Aspen Plus®

Getting Started Modeling Processes with Electrolytes

Version 10.2

Aspen Technology, Inc.

Part Number: Aspen Plus® 10.2
February 2000

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

Aspen Plus Installation Guide for Windows This guide provides instructions on installation of Aspen Plus.

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 Getting Started Modeling Processes with Solids This tutorial includes several hands-on sessions to familiarize you with simulating systems containing solids 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*
- *Input Language Guide*

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   AspenTech customers with a valid license and software maintenance agreement can register to access the **Online Technical Support Center** at **http://support.aspentech.com/**

This web support site allows you to:

- Access current product documentation
- Search for tech tips, solutions and frequently asked questions (FAQs)
- Search for and download application examples
- Submit and track technical issues
- Send suggestions
- Report product defects
- Review lists of known deficiencies and defects

Registered users can also subscribe to our Technical Support e-Bulletins. These e-Bulletins are used to proactively alert users to important technical support information such as:

- Technical advisories

- Product updates and Service Pack announcements

The most up-to-date contact information for your nearest support office is also available on AspenTech's web page at **http://support.aspentech.com/**

The following contact information was current when this product was released:

If you are located in:	Phone Number	Fax Number	E-Mail Address
North America & the Caribbean	+1-617/949-1021	+1-617/949-1724	support@aspentech.com
	+1-888/996-7001 (toll free)		
South America (Argentina office)	+54-11/4393-5308	+54-11/4394-8621	tecnoba@aspentech.com
(Brazil office)	+55-11/5012-0321	+55-11/5012-4442	tecnosp@aspentech.com
Europe, Gulf Region, & Africa (Brussels office)	+32-2/724-0100	+32-2/705-4034	atesupport@aspentech.com
(UK office)	+44-1223/312220	+44-1223/366980	
Japan	+81-3/3262-1743	+81-3/3262-1744	atjsupport@aspentech.com
Asia & Australia (Singapore office)	+65/295-83-30	+65/295-83-25	atasupport@aspentech.com

1   Modeling Electrolyte Chemistry

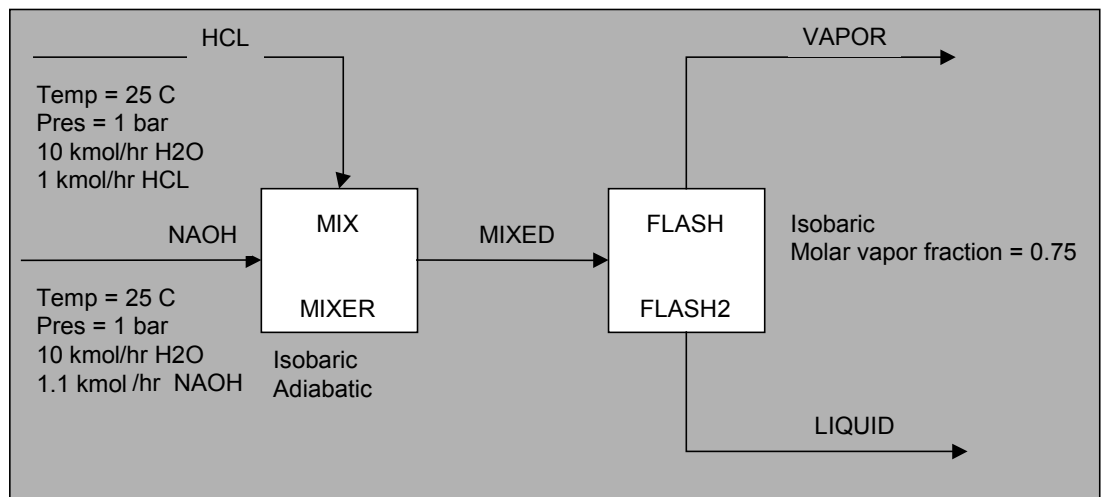In this simulation mix and flash two feed streams containing aqueous electrolytes.

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 simulation.

Electrolyte Chemistry Flowsheet

The process flow diagram and operating conditions for this simulation 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. Use the MIXER model for the mixer and the FLASH2 model for the flash.

HCL

VAPOR

Temp = 25 C
Pres = 1 bar
10 kmol/hr H2O
1 kmol/hr HCL

MIX
MIXER

NAOH

MIXED

FLASH
FLASH2

Isobaric
Molar vapor fraction = 0.75

Temp = 25 C
Pres = 1 bar
10 kmol/hr H2O
1.1 kmol /hr NAOH

Isobaric
Adiabatic

LIQUID

Electrolyte Chemistry

Starting Aspen Plus

To start Aspen Plus:

1. From your desktop, select Start and then select Programs.

2. Select AspenTech, then Aspen Plus 10.2, 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, use an Aspen Plus template.

To select the Template option:

1. Select the Template radio button and click [OK] .

   The **New** dialog box appears.

   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:

1. Select the Electrolytes with Metric Units template.

   Note The default Run Type, Flowsheet, is appropriate for this simulation.

2. Click ` OK ` to apply these options.

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

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

The **Aspen Plus** window is now active.

