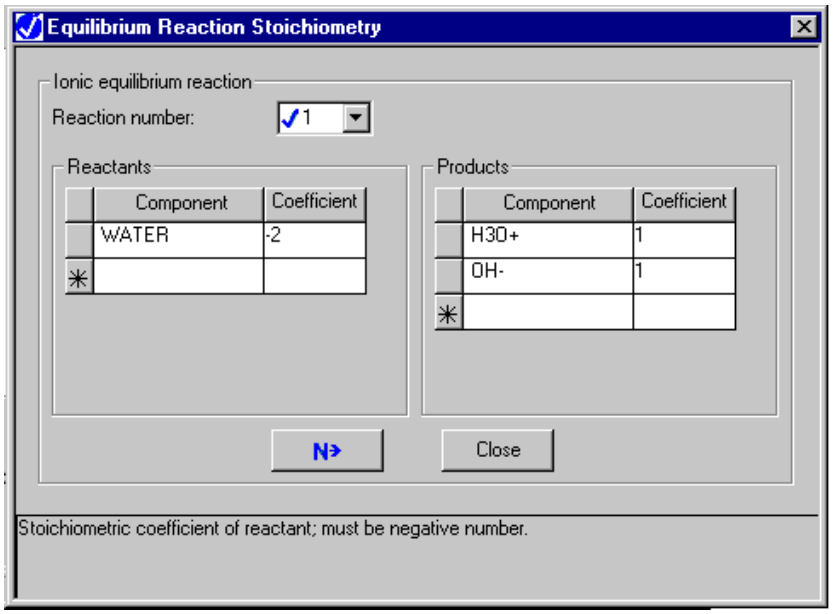
➤ Click Reactions on the Data Browser menu tree, then Chemistry, then Global.

The Reactions Chemistry Global form appears.



➤ To view a particular reaction, click the Reaction and then click the Edit button.

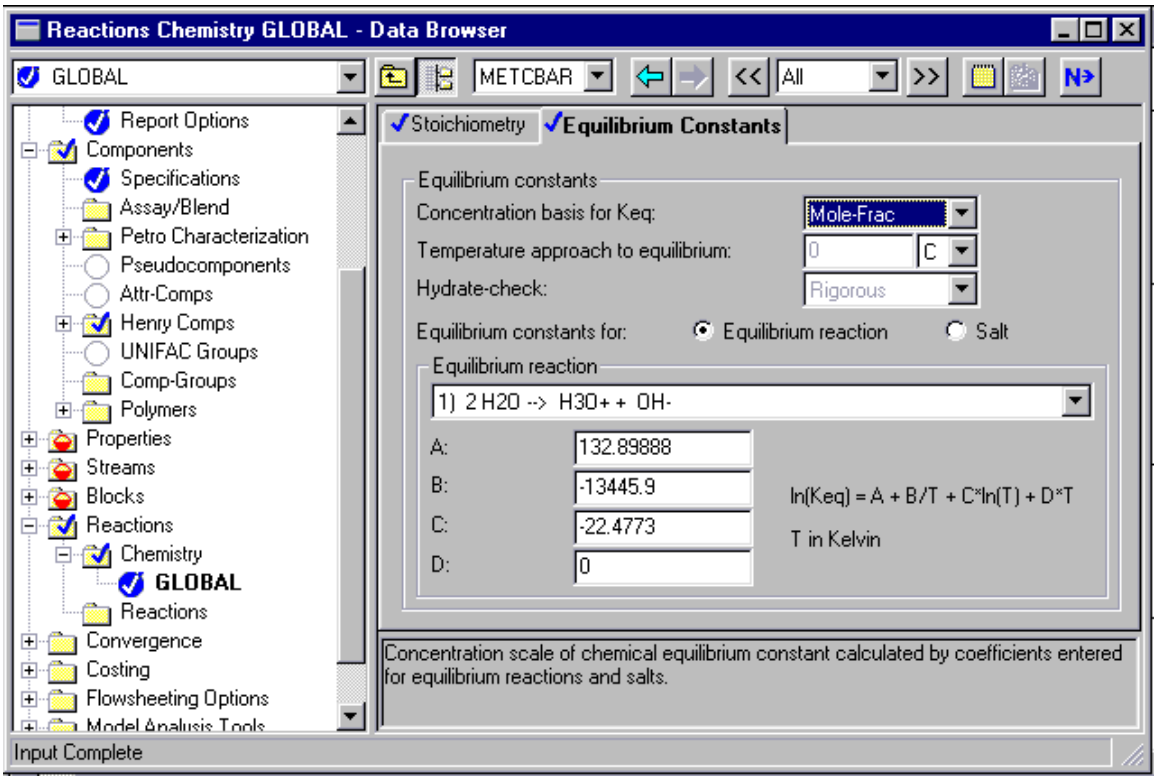
The Equilibrium Reaction Stoichiometry dialog box appears, with the data for the selected reaction that was generated by the Electrolytes Wizard.



The first equilibrium ionic reaction shown is for water dissociation.

➤ Close the dialog box and view the other reactions using the same method.

The optional equilibrium constant coefficients have been automatically retrieved from the Aspen Plus reactions database. The equilibrium constants are located on the Reactions Chemistry Equilibrium Constants sheet.



The Aspen Plus reactions database contains over 600 reactions, which cover virtually all common electrolyte applications.

➤ Click on the arrow to the right of the Equilibrium reaction field to select another equilibrium reaction and view the equilibrium constants.

The second equilibrium ionic reaction is for HCL dissociation. There are no equilibrium constant coefficients for this reaction. Instead of calculating the equilibrium constant directly, Aspen Plus will calculate the chemical equilibrium from the Gibbs free energy of the participating components.

The reaction for NACL(S) precipitation and its equilibrium constant coefficients are also available on this sheet. To view the equilibrium constants for the salt reactions:

➤ Select the Equilibrium constants for: **Salt** option.

➤ Click on the arrow to the right of the Equilibrium reaction field to select any other salt reaction and view the equilibrium constants.

For the complete dissociation reaction of NaOH, no constants are shown. Since this is a complete dissociation reaction, it does not require an equilibrium constant.

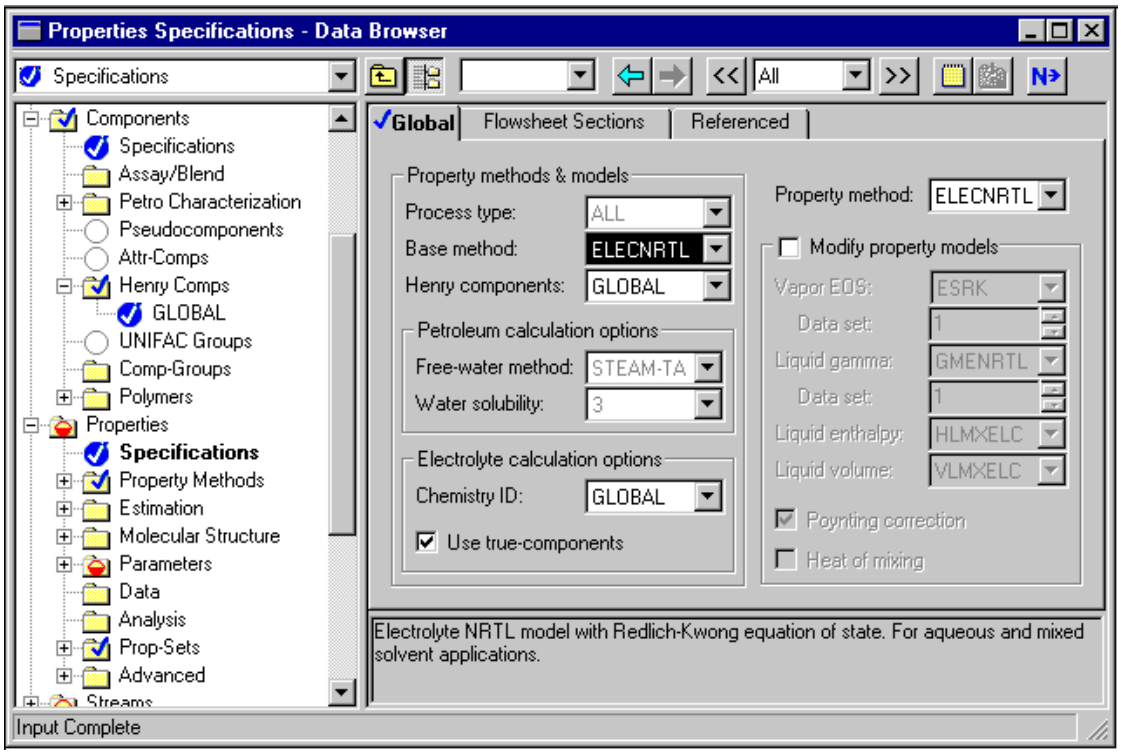
If you had your own equilibrium constant coefficients, or additional reactions you would like to include, you could enter them directly on this form.

Selecting Electrolyte Property Models

The Properties Specifications Global sheet is used to enter the thermodynamic methods used to calculate the properties used in the simulation.

➤ Click Properties on the Data Browser menu tree, then Specifications.

The Properties Specifications Global sheet appears. The Electrolytes Wizard has already completed this form:



The Electrolyte-NRTL activity coefficient model, ELECNRTL, is the recommended option set for simulations with electrolytes. ELECNRTL calculates liquid phase properties from the Electrolyte-NRTL activity coefficient model. Vapor phase properties are calculated from the Redlich-Kwong equation of state.

ELECNRTL can represent aqueous and aqueous/organic electrolyte systems over the entire range of electrolyte concentrations with a single set of binary interaction parameters. In the absence of electrolytes, the model reduces to the standard NRTL model.

Aspen Plus contains a databank of binary interaction parameters between water and over 600 electrolyte ion pairs. If the binary interaction parameters between any solvent and an electrolyte ion pair are missing from the databank, and you do not provide your own values, Aspen Plus provides reasonable default values.

➤ Click the Next button  on the Data Browser window toolbar to continue.

The Binary Interaction form appears for the binary parameters HENRY-1. Next takes you to this form so you can see the Henry's Law parameters retrieved by the electrolytes expert system. If you had your own Henry's Law parameters, you could enter them on this form.

➤ Click the Next button  on the Data Browser window toolbar to continue.

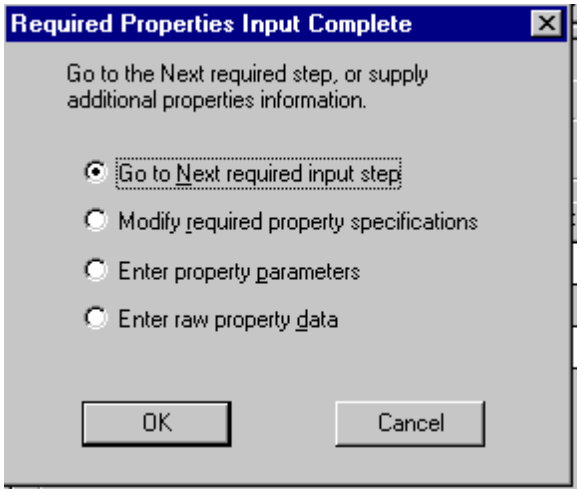
The Binary Interaction form appears for the binary parameters VLCLK-1. Next takes you to this form so that you can see the Clarke density parameters retrieved by the electrolytes expert system. If you had your own Clarke density parameters, you could enter them on this form.

➤ From the Data Browser window, select Electrolyte then Pair.

The Electrolyte Pair forms define the electrolyte pair parameters: GMELCC, GMELCD, GMELCE , and GMELCN. If you had your own pair parameters, you could enter them on these forms.

➤ Click the Next button  on the Data Browser window toolbar to continue.

The Required Properties Input Complete dialog box appears:



Correct representation of physical properties is essential to process modeling. For many simulations, the only physical property specification that you must provide is the selection of an option set. This dialog box shows that the Aspen Plus physical property system has many optional capabilities that you can use to increase the accuracy of the physical property calculations.

Because the Aspen Plus electrolytes database has data for all components and pairs in this simulation, you don't need to provide any optional specifications or data.

Now that the Components and Properties specifications are complete, you can complete the rest of the flowsheet specifications in the same way as for nonelectrolytes. There are no stream or block restrictions in using Aspen Plus electrolytes. You can use all Aspen Plus unit operation models in an electrolytes simulation.

➤ Click OK to move to the next required input.

Entering Stream Data

The Streams Input form for stream HCL appears. Aspen Plus requires two thermodynamic specifications and enough information to calculate the flow rate of each component.

➤ On the Streams Input Specifications sheet for Stream HCL, specify the following:

Temperature	**25 C**
Pressure	**1 Bar**
H2O flow value	**10 kmol/hr**
HCL flow value	**1 kmol/hr**

You entered the flow specifications for this stream in terms of the base components (the apparent components). Although you are using the true component approach in this problem, Aspen Plus can accept stream specifications in terms of the apparent components as well as the true components. Aspen Plus converts the apparent component flow specifications to true component specifications.

➤ Click the Next button  on the Data Browser window toolbar to continue.

The Streams Input form for stream NAOH appears.

➤ On the Streams Input Specifications sheet for stream NAOH, specify the following:

Temperature	**25 C**
Pressure	**1 Bar**
H2O flow value	**10 kmol/hr**
NAOH flow value	**1.1 kmol/hr**

➤ Click the Next button  on the Data Browser window toolbar to continue.

Specifying the Flash Block

The Input Specifications sheet for block FLASH appears. For this problem, you will specify the pressure drop and vapor fraction.

- In the Pressure field, enter **0** (indicating there is no pressure drop).
- Select Vapor fraction from the drop-down list. In the Vapor fraction field, enter **0.75**.
- Click the Next button  on the Data Browser window toolbar to continue.

The Input Flash Options sheet for block MIX appears. As the prompt says, the zero default pressure indicates no pressure drop, which is correct for this problem.

- Click the Next button  on the Data Browser window toolbar to continue.

A dialog box appears telling you that all required input is complete and asking if you want to run the simulation.

Before you run the simulation, you will request that certain optional properties be included in the stream report.

- Click Cancel, to close the dialog box without starting a run.

Specifying Additional Stream Properties

By default, the only component properties that Aspen Plus calculates and reports for this simulation are component mass flows. Since you are using the true component approach, the component flows will be in terms of the components actually present at equilibrium, not the apparent (base) components. To specify additional properties, you will open the Setup Report Options form.

➤ Click Setup on the Data Browser menu tree, then Report Options.

On the Setup Report Options Stream sheet, you specify the stream properties to be calculated and reported. For this session you will request that component mass fractions be calculated and reported.

➤ Click the Stream tab.

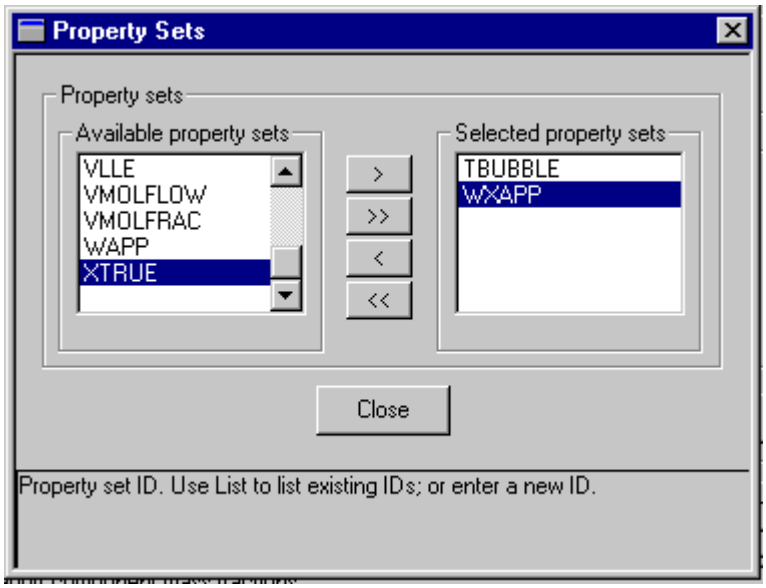
➤ Under Fractions Basis, click Mass.

You can also define additional stream properties to be calculated and reported, using Aspen Plus Property Sets. Aspen Plus provides a number of built-in Property Sets based on the Application Type you selected. You can also define your own Property Sets. In this problem, you will use a built-in Property Set to report the bubble point of each stream, and a second built-in Property Set to report the mass fractions of the apparent components in each stream.

➤ Click the Property Sets button.

The Property Sets dialog box appears.

➤ Select TBUBBLE and WXAPP from the Available Property Sets and move to the Selected Property Sets using the Move button >.



➤ Click Close.

➤ Click the Next button N> on the Data Browser window toolbar to continue.

Running the Simulation

The Required Input Complete dialog box appears.

➤ Since you have finished entering all required input, click OK, to run the simulation.

The Control Panel appears.

As the run proceeds, status messages appear in the Control Panel. It takes about a minute for Aspen Plus to process input specifications and perform the simulation.

Aspen Plus has a special databank that is searched only when you use the ELECNRTL option set, as in this session. Some physical property parameters in this databank may be different from the parameters in the standard non-electrolyte databanks. The values of the physical property parameters in the special databank were determined to provide a better fit for electrolyte systems, and are not generally applicable.

When values are retrieved from this special databank, Aspen Plus generates messages in the Control Panel to inform you what properties are retrieved for which components.

When the calculations finish, the message *Results Available* appears in the status area at the bottom right of the main window.

➤ Use the vertical scroll bar to the right of the Control panel window to see the messages.

You can now examine the results of your run.

Examining Simulation Results

To view the results of the simulation:

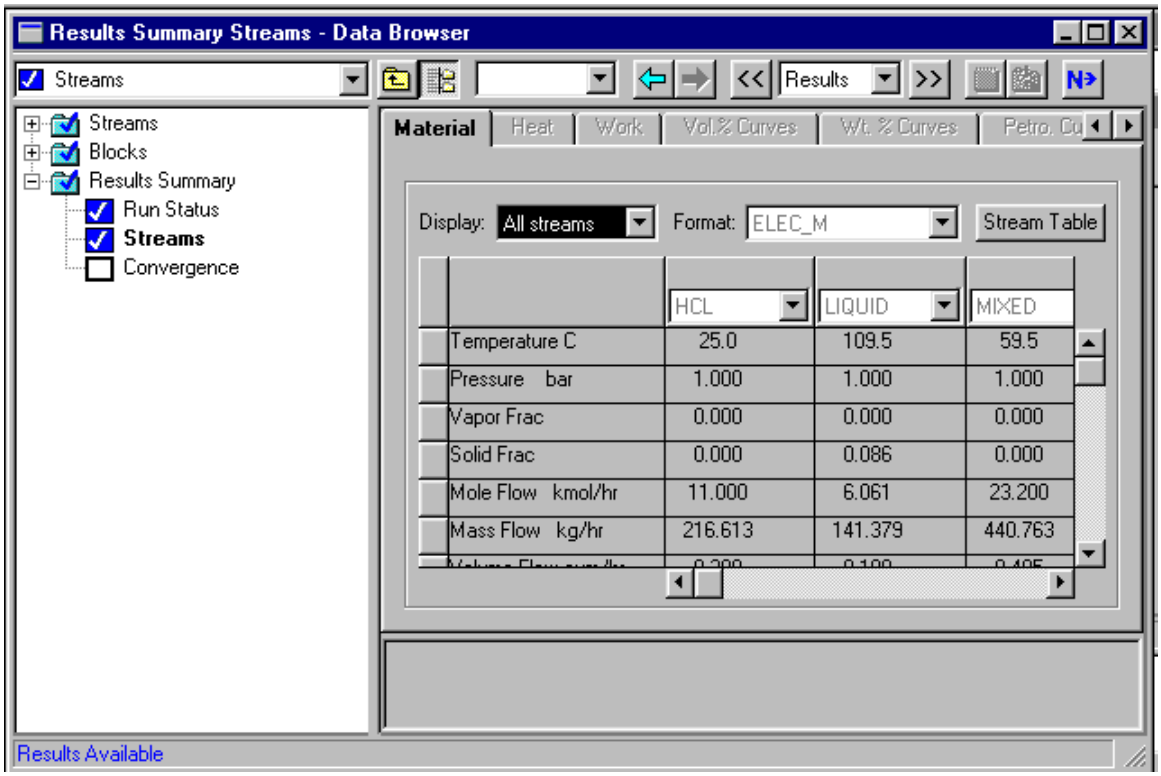
➤ Click the Check Results button on the Control Panel.

The Run Status Data Browser appears, indicating that the simulation completed normally.

➤ Use the Next form button >> to move to the next form with results.

The Results Summary Streams form appears.

➤ Review the results on this form. Since this is a scrolling form, click the arrow in the lower right corner of the form to review results that are off the screen.



Since you selected the True Component approach, results for Mass Flow and Mass Frac are in terms of true components.

Although you specified the flow rates in terms of the apparent components (1 kmol/hr HCL and 10 kmol/hr H2O), Aspen Plus calculated the flow rates of the true components. In stream HCL, there is only a trace of molecular HCL remaining. Virtually all of the HCL is dissociated into $H3O^+$ and CL^-. Since the HCL dissociation consumes a mole of water, the overall H2O flow rate is reduced from 180 kg/hr (10 kmol/hr) to 162 kg/hr (9 kmol/hr).

You also specified the NAOH stream in terms of apparent components (1.1 kmol/hr NAOH and 10 kmol/hr H2O). NAOH dissociates completely into NA^+ and OH^-. This is reflected by the complete disappearance of molecular NAOH in this stream.

Stream HCL and Stream NAOH are added together in block MIX to form Stream MIXED. Because water dissociation is included as one of electrolytes reactions, MIX allows $H3O^+$ and OH^- to recombine to form water. The heat of this reaction raises the temperature of Stream MIXED from 25 C (the temperature of both inlets) to 61 C. This demonstrates that the heat of electrolyte reactions (including the heat of mixing) is automatically included in Aspen Plus electrolytes calculations.

Stream MIXED feeds a Flash2 block where water is boiled off. Because ions and precipitated salts are nonvolatile, Stream VAPOR only contains pure water. As the ions are concentrated in Stream LIQUID, the solubility limit of NACL in water is exceeded, causing 30 kg/hr of molecular NACL(S) to precipitate.

Examine the bubble temperature for stream MIXED and stream LIQUID. Stream MIXED is subsaturated in NACL and stream LIQUID is saturated with NACL. Aspen Plus correctly calculates the bubble point of LIQUID (110 C) as greater than the bubble point of MIXED (103 C), which is greater than the boiling point of pure water at 1 bar (99.6 C).

Compare the apparent mass fractions for the liquid phase with the true component mass fractions in stream LIQUID. Even though stream LIQUID has precipitated NACL(S), the apparent mass fraction of NACL(S) is zero because Aspen Plus does not consider precipitated salts to be apparent components. The apparent mass fractions of the ions NA+, H3O+, OH-, and CL- are also zero. Precipitated salts and ions can only be true components.

Since the precipitated NACL(S) is not an apparent component, it is represented in the apparent component approach in terms of the original species that combined to form NACL(S): NAOH, and HCL. This is why the apparent component basis mass fraction of NAOH is 0.209 even though the true component basis mass fraction of NAOH is zero.

You have now viewed the most relevant results for an electrolytes simulation.

This simulation has other Results forms. You can use the browse button  to view them, if you choose.

Exiting Aspen Plus

To exit from Aspen Plus:

➤ From the File menu, select Exit.

➤ When the dialog box appears asking if you want to save the run, select No to exit without saving the run;
– or –
if you want to save the run, select Yes and enter a Run ID when prompted.

This simulation is delivered as backup file *elec1* in the online Aspen Plus Examples Library. You can use this backup file to check your results.

❖ ❖ ❖ ❖

2 Modeling a Sour Water Stripper

In this session you will use a distillation column to strip NH_3 and H_2S from a sour water feed stream.

You will:

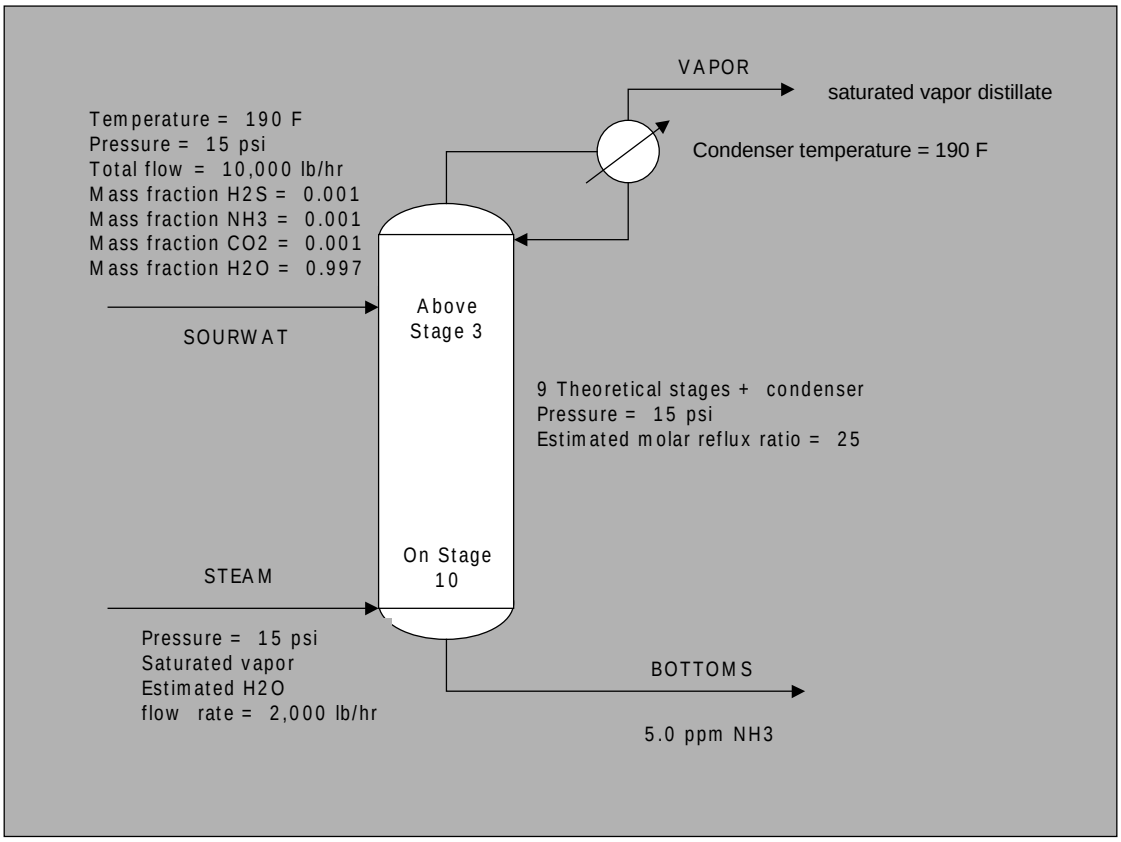
- Modify the generated Chemistry
- Use the apparent component approach for electrolytes
- Define a stream property (Property Set)
- Convert the simulation from the apparent approach to the true approach

Allow about 45 minutes to do this session.