Drawing the Graphical Simulation Flowsheet

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

1. From the Aspen Plus menu bar, select Tools and then select Options.
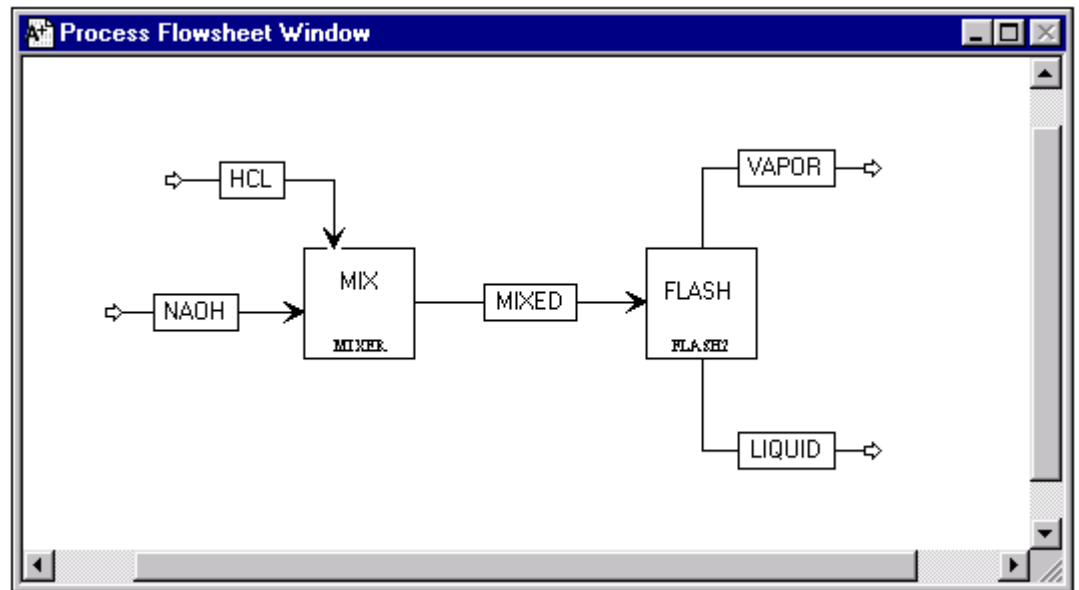
   The **Options** dialog box appears.

2. Select the **Flowsheet** tab.

3. Deselect the Automatically Assign Block Name with Prefix and the Automatically Assign Stream Name with Prefix options.
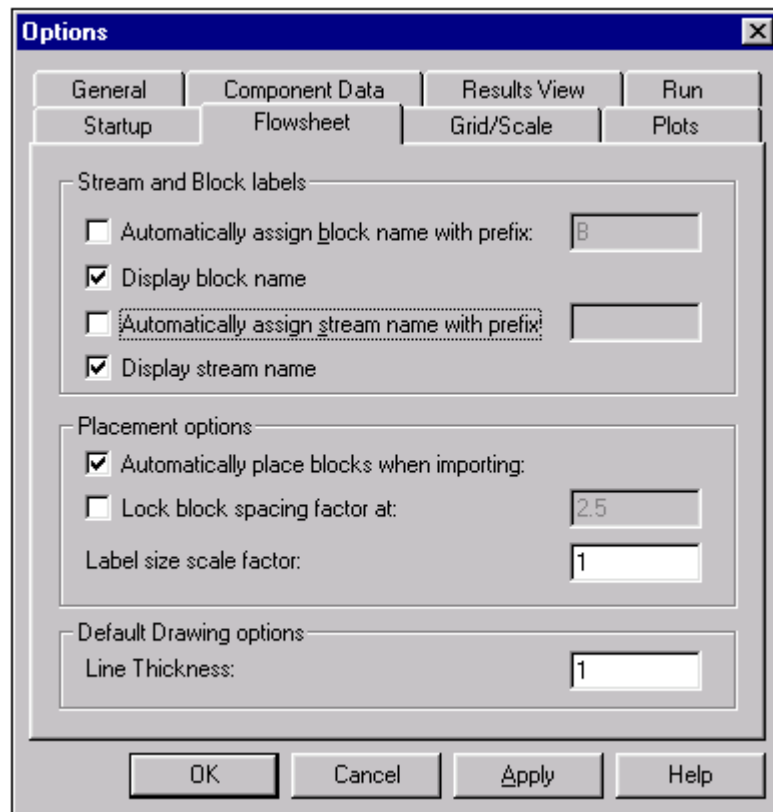
4. Click [OK] to close the **Options** dialog box and apply the changes.

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

5. Place the flowsheet blocks and streams to create the graphical simulation flowsheet as follows:

6. Click [N→] to guide you to the next required input.

The **Flowsheet Complete** dialog box appears.

7. 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 sheets.

Use this sheet 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 template.

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

It is always good practice to enter a title for the simulation.

1. In the Title field, enter Getting Started with Electrolytes - Simulation 1.

   The Electrolytes with Metric Units application type sets the following global defaults for electrolytes applications:
   - The Input data and Output results fields are populated with METCBAR units (Metric units with temperature in degrees Centigrade and pressure in bars)
   - The Flow basis field is populated with Mass for all flow inputs

To specify flows on a mole basis for this simulation:

1. At the Flow basis field, click [▼] and select Mole.
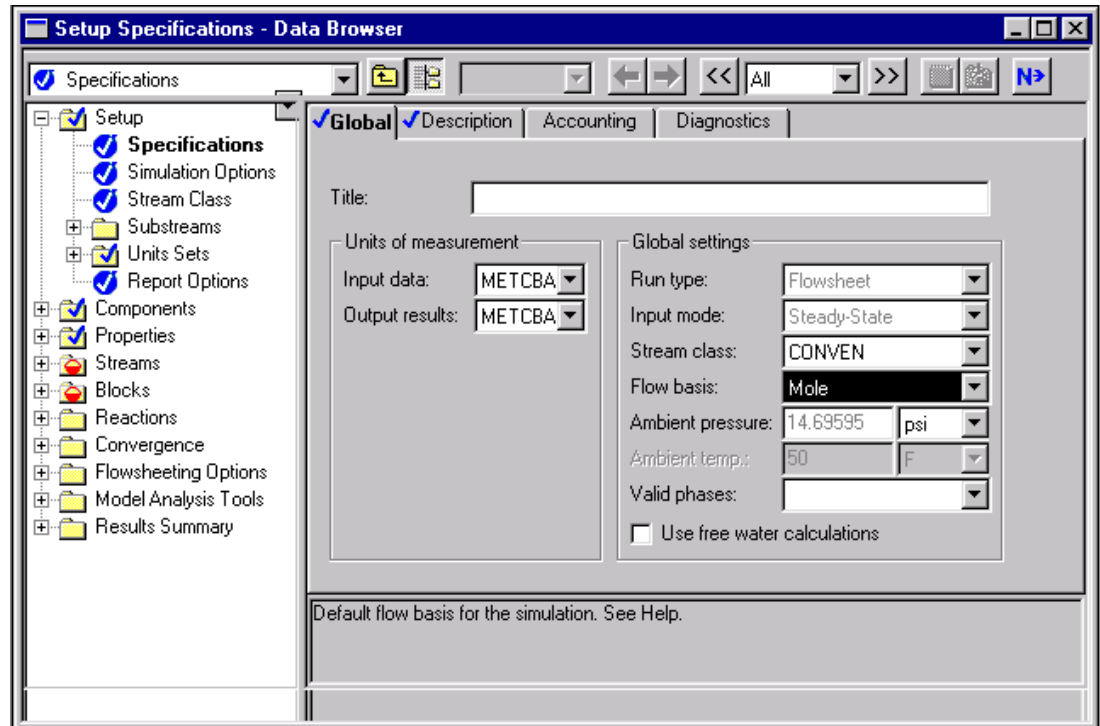
Based on the Electrolytes with Metric Units template, Aspen Plus displays the following defaults for calculating and reporting stream properties:

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

To review the report options specified in the selected template:

1. From the Data Browser, select the **Setup Report Options** sheet.

2. Select on the **Stream** tab.

Note   You will return to this sheet and specify stream properties later in this simulation.

To move to the next required input:

1. From the Data Browser, select the **Components** folder and then select Specifications.
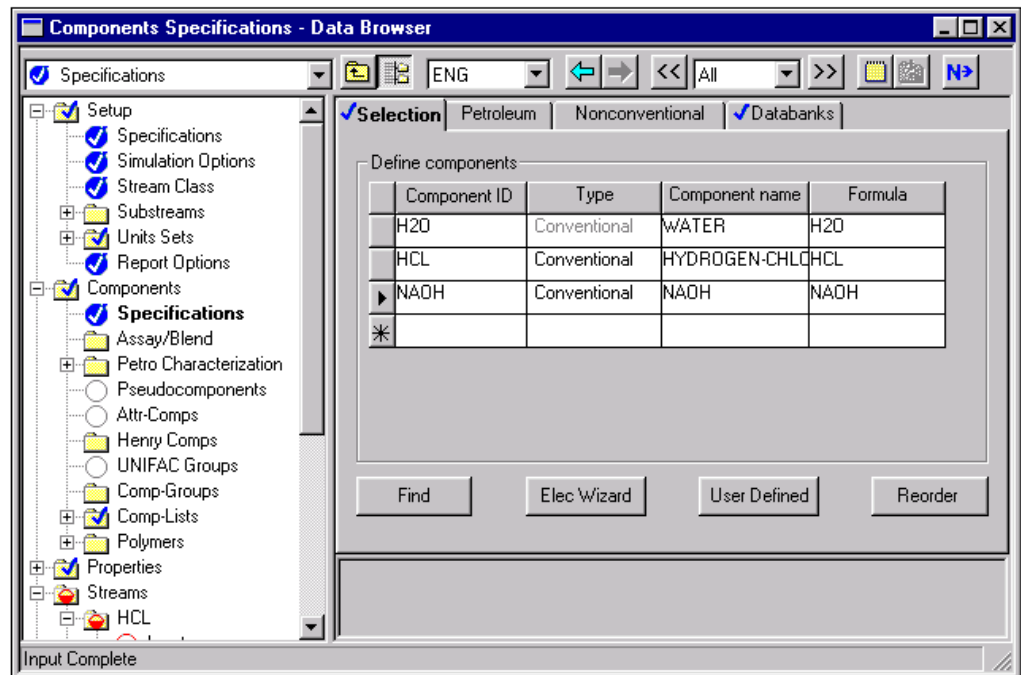
Specifying Components

The **Components Specifications Selection** sheet appears.

The apparent (or base) components for this simulation are H₂O, HCL, and NaOH.

Note   Because you chose an electrolytes template, water already appears on the sheet.

1. Enter the remaining components (HCL and NAOH) as following:

H2O	Water
HCL	Hydrogen-Chloride
NAOH	NAOH

To rename H20 to water:

1. In the Component ID field, select H20 and enter Water.

2. When the **Aspen Plus** dialog box appears, click Rename .

3. Click Elec Wizard .

The **Electrolytes Wizard** dialog box appears.

**Note** Use this wizard for defining automatic chemistry generation.

The Electrolytes Wizard

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.

1. From the **Electrolytes Wizard** dialog box, click [Next >] .

   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.

2. Click [>>] to move all components in the **Available components** column to the **Selected components** column.

3. Click [Next >] to continue.
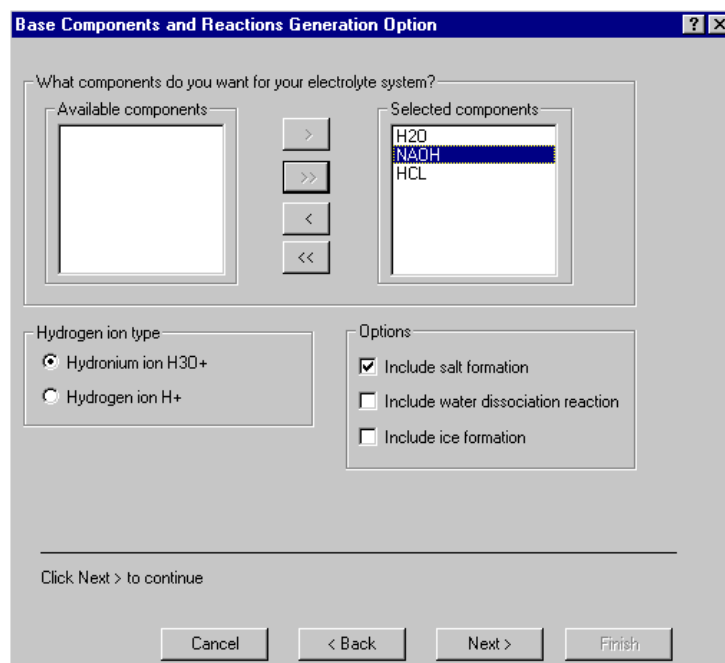
The **Generated Species and Reactions** dialog box appears:
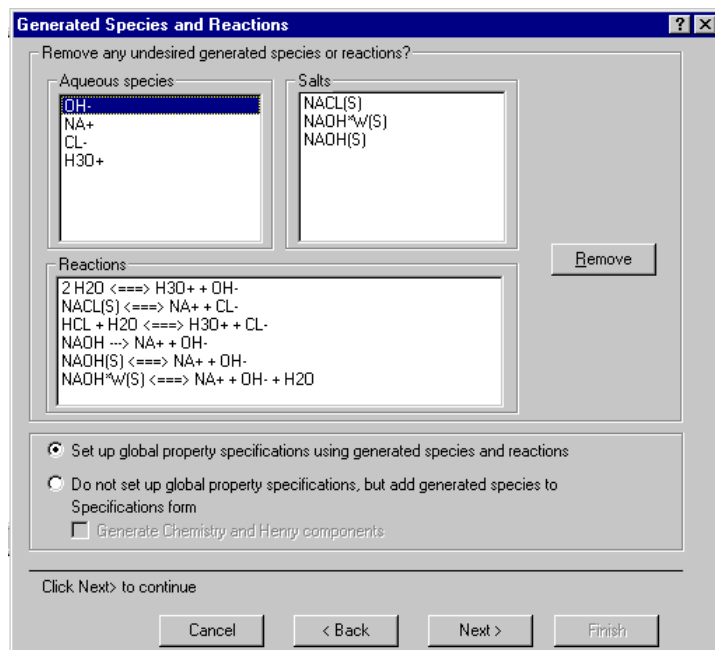
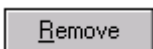Aspen Plus generates all possible ionic and salt species, and reactions for the H2O-NAOH-HCL system.

In the Reactions section in the **Generated Species and Reactions** dialog box, different style arrows denote the following reaction types:

<<===>>   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.

4. Click [Remove] to eliminate any of the generated species and reactions.

Note   In this simulation, the NaOH and the NaOH*W salts are not relevant.

To remove these salts from the solution chemistry:

1. From the Salts list, select NaOH(S) and NaOH*W(S).

2. Click Remove .

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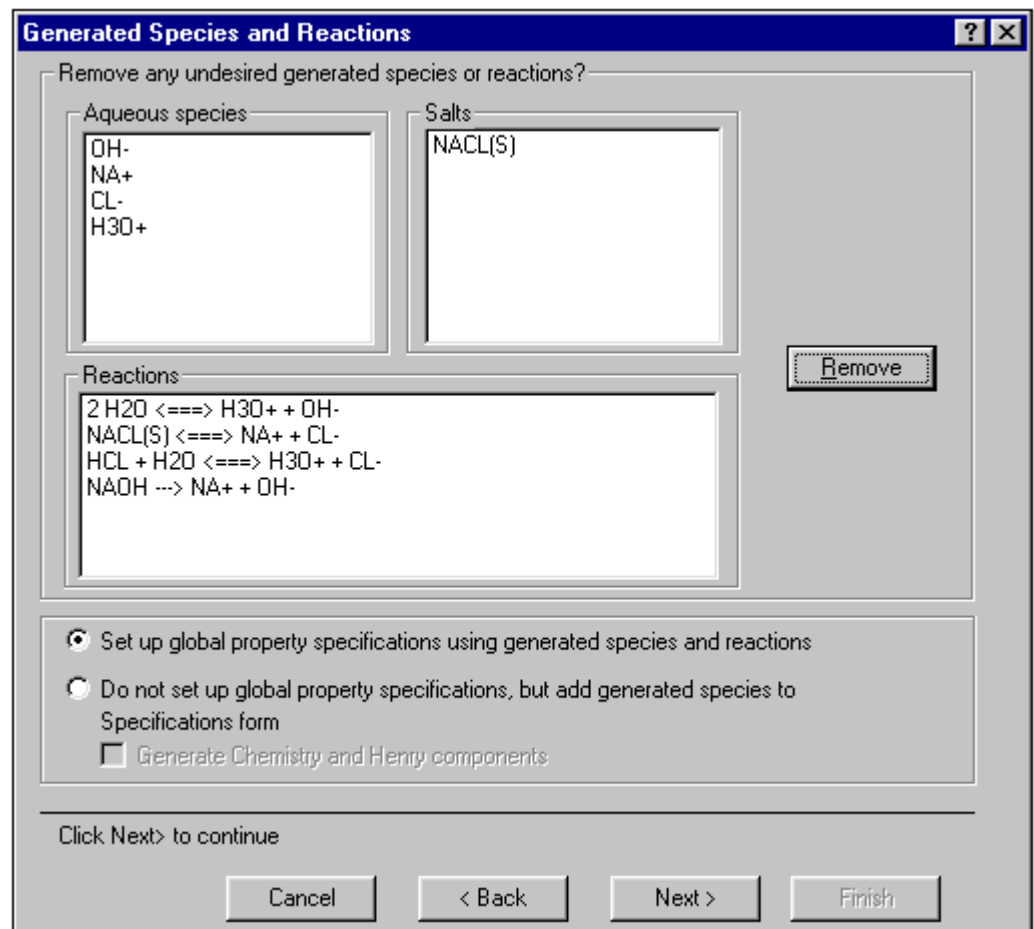
Note Any time you know that a reaction can be neglected
because of expected process conditions, remove it from the
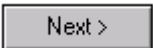solution chemistry to decrease the execution time required
for your simulation.

3. On the **Generated Species and Reactions** dialog box click [Next >] 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.

4. Select the radio button next to the True component approach field.

   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 sheeted 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 simulation.

5. Click [Next >] to move to the next dialog box.

   The **Summary** dialog box appears, providing Aspen Plus electrolytes expert system information.