Sour Water Stripper Flowsheet

The process flow diagram and operating conditions for this session are shown in the Process Diagram: Sour Water Stripper. Two feed streams, one containing sour water, the other steam, are fed to a stripper to remove CO_2, H_2S, and NH_3 from the sour water. You will use RadFrac to simulate the stripper.

Process Diagram: Sour Water Stripper



The specifications for the column are:

- 10 theoretical stages total (includes one for the condenser)
- Distillate product as saturated vapor (partial condenser)
- Initial estimate for molar reflux ratio = 25
- No reboiler
- Feed stream SOURWAT above stage 3
- Feed stream STEAM on stage 10
- Column pressure of 15 psi (isobaric)
- Vary the reflux ratio and stream STEAM feed rate to achieve a bottoms product with 5 ppm (mass) of NH3 and a condenser temperature of 190 F

Starting Aspen Plus

To start Aspen Plus:

➤ From your desktop, click Start and then select Programs.

➤ Select AspenTech, then Aspen Plus 10.1-0, then Aspen Plus User Interface.

Note If the Connect to Engine dialog box appears, see Appendix A.

The Aspen Plus Startup dialog box appears. Aspen Plus displays a dialog box whenever you must enter information or make a selection before proceeding. In this simulation, you will use an Aspen Plus template.

➤ To select the Template option, point the mouse to the Template radio button and click the left mouse button.

➤ Click OK to apply this option.

The New dialog box appears.

You use the New dialog box to specify the Application Type and the Run Type for the new run. Aspen Plus uses the Application Type you choose to automatically set various defaults appropriate to your application.

To specify the Application Type and Run Type for the new run:

➤ Select the Electrolytes with English Units template.

➤ The default Run Type, Flowsheet, is appropriate for this session. Click OK to apply these options.

It will take a few seconds for Aspen Plus to apply these options.

Note If the Connect Host dialog box appears, see Appendix A.

The Aspen Plus Main window is now active.

Drawing the Graphical Simulation Flowsheet

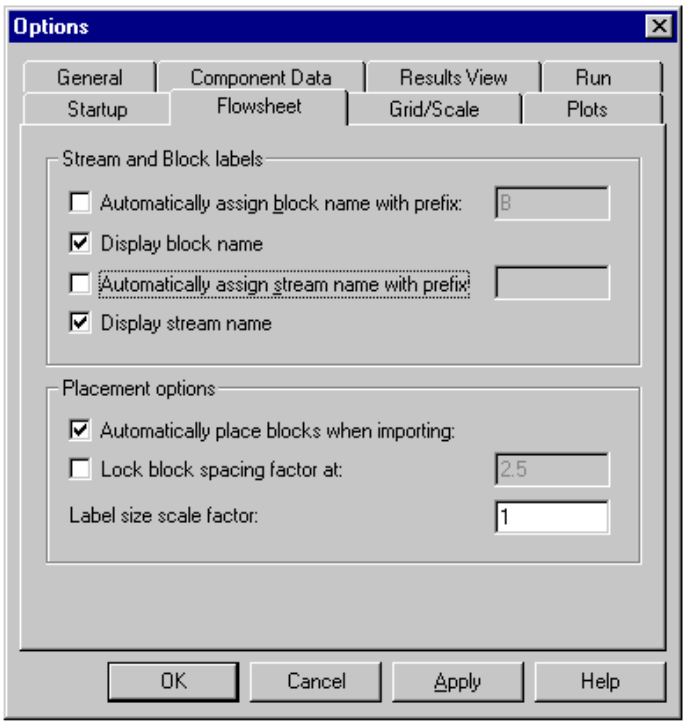
In this session you will begin to build the process flowsheet. Since you will enter your own block and stream IDs, you must turn off the default Create auto block ID and Create auto stream ID options, which provide these IDs automatically.

➤ From the Aspen Plus Tools menu, select Options.

The Options dialog box appears.

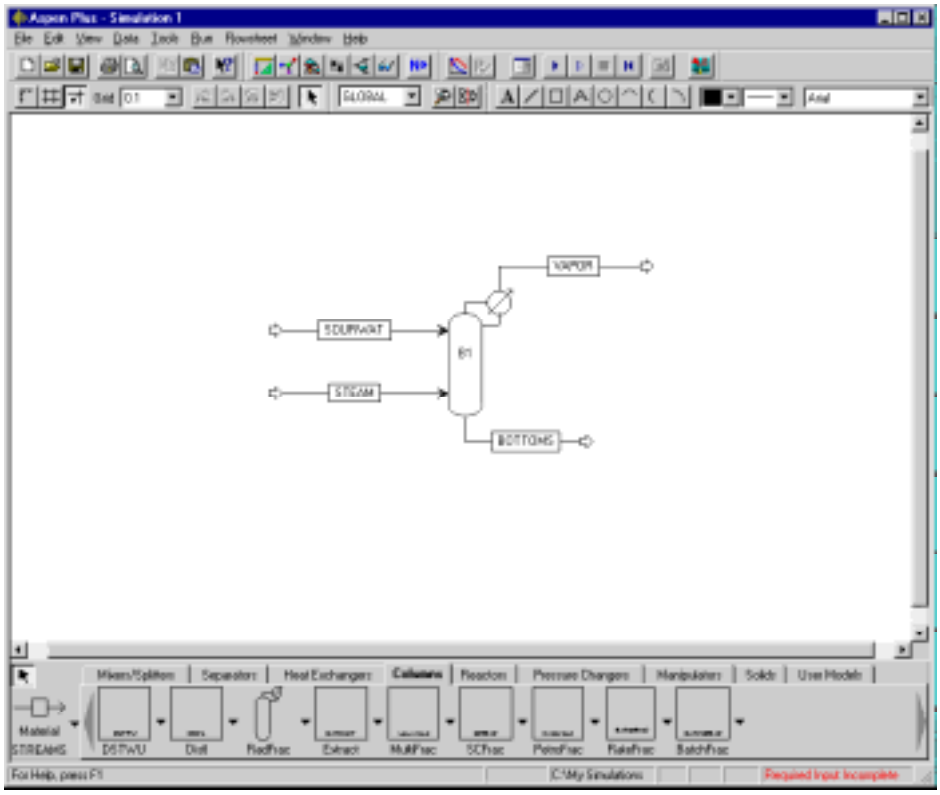
➤ Select the Flowsheet tab.

➤ Deselect the Automatically Assign Block Name with Prefix and the Automatically Assign Stream Name with Prefix options.



➤ Click OK to close the Options dialog box and apply the changes.

➤ Place the flowsheet blocks and streams to create the graphical simulation flowsheet shown below.



➤ Use Next (click the Next button  on the main window toolbar) to guide you to the next required input.

The Flowsheet Connectivity is Complete dialog box appears.

➤ Click OK, to continue.

Specifying Title, Stream Properties, and Global Options

The Data Browser window appears. The Setup Specifications form displays defaults Aspen Plus uses for other forms. You will use this form to give your simulation a title, and to review the stream properties and global options that were set when you selected the Electrolytes with English Units Application Type.

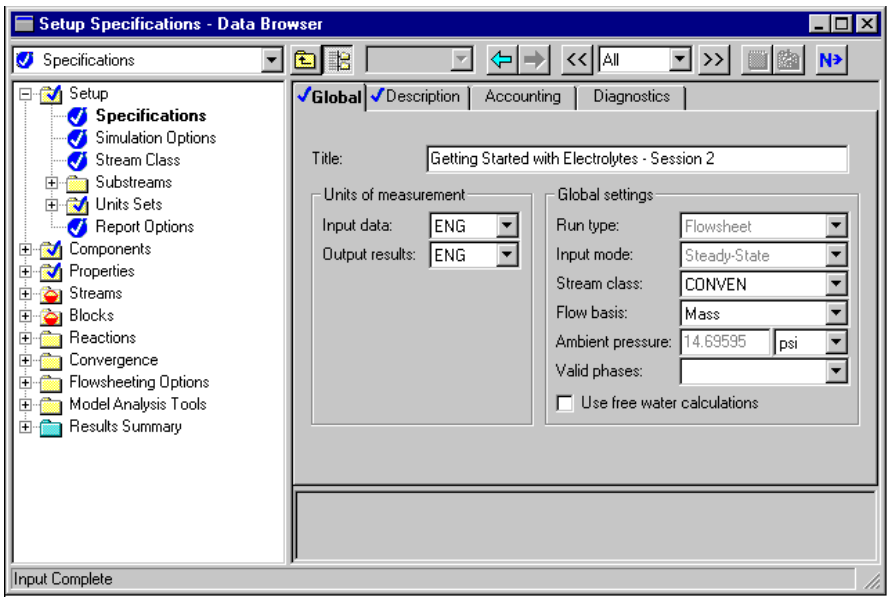
The Run Type field displays Flowsheet, which is appropriate for this session.

The Electrolytes with English Units Application Type sets the following global defaults for electrolytes applications:

- ENG units (English units)
- Mass Flow basis for all flow inputs

It is always good practice to describe your problem by entering a title for the simulation. To select the template option, click the Template option button.

➤ Enter the title **Getting Started with Electrolytes – Session 2**.



Since you chose the Electrolytes with English Units Application Type when you started this session, Aspen Plus has set the following defaults for calculating and reporting stream properties:

- Flow and Fraction Basis of Mass: Aspen Plus will report the component flow rates on a mass flow basis.
- ELEC_E Stream Format: Aspen Plus formats the Stream Summary form for electrolytes.

To review the report options specified in the selected Template:

➤ In the menu tree of the Data Browser window, click the Report Options form in the Setup folder.

➤ Click on the Stream tab to view the Stream sheet.

To move to the next required input sheet:

➤ Click Components on the Data Browser menu tree, then Specifications.

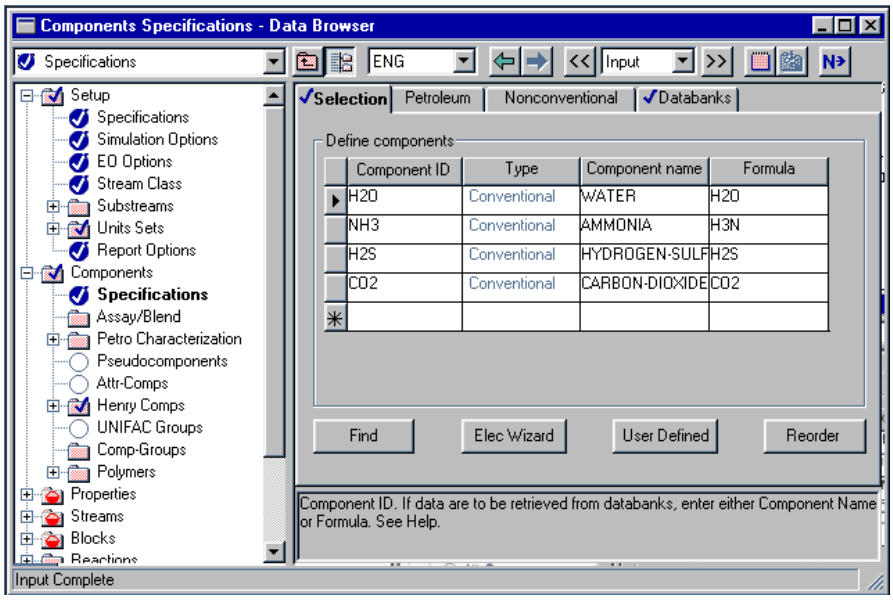
Specifying Components

The Components Specifications Selection sheet appears.

The apparent (or base) components for this session are H2O, NH3, H2S, and CO2. Because you chose an electrolytes Application Type, water already appears on the form.

Because the formula for ammonia is represented as H3N in the Aspen Plus databank, you must identify NH3 by entering either the component name (ammonia) or the formula (H3N).

➤ Enter the remaining components as shown below.



➤ Click the Elec Wizard button.

The Electrolytes Wizard dialog box, for defining automatic chemistry generation, appears.

The Electrolytes Wizard

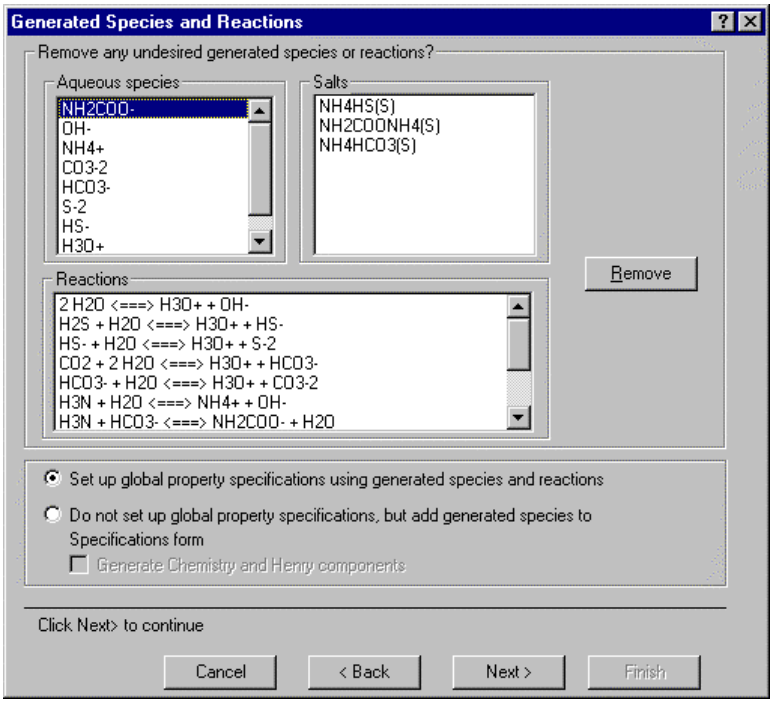
You use the Electrolytes Wizard dialog box to define the ionic species that can be generated from the base components you specified on the Components Specifications form, and to generate the reactions that occur among these components in the liquid phase.

➤ Click the Next > button.

➤ Move all components to the Selected components area by using the Move All button >>.

➤ Click the Next > button to continue

The Generated Species and Reaction dialog box appears.



Aspen Plus generates all possible ionic species and reactions for the H2O-NH3-H2S-CO2 system.

In the Generated Reactions list, different-style arrows denote the type of reaction.

<<===>> Denotes ionic equilibrium and salt precipitation

--->> Denotes complete dissociation

For this simulation, you know that ammonium carbamate formation can be neglected. To remove ammonium carbamate formation from the solution chemistry:

➤ Select NH2COO- aqueous species.

➤ Click the Remove button to the right of the Generated Reactions list.

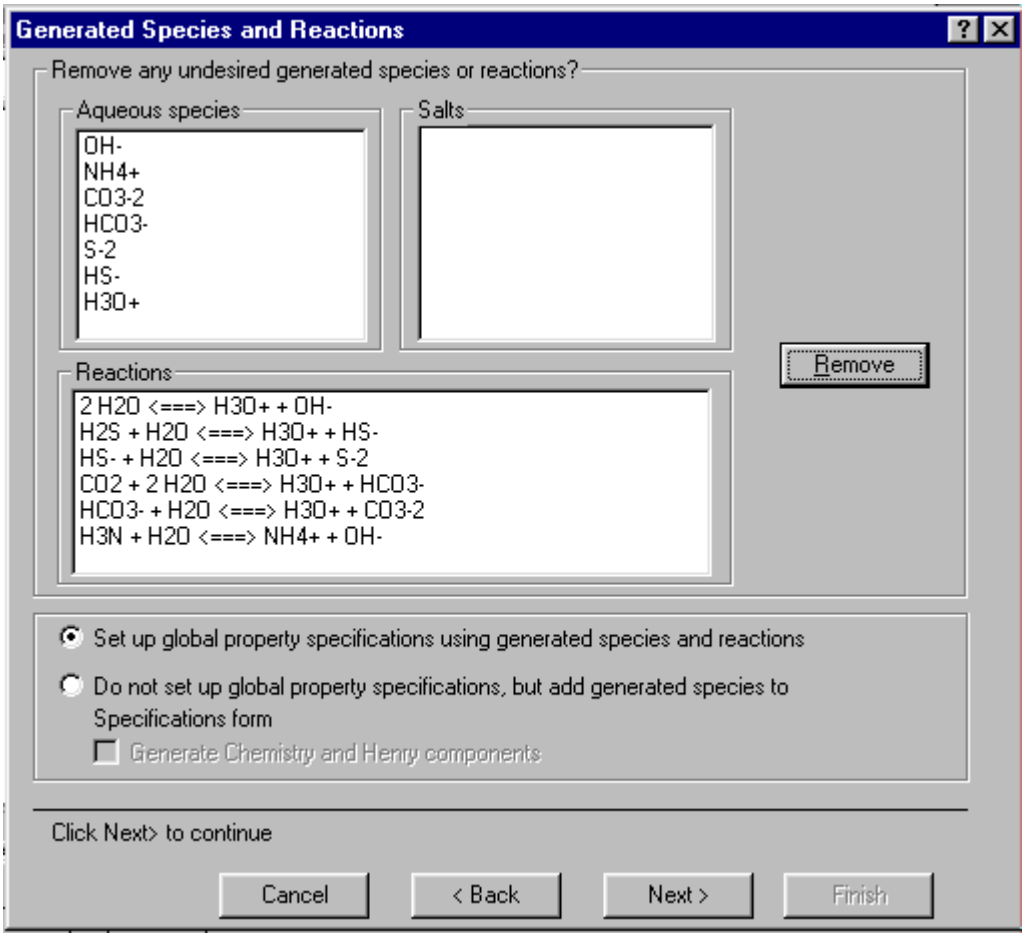
Now that you have removed NH2COO- from the Generated Aqueous Species list, Aspen Plus automatically removes all reactions involving NH2COO- from the Reactions list.

The salts are also not relevant.

To remove the salts from the solution chemistry:

➤ Select NH4HS(S) and NH4HCO3(S) from the Salts list.

➤ Click the Remove button to the right of the Generated Reactions list.



Note Any time you know that a reaction can be neglected because of expected process conditions, you should remove it from the solution chemistry, to decrease the execution time required for your simulation.

In this example, only ionic equilibrium reactions are generated. The remaining six generated reactions represent partial dissociation of water, partial dissociation of H_2S to HS^- and S^{-2}, partial dissociation of CO_2 to HCO_3^- and CO_3^{-2}, and partial dissociation of NH_3 to NH_4^+.

➤ Click Next > on the Generated Species and Reactions dialog box to accept the generated species and reactions.

The Simulation Approach dialog box appears, allowing you to choose between the true species approach and the apparent component approach. For this problem you use the apparent component approach.

When you use the apparent component approach, Aspen Plus solves the equations describing solution chemistry as part of the physical property calculations. Aspen Plus modifies the physical properties of the apparent components to account for the reactions described by the solution chemistry. The ions and precipitated salts are not seen by the unit operation models.

The apparent component approach also defines how Aspen Plus reports simulation results. The component flow rates for ions are not reported. Instead, Aspen Plus reports the component flow rates of the apparent components as if no dissociation occurred.

For example, the generated Chemistry for this system specifies that H_2S partially dissociates into HS^- and S^{-2}. If you choose the apparent component approach, Aspen Plus will report a value for the mole flow rate of H2S that includes molecular H_2S, HS^-, and S^{-2}.

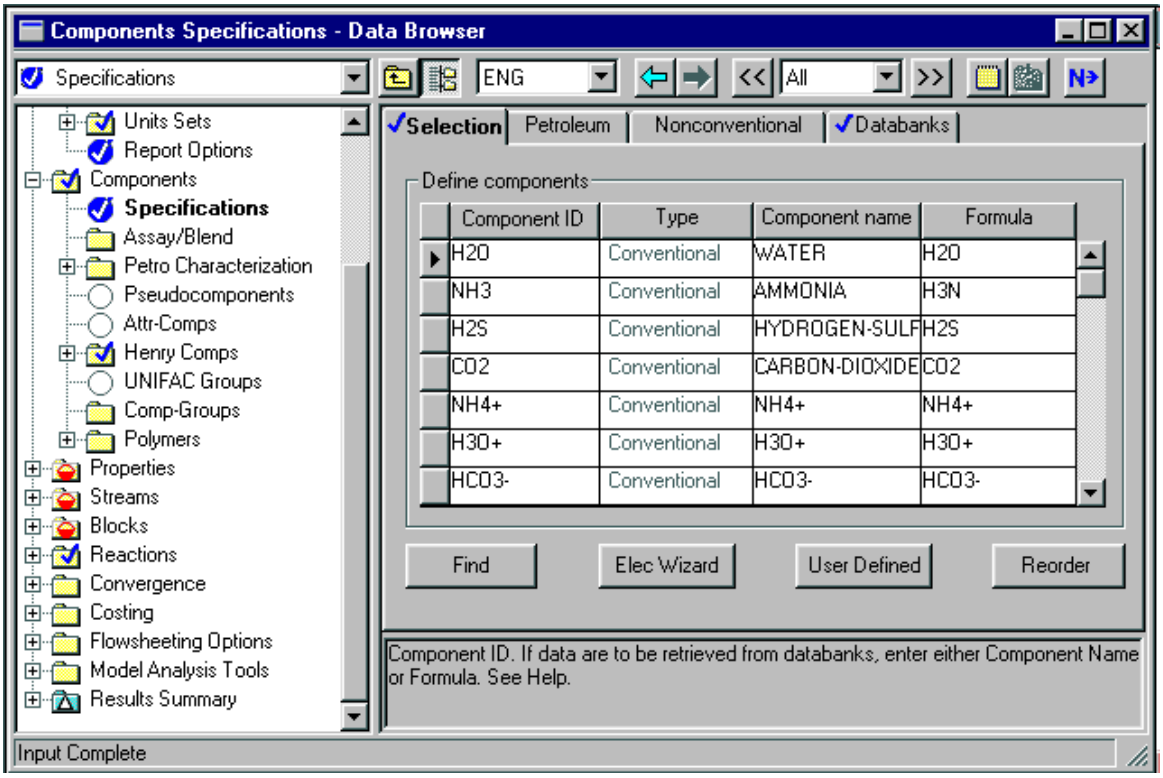
➤ Select Apparent component approach.

➤ Click Next > to move to the next dialog box.

The Summary dialog box appears, telling you what the Aspen Plus electrolytes expert system has done.

➤ Click Finish to close the dialog box.

On the Components Specifications form, Aspen Plus has now added the generated electrolyte components. Since all components are databank components, Aspen Plus will automatically retrieve all relevant physical property parameters.



➤ Click the Next button  on the Data Browser window toolbar to continue.

The Components Henry Comps Global sheet appears for the Henry Comps group GLOBAL, which was defined by the electrolytes expert system. Next guides you to this form so that you can see which components have been declared as Henry's Law components by the electrolytes expert system. If you had additional Henry's Law components in your simulation (such as nitrogen and oxygen), you could add them to the list on this form.

Examining Generated Chemistry

In the previous step, the Aspen Plus Electrolytes Wizard automatically generated the chemistry definition for your problem and named it GLOBAL.

To examine the generated Chemistry:

➤ Click Reactions on the Data Browser menu tree, then Chemistry, then Global.