6. 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 automatically retrieves all relevant physical property parameters. Note that the salt NACL(S) is identified as type Solid.
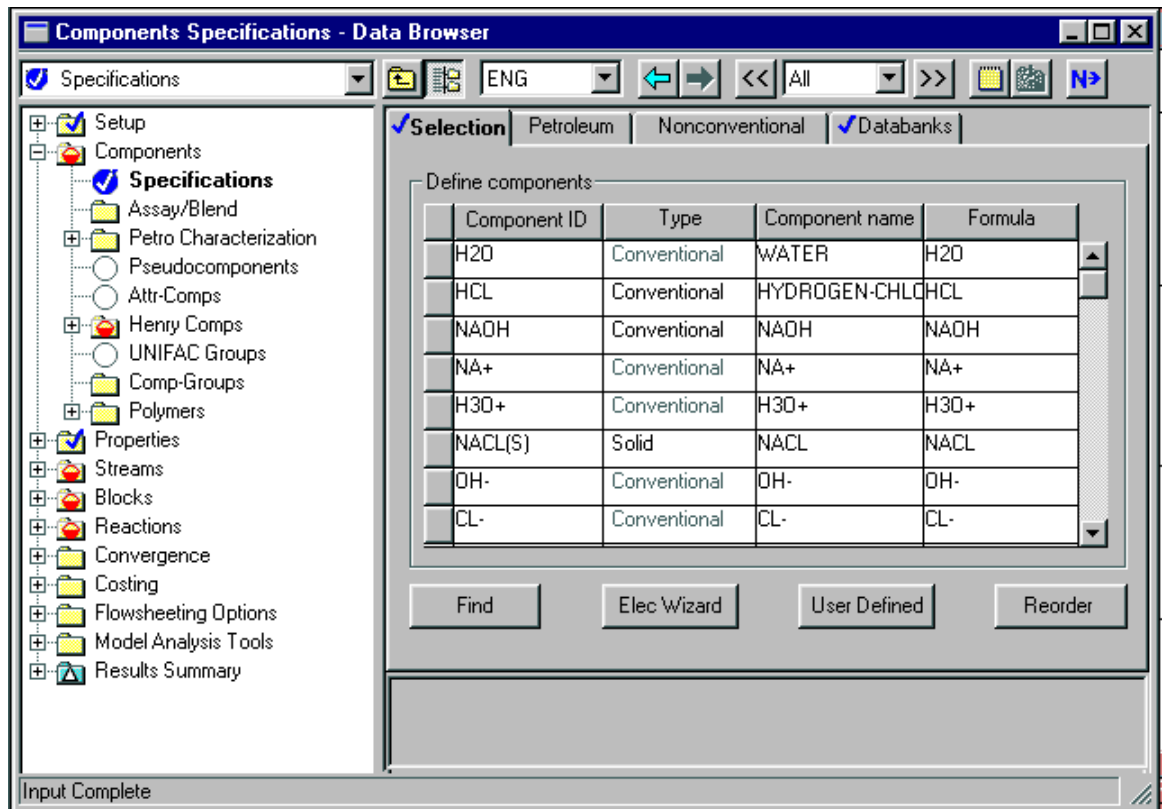
7. Click to continue.

The **Components Henry Comps Global** sheet appears, which was defined by the Electrolytes Wizard. Use this sheet to 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 sheet.

Examining Generated Chemistry

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

To examine the generated Chemistry:

1. From the Data Browser, select the **Reactions** folder.

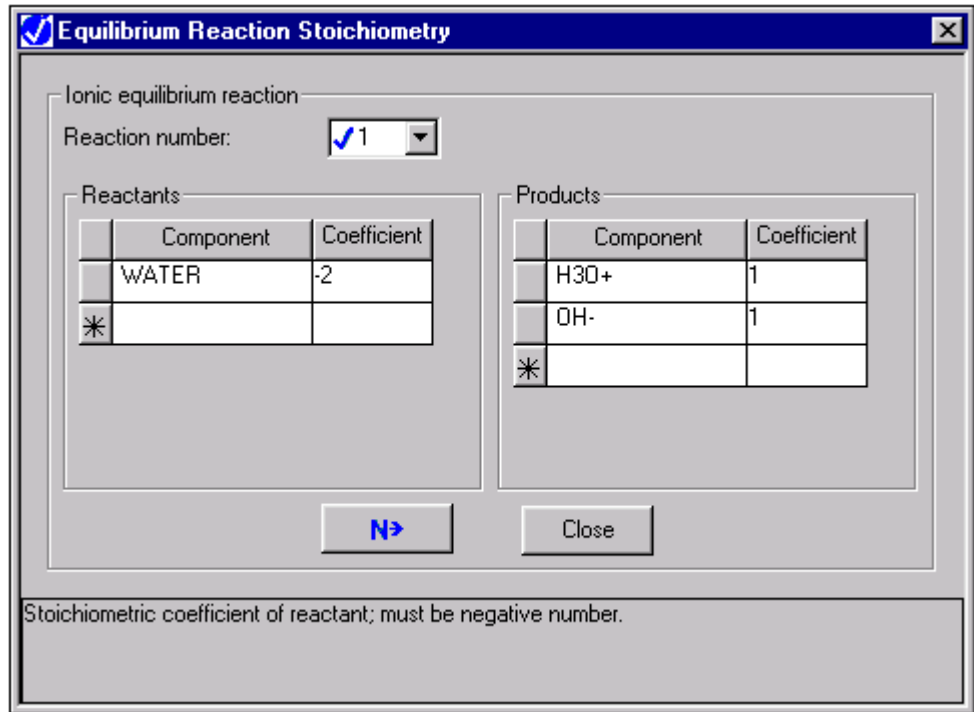2. From the **Reactions** folder, select Chemistry and then Global.