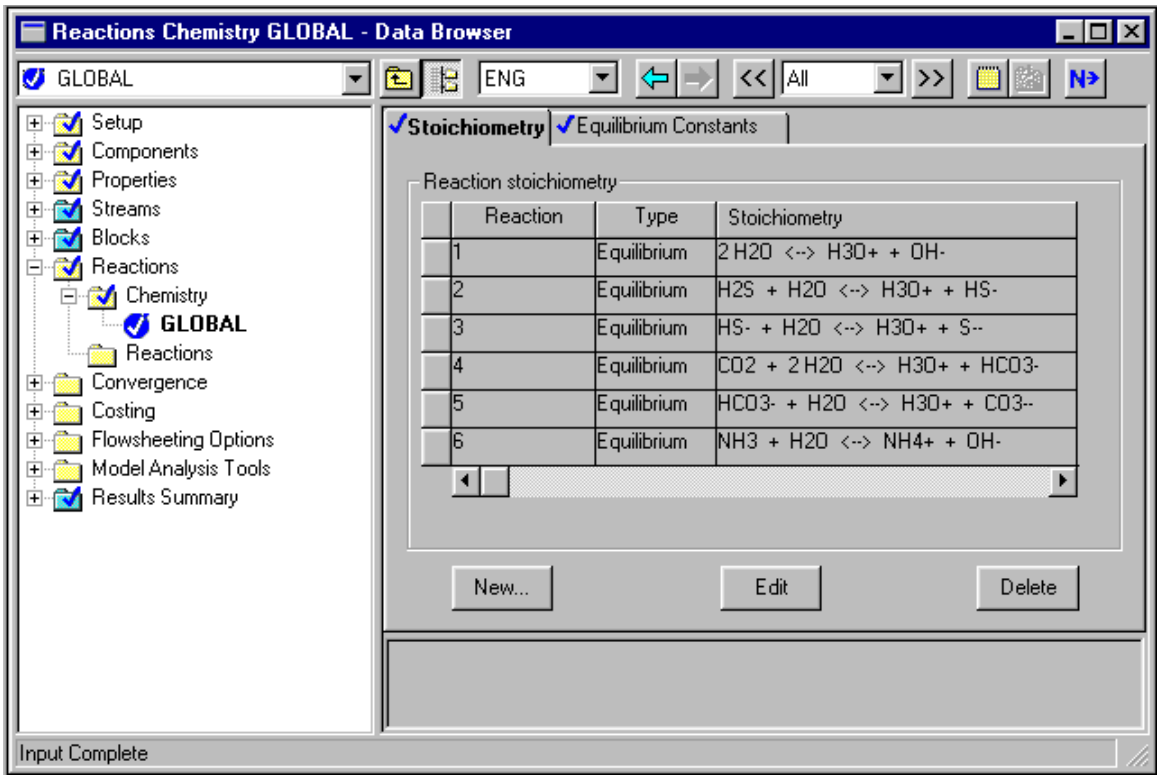
The Reactions Chemistry Global form appears.

➤ To view the generated chemistry, select the Reaction and click the Edit button.

The Reaction Stoichiometry dialog box appears, with the data for the selected reaction that was generated by the Electrolytes Wizard.

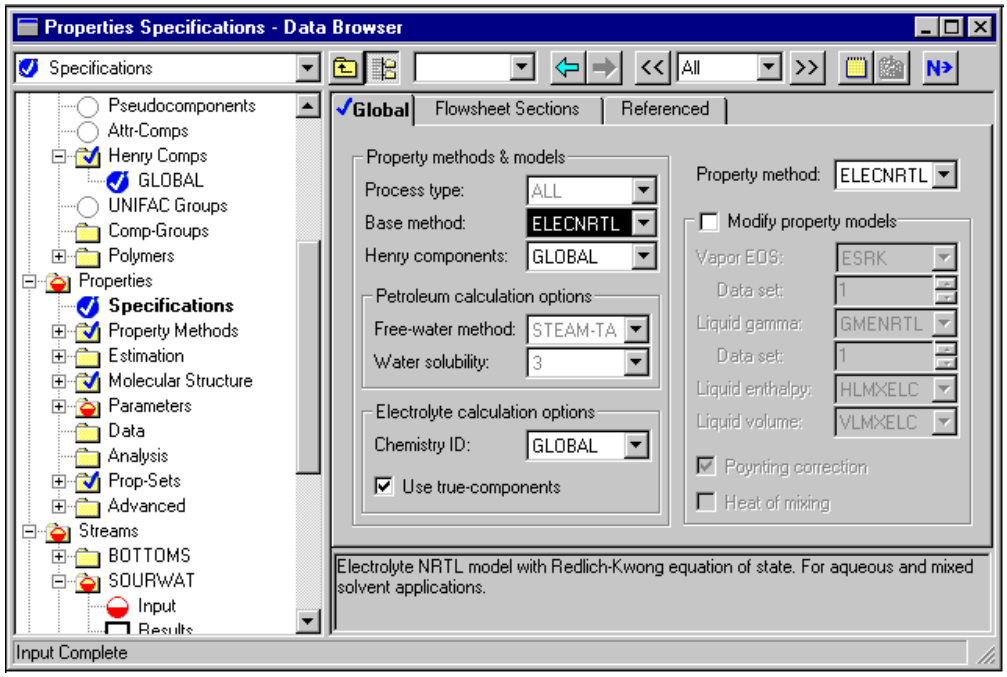
➤ View the remaining reactions using the same method.

All six reactions have equilibrium constant that have been retrieved from the Aspen Plus reactions database.



➤ Click Properties on the Data Browser menu tree, then Specifications.

The Properties Specifications form appears. The Electrolytes Wizard has already completed this form.



➤ Ensure the Use True-Components box is checked.

➤ Click the Next button on the Data Browser window toolbar to continue.

The Binary Interaction form appears for the binary parameters HENRY-1. Next takes you to this form so that you can see the Henry's Law parameters retrieved by the electrolytes expert system. If you had your own Henry's Law parameters, you could enter them on this form.

➤ Click the Next button on the Data Browser window toolbar to continue.

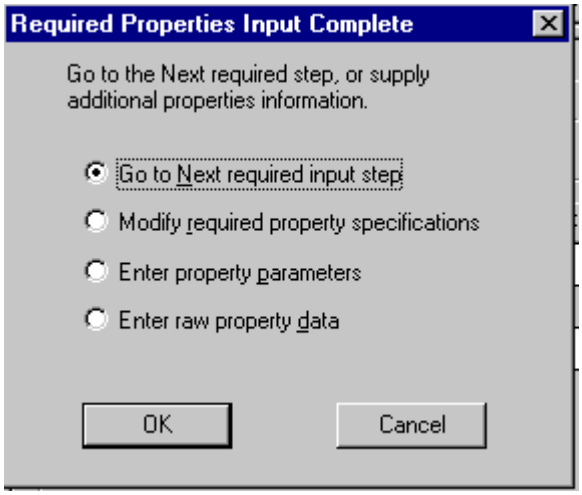
The Binary Interaction form appears for the binary parameters NRTL-1. Next takes you to this form so that you can see the molecule-molecule interaction parameters retrieved by the electrolytes expert system. If you had your own molecule-molecule interaction parameters, you could enter them on this form.

➤ From the Data Browser window, select Electrolyte then Pair.

The Electrolyte Pair forms define the electrolyte pair parameters: GMELCC, GMELCD, GMELCE, and GMELCN. If you had your own pair parameters, you could enter them on these forms.

➤ Click the Next button on the Data Browser window toolbar to continue.

The Required Properties Input Complete dialog box appears:



Correct representation of physical properties is essential to process modeling. For many simulations, the only physical property specification that you must provide is the selection of an option set. This dialog box shows that the Aspen Plus physical property system has many optional capabilities that you can use to increase the accuracy of the physical property calculations.

Because the Aspen Plus electrolytes database has data for all components and pairs in this system, you don't need to provide any optional specifications or data.

Now that the Components and Properties specifications are complete, you can complete the rest of the flowsheet specifications in the same way as for nonelectrolytes. You can use all Aspen Plus unit operation models in an electrolytes simulation.

➤ Click OK to close the dialog box and move to the next required input.

Entering Stream Data

The Streams Input form for stream SOURWAT appears. Aspen Plus requires two thermodynamic specifications and enough information to calculate the molar flow rate of each component.

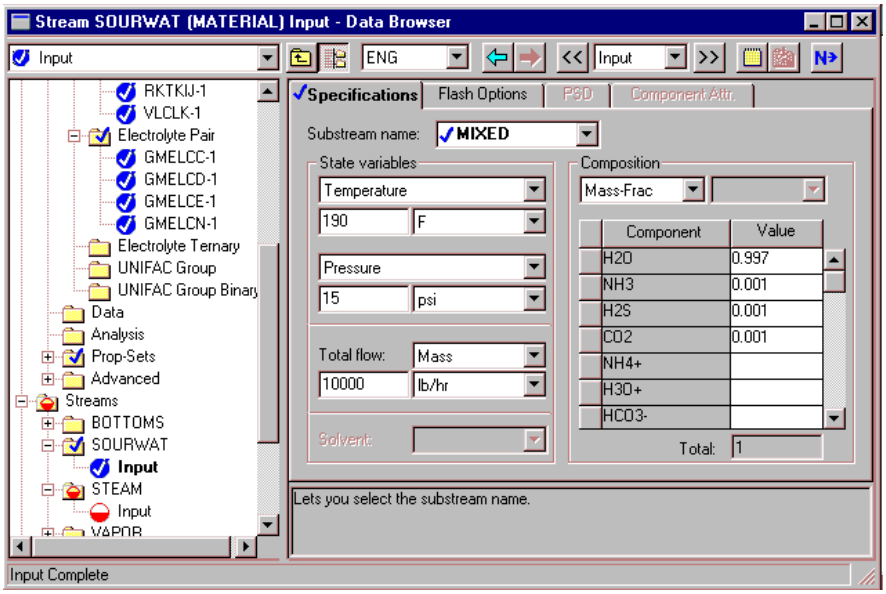
➤ On the Specifications sheet for Stream SOURWAT, enter the following specifications:

Temperature	**190 F**
Pressure	**15 PSI**
Total flow Mass	**10000 LB/HR**

➤ In the Composition box, select Mass-Frac from the list.

➤ Enter the following mass fractions:

H2O	**0.997**
NH3	**0.001**
H2S	**0.001**
CO2	**0.001**

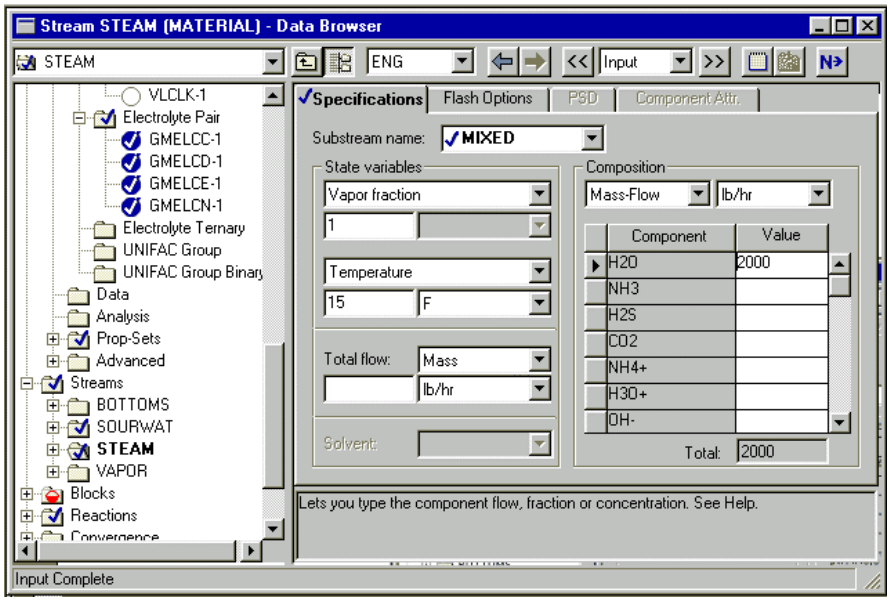


➤ Click the Next button  on the Data Browser window toolbar to continue.

The Streams Input form for stream STEAM appears.

➤ On the Specifications sheet for stream STEAM, enter the following specifications:

Pressure	**15 PSI**
Vapor Fraction	**1**
Composition	**Mass-Flow**
H2O Mass flow value	**2000 LB/HR**



➤ Click the Next button  on the Data Browser window toolbar to continue.

Specifying the RadFrac Block

The Blocks Setup form for block B1 appears.

To review the types of specifications that you can make for a RadFrac block:

➤ Use Help on the RadFrac Setup form.

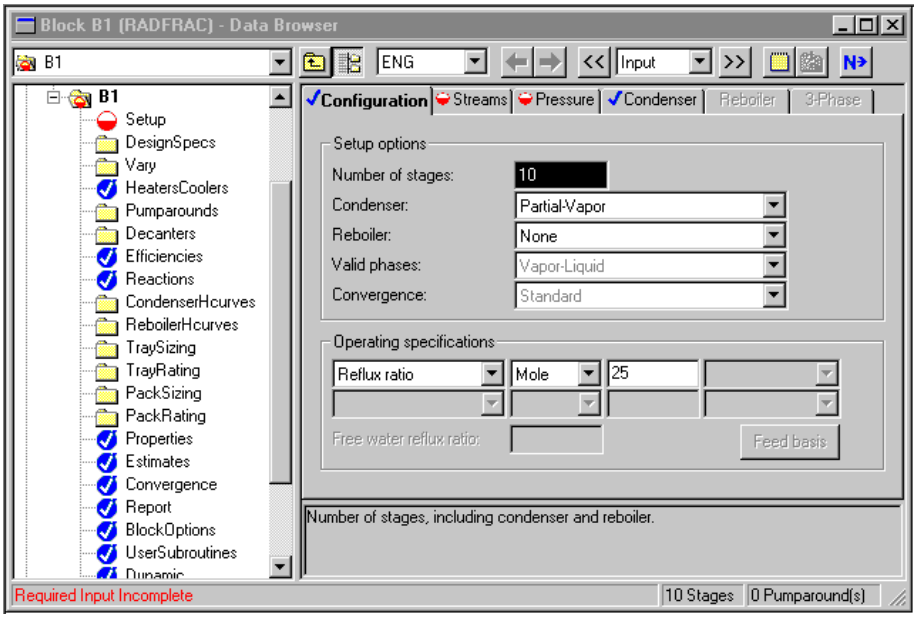
➤ Review the types of specifications, then close the Help window when you are ready to continue.