The **Reactions Chemistry Global** sheet appears:
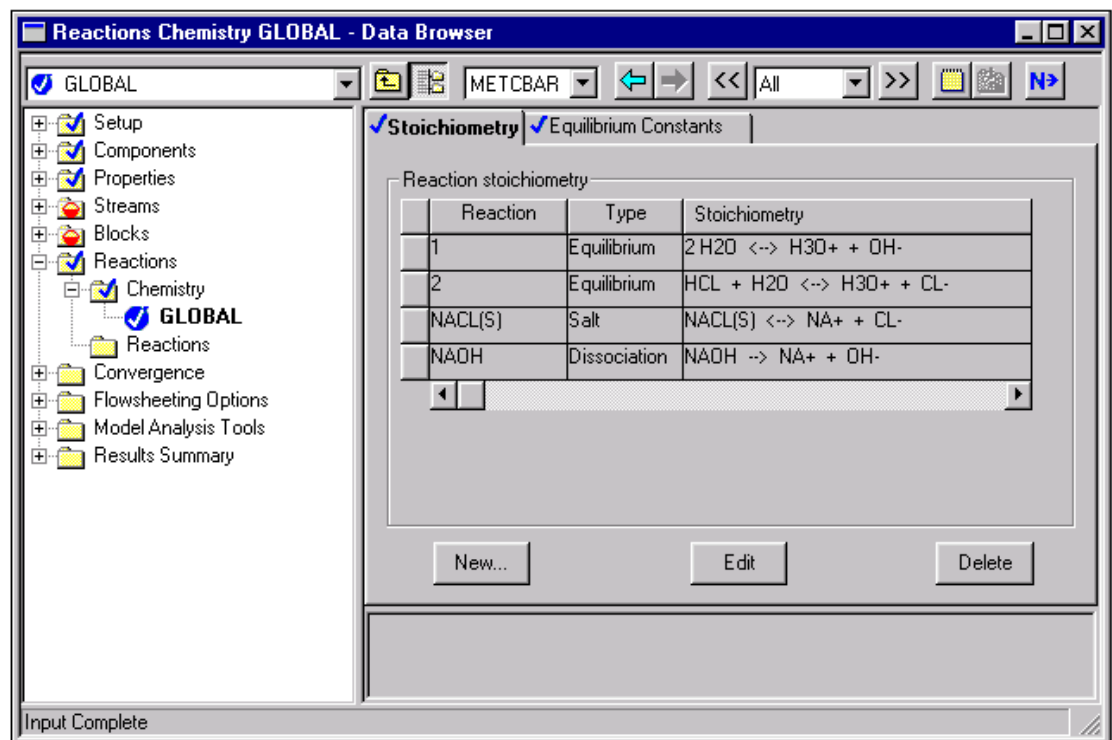
**To view a particular reaction:**

1. Select a Reaction and click [Edit] .

The **Equilibrium Reaction Stoichiometry** dialog box appears, with the data for the selected reaction.

The first equilibrium ionic reaction shown is for water dissociation.

2. Close the dialog box and view the other reactions using the same steps.

3. Select the **Equilibrium Constants** sheet.

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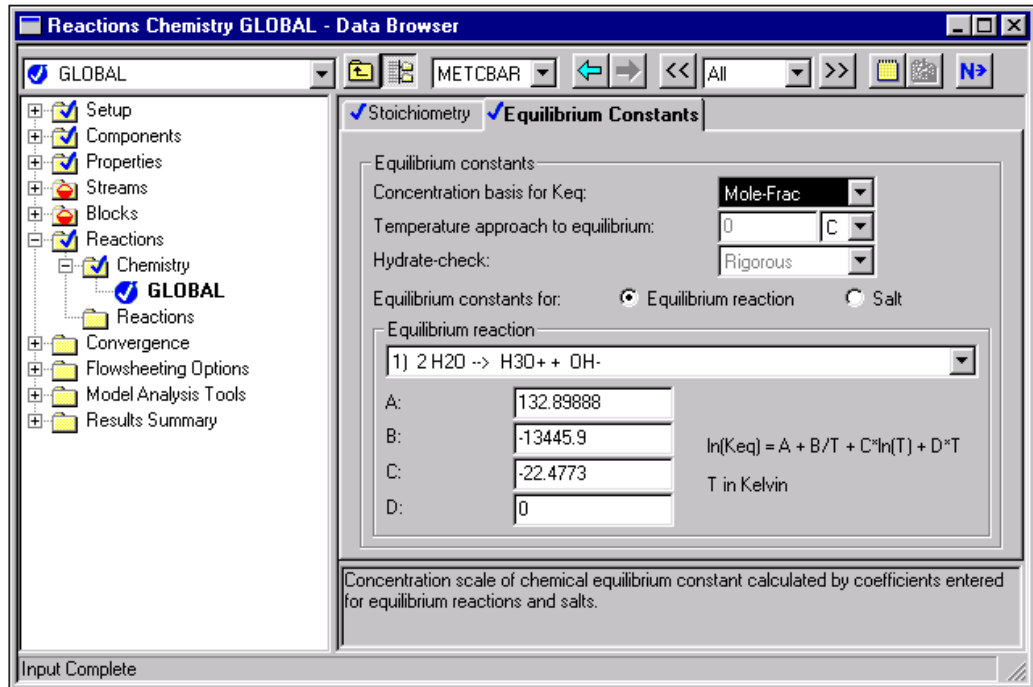
The Aspen Plus reactions database contains over 600 reactions, which cover virtually all common electrolyte applications.

4. Click ⬛ 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:

1. At the Equilibrium constants for field, select the radio button next to the Salt field.

2. Click ⬛ 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.

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

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.