➤ On the Blocks B1 Setup Configuration sheet specify the following:

Number of stages	**10 (9 theoretical stages and condenser)**
Condenser	**Partial-Vapor**
Reboiler	**None**

In the Operating Specifications list, select **Reflux Ratio, Mole** and specify **25** as the initial estimate for reflux ratio

The Blocks B1 Setup Configuration sheet is complete:



➤ Click the Next button  on the Data Browser window toolbar to continue.

The Blocks B1 Setup Streams sheet appears. Use this form to describe how the streams are connected to the RadFrac block.

- Specify that Stream SOURWAT is fed to Stage 3 with the Above-Stage Feed convention.

- Specify that stream STEAM is fed to Stage 10 with the On-Stage feed convention.

Because stream VAPOR is connected to the vapor distillate port, Aspen Plus automatically assigns stream VAPOR as a vapor phase product from stage 1. Similarly, Aspen Plus assigns stream BOTTOMS as a liquid phase product from stage 10. The Blocks B1 Setup Streams sheet does not accept flow specifications for distillate product or bottoms product streams.

- Click the Next button  on the Data Browser window toolbar to continue.

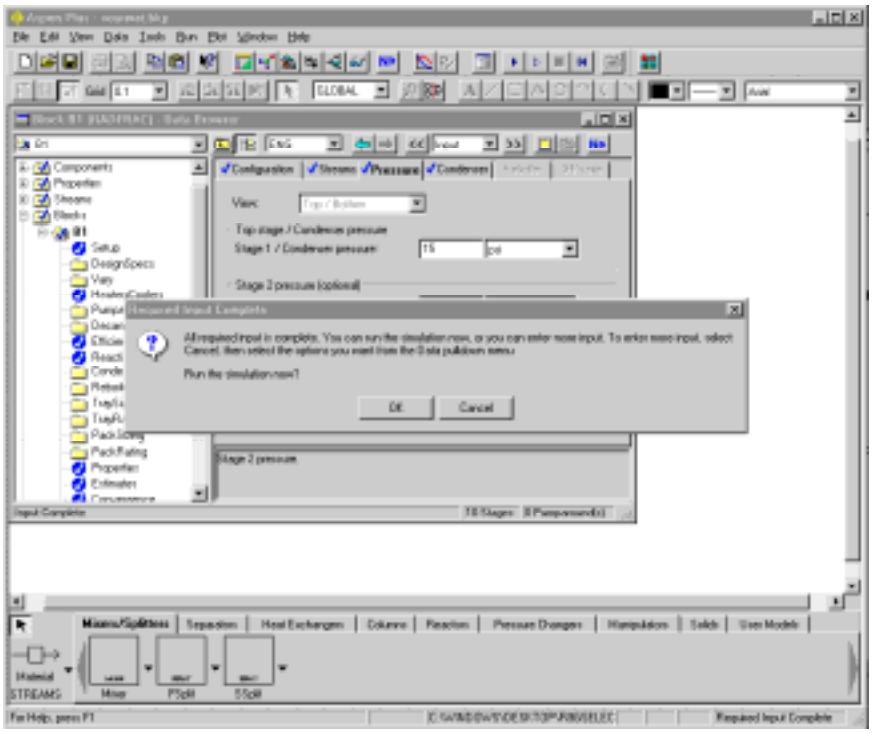
The Setup Pressure sheet appears.

To specify that this column operates isobarically at 15 psia:

- On the first row of the form, enter a pressure of 15 PSI for Stage 1.

- Click the Next button  on the Data Browser window toolbar to continue.

The Required Input Complete dialog box appears, indicating that all required input specifications for RadFrac Block B1 have been entered:



➤ Click Cancel to close the dialog box.

You can now enter optional specifications. For this column, you have two design specifications:

Spec1	Concentration of NH3 in BOTTOMS	50 ppm
Spec2	Condenser Temperature	190°F

➤ To define the first design specification, click the Blocks B1 Design Specs folder.

The Design Specs Object Manager appears.

➤ Click New.

➤ In the dialog box that appears, click OK to accept the default ID, 1.

The Design Specs 1 form appears.

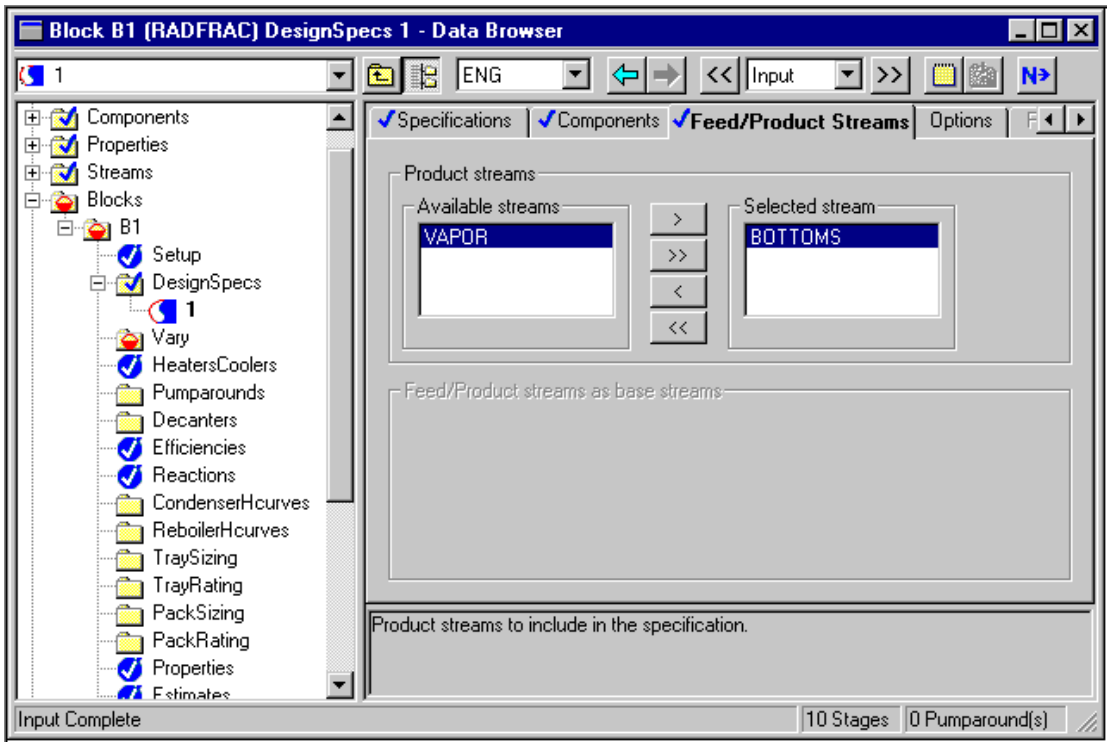
➤ In the Type field on the Specifications sheet, use the drop-down list and select Mass purity, then enter the value **5.0E-6**.

You must specify where this specification is to be applied, and what component and phase it applies to:

- On the Components sheet, select AMMONIA as the Component.

- On the Feed/Product Streams sheet, select the BOTTOMS stream.

The Design Specs 1 form is complete:



- To define another design specification, click the Design Specs folder in the Data Browser window.

The Design Specs Object Manager appears again.

➤ Click New, then OK.

A new Design Specs form appears.

➤ Enter, or use List to select, the following specifications:

Type	**Stage temperature**
Value	**190 F**
Stage	**1**

➤ Click the Next button  on the Data Browser window toolbar to continue.

The Vary Object Manager appears. You need to define two manipulated variables to meet the two design specifications. In this problem you will keep free the steam feed rate and the reflux ratio specifications provided on the Blocks B1 Setup form. Aspen Plus will adjust the steam feed rate and reflux ratio to achieve the NH_3 bottoms concentration specification and the condenser temperature specification.

➤ To define the first manipulated variable, click New, then OK.

The Vary 1 form appears.

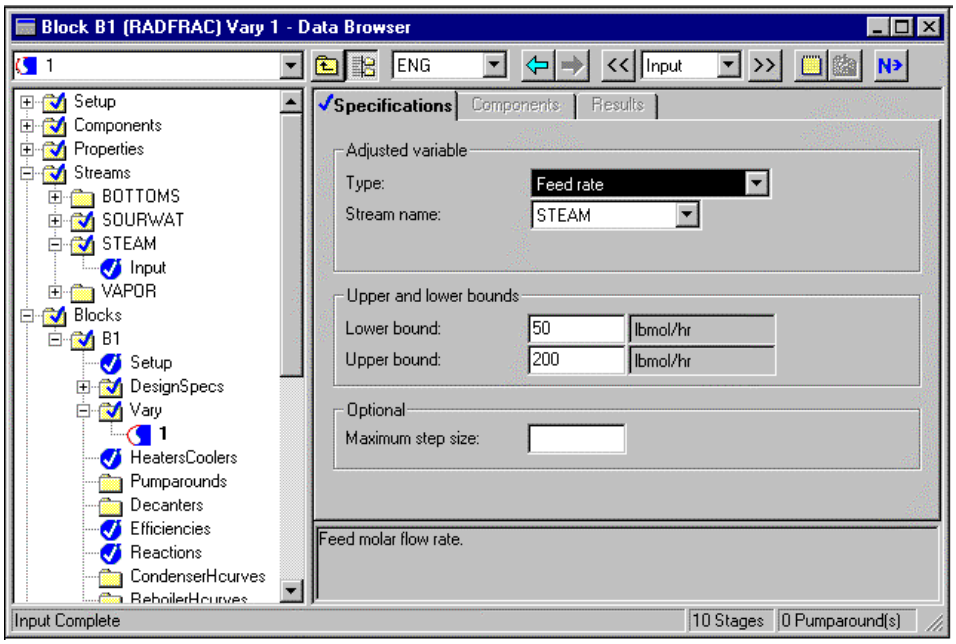
On the Vary 1 form, you can tell Aspen Plus which input variables you want to keep free in order to meet the design specifications you provide.

➤ Enter, or use List to select, the following values:

Type	**Feed rate**
Stream name	**STEAM**
Lower bound	**50 lbmol/hr**
Upper bound	**200 lbmol/hr**

On the Streams STEAM form you specified a Mass-Flow for Stream STEAM.

However, when you select the variable type Feed rate on the Vary 1 form, Aspen Plus assumes the Feed rate to be on a mole basis. In this case, varying the Feed rate on a mole basis from 50-200 (lbmol/hr) is equivalent to varying the Mass flow from 900-3600 (lb/hr).



➤ To define the second manipulated variable, click the Vary folder in the Data Browser window, select New, then OK.

➤ Enter, or use List to select, the following values:

Type	**Reflux ratio**
Lower bound	**15**
Upper bound	**50**

As with Feed rate, Aspen Plus always varies the reflux ratio on a mole basis, even if you specify a Mass Reflux ratio on the Blocks B1 form.

➤ Click the Next button N→ on the Data Browser window toolbar to continue.

Aspen Plus displays the Required Input Complete dialog box, indicating that all required specifications are complete.

➤ Click Cancel.

By default, Aspen Plus displays results only for stages that have feeds, products, heaters, or a maximum or minimum flow, and for the stages immediately above and below those stages. You will modify the default stage report so that results are reported for all stages.

➤ To change the report, select Blocks B1 Report.

➤ Click on the Profile Options tab.

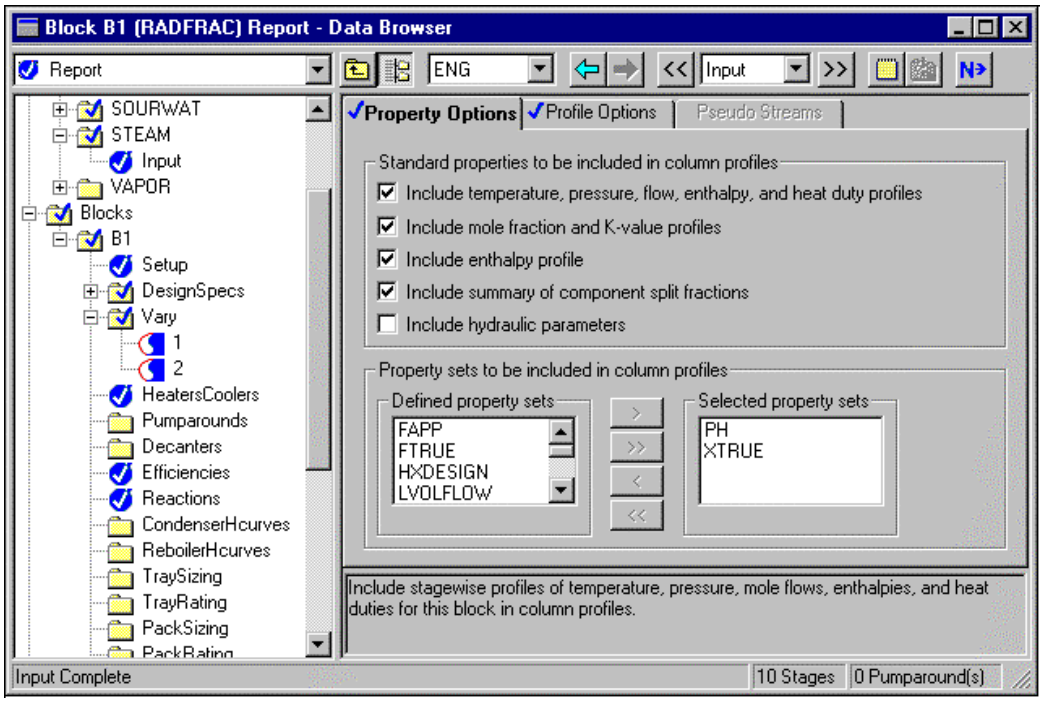
➤ On the Report Profile Options sheet, click the All Stages radio button.

By default, Aspen Plus reports only temperature, pressure, total mole flows, enthalpy, mole fractions and K-values for the selected trays. You can request that additional properties be reported by selecting additional property sets on the Property Options sheet.

You will specify that Aspen Plus report pH and true component mole fractions, using two built-in Property Sets.

➤ Click on the Properties tab.

➤ On the Report Properties sheet, move PH and XTRUE from the Defined property sets area to the Selected property sets area using the Move button >.



➤ Click the Next button N> on the Data Browser window toolbar to continue.

Running the Simulation

The Required Input Complete dialog box appears.

➤ Since you have entered all required specifications, click OK to run the simulation.

The Control Panel appears.

As the run proceeds, messages appear in the Control Panel. It takes a few minutes for Aspen Plus to process input specifications and perform the simulation.

As in session 1, Aspen Plus displays messages indicating that some properties have been retrieved from a special databank.

When the calculations finish, the message *Results Available* appears in the status area at the right of the main window toolbar.

➤ When the message *Results Available* appears in the toolbar, close the Control Panel by clicking the Close button.

You can now examine the results of your run.

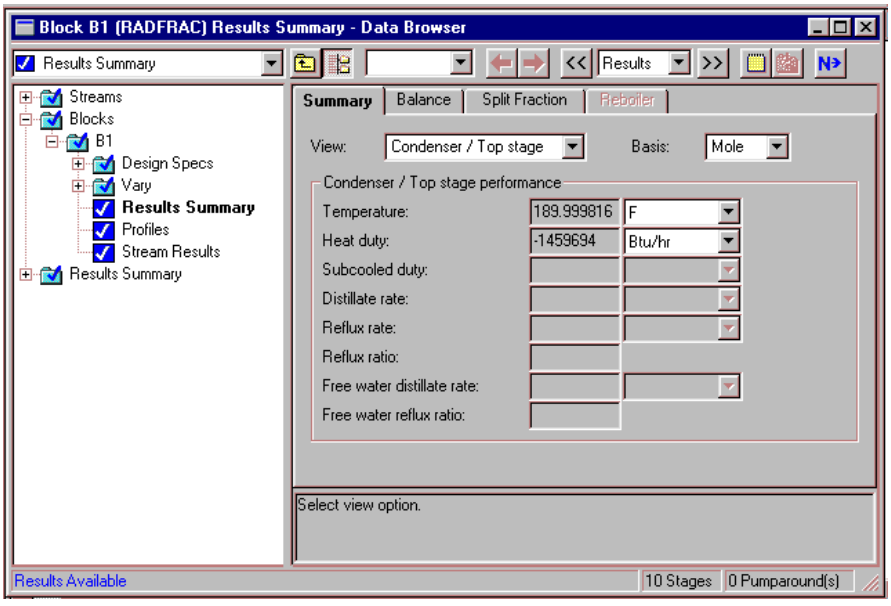
Examining Simulation Results

Aspen Plus generates many results for this simulation. You can examine any results of interest to you. This session guides you through a review of some of the simulation results.

To view RadFrac results:

- On the graphical simulation flowsheet, select the RadFrac block.
- To display the block shortcut menu, right-click inside the RadFrac block.
- Select Results from the menu.

The Blocks B1 Results Summary Summary sheet appears. This sheet reports the flows, temperatures, and duties for the top and bottom stage of the column.



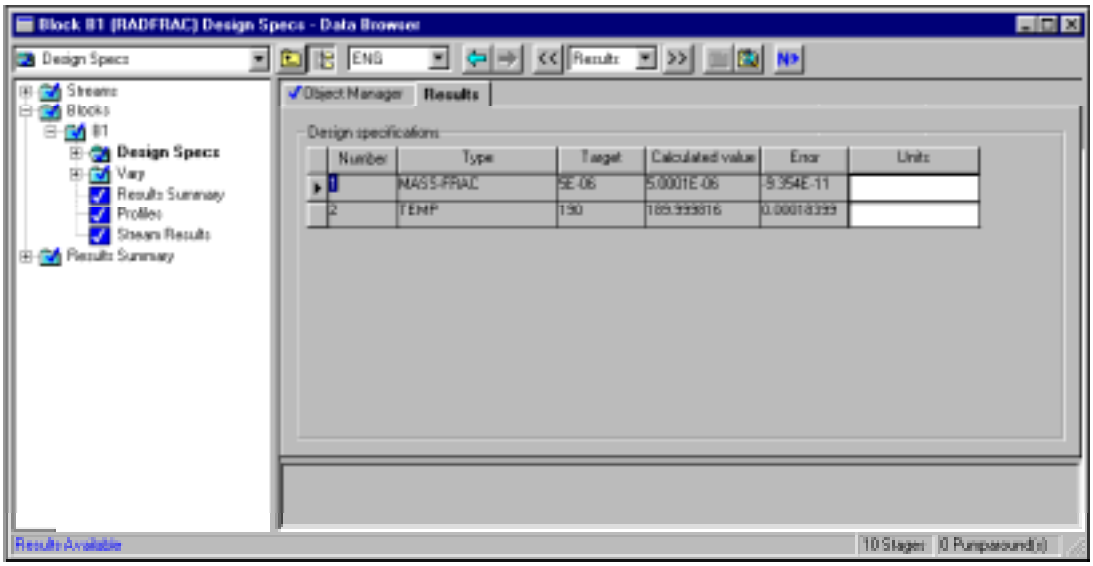
- Click the browse forward button >> to move to the next form with results.

The Balance sheet appears. The block is in mass balance, but is not in enthalpy balance, because heat is being removed from the RadFrac block in the condenser. The enthalpy would have balanced if you had assigned a heat stream to the condenser duty.

A summary of the results of the design specifications is located on the Design Specs Results sheet. This sheet reports the specified values and the final values for all of the design specifications. To view these results:

➤ Click the Design Specs folder in the Data Browser window.

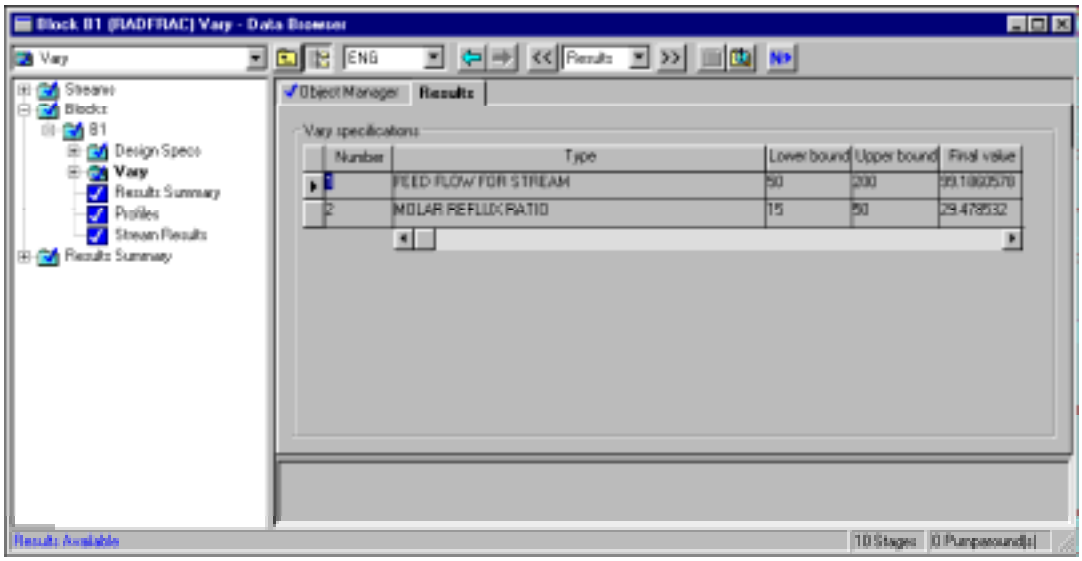
➤ Click the Results tab to view the Design Specs results.



A summary of the results of the manipulated variables is located on the Vary Results sheet. This sheet reports the specified bounds and the final values for all of the manipulated variables. To view these results:

➤ Click the Vary folder in the Data Browser window.

➤ Click the Results tab to view the Vary results.

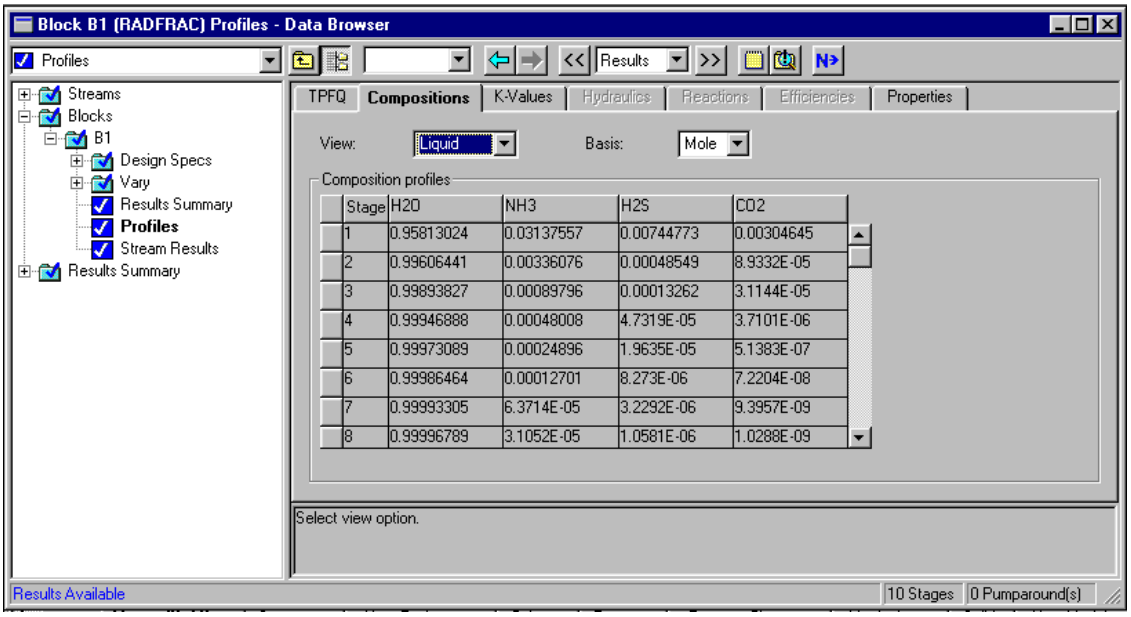


The Profiles Compositions sheet lists the mole fractions of each component for every stage. Since you chose the apparent component approach for this simulation, only the apparent components are reported. To view these results:

➤ Click the Profiles folder in the Data Browser window.