1. From the Data Browser, select the **Properties** folder and then select Specifications.

The **Properties Specifications Global** sheet appears. The Electrolytes Wizard has already completed this sheet:
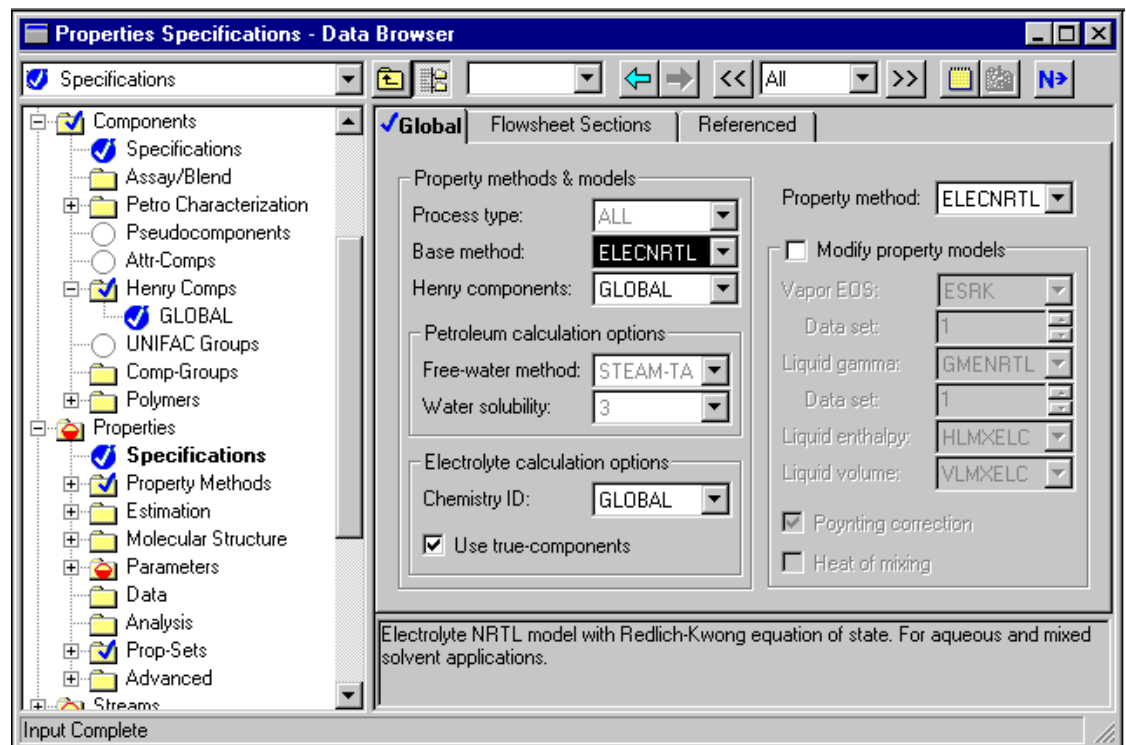
The Electrolyte-NRTL activity coefficient model, ELECNRTL, is the recommended option set for simulations with electrolytes. ELECNRTL calculates liquid phase properties from the Electrolyte-NRTL activity coefficient model. Vapor phase properties are calculated from the Redlich-Kwong equation of state.

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 values, Aspen Plus provides reasonable default values.

2. Click ![N→] to continue.

The **Binary Interaction HENRY-1** sheet appears.

Use this sheet to view the Henry's Law parameters retrieved by the electrolytes expert system. If you had your own Henry's Law parameters, enter them on this sheet.

3. Click ![N→] to continue.

The **Binary Interaction VLCLK-1** sheet appears.

Use this sheet to view the Clarke density parameters retrieved by the electrolytes expert system. If you had your own Clarke density parameters, enter them on this sheet.

4. From the Data Browser, select the **Electrolyte Pair** folder.

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

5. Click ![N→] to continue.

The **Electrolyte Pair GMELCC-1 Input** sheet appears.

6. Click ![N→] to continue.

The **Electrolyte Pair GMELCD-1 Input** sheet appears.
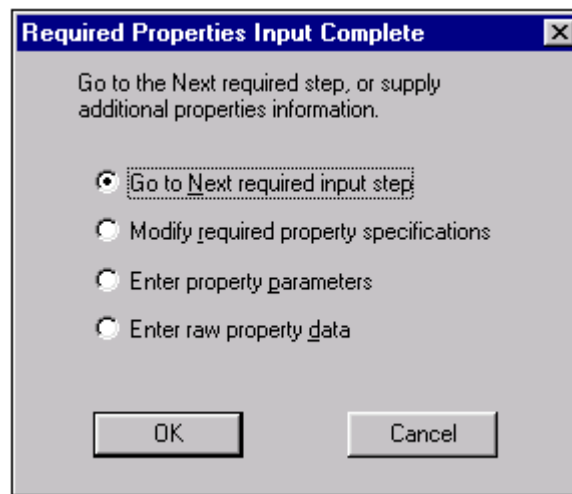
7. Click ![N→] to continue.

The **Electrolyte Pair GMELCE-1 Input** sheet appears.

8. Click ![N→] to continue.

The **Electrolyte Pair GMELCN-1 Input** sheet appears.

9. Click ![N→] 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 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, 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. Use all Aspen Plus unit operation models in an electrolytes simulation.

10. Click [OK] to move to the next required input.

Entering Stream Data

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

1. On the **Streams HCL Input Specifications** sheet, enter 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 simulation, 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.

2. Click [N→] to continue.

    The **Streams NAOH Input** sheet appears.

3. On the **Streams NAOH Input Specifications** sheet, enter the following:

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

4. Click [N→] to continue.

Specifying the Flash Block

The **FLASH Input Specifications** sheet appears. For this simulation, specify the pressure drop and vapor fraction.

1. In the Temperature field, click [▼], select Vapor fraction, and then enter 0.75.

2. In the Pressure field, enter 0 (indicating there is no pressure drop).

3. Click [N→] to continue.

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

4. Click [N→] to continue.

   The **Required Input Complete** dialog box appears informing you that all required input is complete and asking if you want to run the simulation.

   Before running the simulation, request that certain optional properties be included in the stream report.

5. Click [Cancel] to close the dialog box without running the simulation.

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:

1. From the Data Browser, select the **Setup** folder and then select Report Options.

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

2. Select the **Stream** tab.

3. Under Fractions Basis, select the checkbox next to Mass.
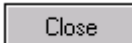
   You can also define additional stream properties to be calculated and reported, using Aspen Plus Property Sets. Aspen Plus provides a number of built-in Property Sets based on the Application Type you selected. You can also define your own Property Sets. In this simulation, you will use a built-in Property 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.