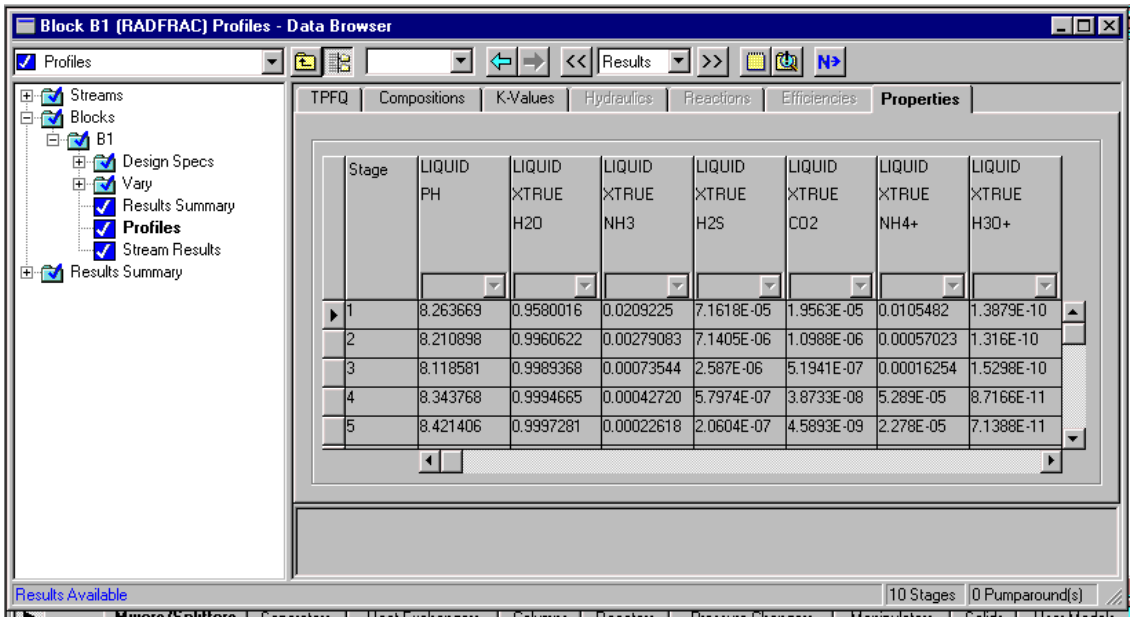
➤ Click the Compositions tab to view the results.

➤ Click the View list box and select Liquid.



The Profiles Properties sheet reports the actual composition of molecular components and ions. To view these results:

➤ Click the Properties tab.



Consider the results for Stage 1. The true composition of NH3 and NH4+ sum to 0.03147 on Stage 1. This value is slightly different from the apparent mole fraction of NH3 reported on the Compositions sheet: 0.03138. This slight difference is caused by the solution chemistry.

In general, the total number of moles is not conserved by solution chemistry. In this simulation, the fourth equilibrium reaction consumes 3 moles of reactants and generates two moles of products:

$CO2 + 2H2O <<===>> H3O+ + HCO3^-$

The total number moles on an apparent component basis will be different from the total number of moles on a true component basis. Thus X_{NH3} (apparent basis) is not exactly equal to X_{NH3} (true basis) + X_{NH4+} (true basis).

The liquid composition of apparent NH3 on stage 1 is:

X_{NH3} = 0.0314

➤ Click the Compositions tab.

➤ Click View and select Vapor.

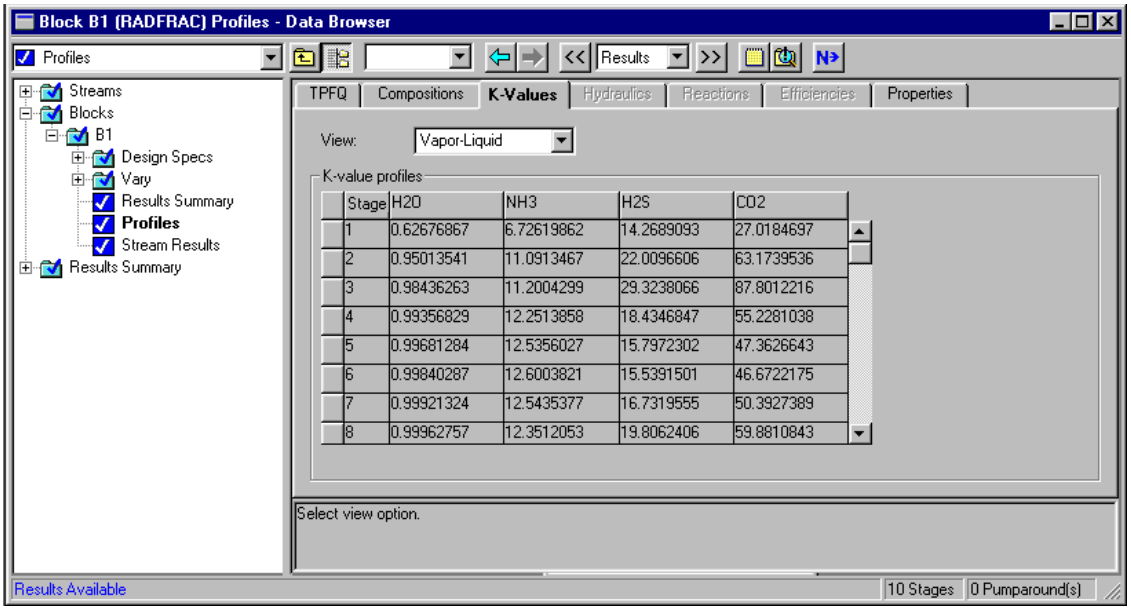
The vapor composition of apparent NH3 on stage is:

Y_{NH3} = 0.2112

From these two values, you can calculate a K-value for NH3 on stage 1:

$K = Y_{NH3}/X_{NH3} = 6.73$

➤ On the Blocks B1 Profiles form, click the K-Values tab.



The K-value for NH3 on stage 1 is 6.73. These results demonstrate that when you use apparent components, Aspen Plus also reports the K-values calculated by RadFrac (or any flash) on an apparent basis.

➤ Close all open windows.

Converting to True Components

Choosing between the true component approach and the apparent component is a matter of personal preference. For all problems, the simulation results should be equivalent. To demonstrate this, you will convert this simulation from the apparent component approach to the true component approach.

To convert the simulation to the true component approach, you must tell Aspen Plus to use the true component approach, and you must adapt the Design Spec in the RadFrac block (5 ppm mass apparent NH3 in the bottoms).

To tell Aspen Plus to use the true component approach:

- From the Aspen Plus Data menu, select Properties.
- Select the Use True-Components check box.

For the RadFrac block, you entered a desired specification of 5.0 ppm (mass) of apparent NH3 in the bottoms. However, this specification is incorrect for the true component approach, because a significant portion of the apparent NH3 is present as $NH4^+$.

To revise the RadFrac design specification to apply to the apparent composition of NH3:

- On the graphical simulation flowsheet, select the RadFrac block.
- To display the block shortcut menu, right-click inside the RadFrac block.
- Select Input from the menu.
- Click the Design Specs folder in the Data Browser window.

The Design Spec Object Manager appears.

- Select Design Spec ID 1, and click Edit.

The Design Spec Specifications sheet appears. You will modify Design Spec 1 to specify a stream property for the apparent mass fraction of NH3.

➤ In the Type field, use the drop-down list and select Property value to replace Mass purity.

➤ In the Value field, enter **5.0E-6**.

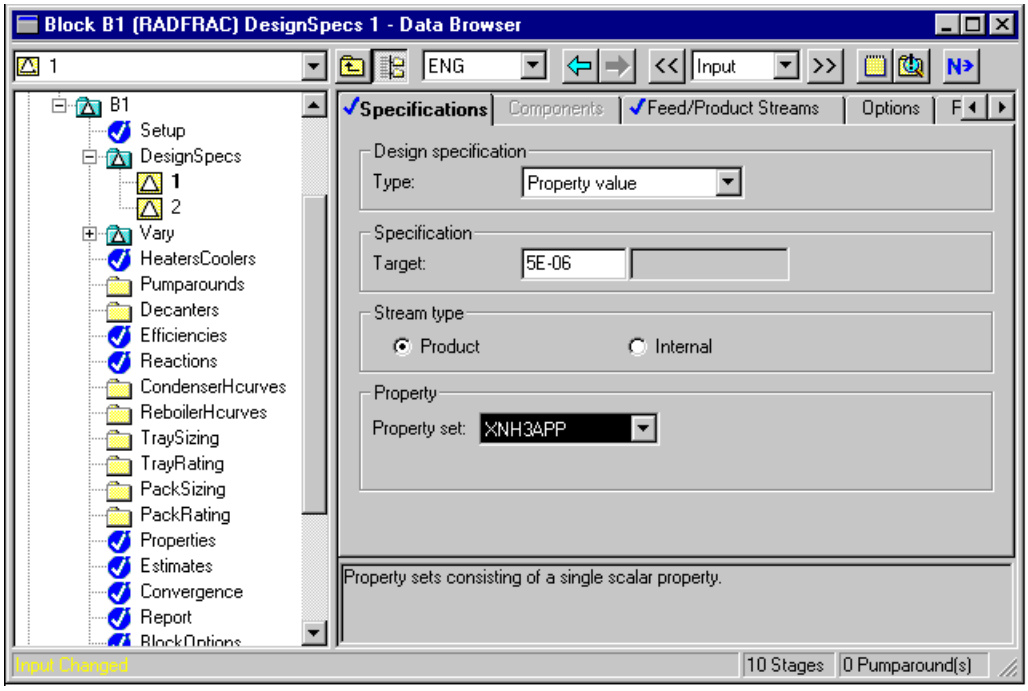
➤ In the Property set field, right-click and select New from the list.

➤ Enter **XNH3APP** as the New property set.

➤ Click OK.

➤ Click on the Feed/Product Streams tab.

➤ On the Feed/Product Streams sheet, move the BOTTOMS stream from the Available streams area to the Selected stream area using the Move button [>].



➤ Click the Next button to move to the next required input.

The Properties Prop-Sets XNH3APP form appears.

Aspen Plus will use this Property Set to calculate the apparent mass fraction of NH3 in the liquid phase.

- Click on the Search button.
- In the Search Physical Properties dialog box, type **apparent component mass fraction** in the field and click on the search button.
- Select **Apparent component mass fraction** alias WXAPP from the list of Physical property names that appears.
- Click on the Add button.
- Click on the Ok button.
- Click on the Qualifiers tab.
- Click in the Phase field on the Qualifiers sheet, and select **Liquid** from the list.
- Click in the Component field, and select **NH3** from the list.
- Click the Next button  on the Data Browser window toolbar to continue.

The Required Properties Input Complete dialog box appears.

- Click OK.

Running the True Component Simulation

A dialog box appears telling you that all specifications are complete and the simulation can be run.

➤ Click OK.

When the calculations finish, the message *Results Available* appears in the status area at the right of the Main Window toolbar.

➤ Close all open windows, and the Control Panel.

To view selected results of the true component simulation:

➤ On the graphical simulation flowsheet, select the RadFrac block.

➤ To display the block shortcut menu, right-click inside the RadFrac block.

➤ Select Results from the menu.

➤ Click the Profiles folder in the Data Browser window.

➤ Click the Compositions tab to view the results.

➤ Click the View list box and select Liquid.

This form reports the liquid phase mole fraction for all components, including the ions. Stage 1 reports the following compositions:

$X_{NH3} = 0.02093$

$X_{NH4+} = 0.01054$

➤ Select Vapor from the View field in the upper left corner of the sheet.

Note that all ions have a mole fraction of zero in the vapor phase. Stage 1 reports the following composition:

$Y_{NH3} = 0.21115$

From these values, a stage 1 K-value for NH3 can be calculated.

$K = Y_{NH3}/X_{NH3} = 10.09$

➤ On the Blocks B1 Profiles form, click the K-Values tab.

On stage 1, the reported K value for NH3 matches the value you just calculated. This demonstrates that when true components are used, the K-values calculated by RadFrac (or any flash) are also reported on a true basis.

Note that the K-value calculated in the apparent simulation is not equal to the K-value calculated in the true simulation due to the partial dissociation of ammonia.

The table below compares a number of the values calculated in the true component simulation and the apparent component simulation.

	Apparent	True
Condenser duty (BTU/HR)	-1.46E6	-1.46E6
Condenser Temperature (F)	190	190
Bottom Stage Temperature (F)	213	213
Steam Feed Rate (lb/hr)	1787	1787
Molar Reflux Ratio	29.5	29.4

All values are virtually identical. This demonstrates that the results calculated by the true approach and the apparent approach are equivalent, even if they are not numerically equal.

Exiting Aspen Plus

To exit from Aspen Plus:

➤ From the File menu, select Exit.

➤ When the dialog box appears asking if you want to save the run, select No to exit without saving the run;
– or –
select Yes if you want to save the run, and enter a Run ID when prompted.

This simulation (using the apparent approach) is delivered as backup file *elec2* in the Aspen Plus Examples Library. You can use this backup file to check your results.

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A Connecting to the Aspen Plus Simulation Engine

If either of the following conditions exist, you will be prompted to specify the host computer for the Aspen Plus simulation engine after you start the Aspen Plus User Interface:

- The simulation engine is not installed on your PC.
- The simulation engine is installed on your PC, but the Activator security device is not connected to your PC.

In these cases, the Connect to Engine dialog box appears.

➤ Click the Server Type list box and select the type of host computer for the simulation engine.

If you choose Local PC as the server for the simulation engine, you do not need to enter any more information into the dialog box.

➤ Click OK to continue.

If you choose UNIX host, OpenVMS host, or Windows NT server as the server for the simulation engine:

➤ Enter the node name of the computer on which the Aspen Plus simulation engine will execute.

➤ Enter your User Name, Password, and Working Directory, and click OK.

When the network connection is established, a message box appears saying Connection Established.

If the Connection Established message does not appear, see your Aspen Plus system administrator for more information on network protocols and host computers for the Aspen Plus simulation engine.