4. Click [Property Sets].

The **Property Sets** dialog box appears.

5. From the **Available Property Sets** column, select TBUBBLE and WXAPP.

6. Click [>] to move the selected property sets to the **Selected Property Sets** column.
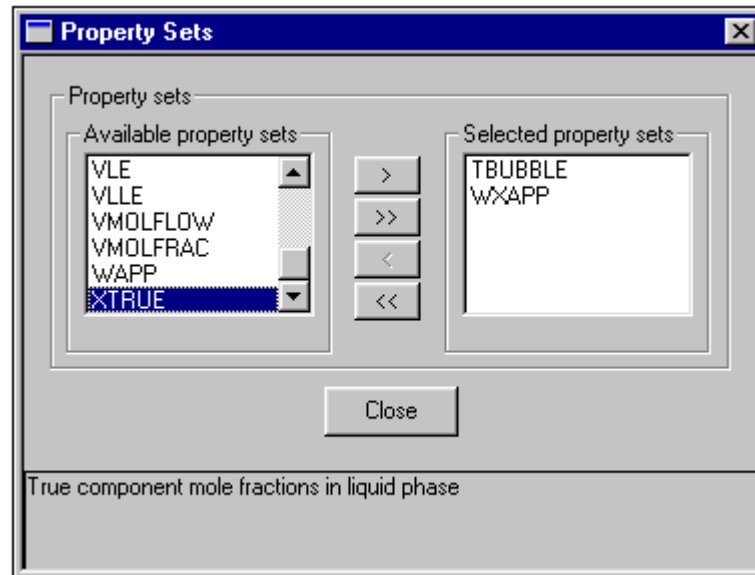
7. Click [Close] .

8. Click [N⇒] to continue.

Running the Simulation

The **Required Input Complete** dialog box appears.

1. 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 persheet the simulation.

    Aspen Plus has a special databank it searches only when you use the ELECNRTL option set, as in this simulation. 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.

2. Use the vertical scrollbar to the right of the Control Panel window to see the messages.

3. Examine the results of your run.

Examining Simulation Results

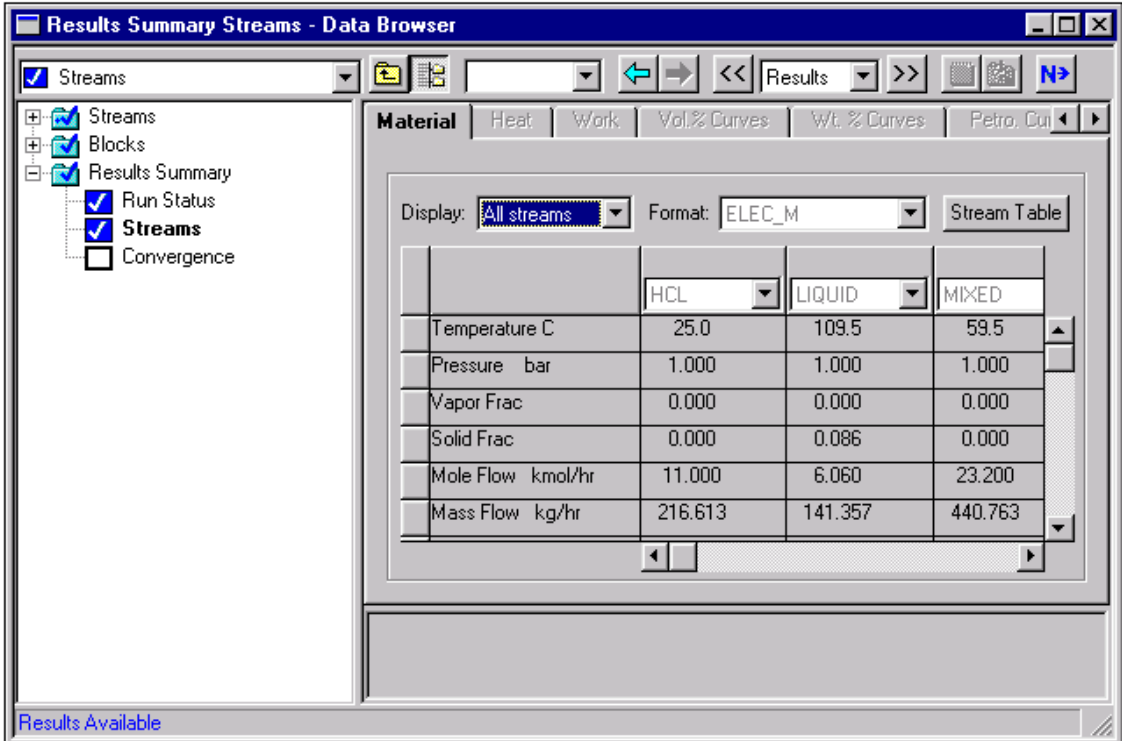**To view the results of the simulation:**

1. From the Control Panel, click [✓].

   The **Run Status Summary** sheet appears, indicating that the simulation completed normally.

2. Click [>>] to move to the next results sheet.

   The **Results Summary Streams** sheet appears.

3. Review the results on this sheet.

4. Use the horizontal scrollbar on the bottom of the sheet 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 sheet Stream MIXED. Because water dissociation is included as one of electrolytes reactions, MIX allows $H3O^+$ and OH^- to recombine to sheet 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 sheet 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.

Note   This simulation has other Results sheets. Click to view them, if you choose.

Exiting Aspen Plus

To exit from Aspen Plus:

1. From the Aspen Plus menu, select File and then select Exit.

   The **Aspen Plus** dialog box appears.

2. Click No .

   – or –

   Click 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 *elec1* in the Aspen Plus Examples Library. Use this backup file to check your results.

❖   ❖   ❖   ❖

2   Modeling a Sour Water Stripper

In this simulation, 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 simulation.

Sour Water Stripper Flowsheet

The process flow diagram and operating conditions for this simulation 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. Use RadFrac to simulate the stripper.
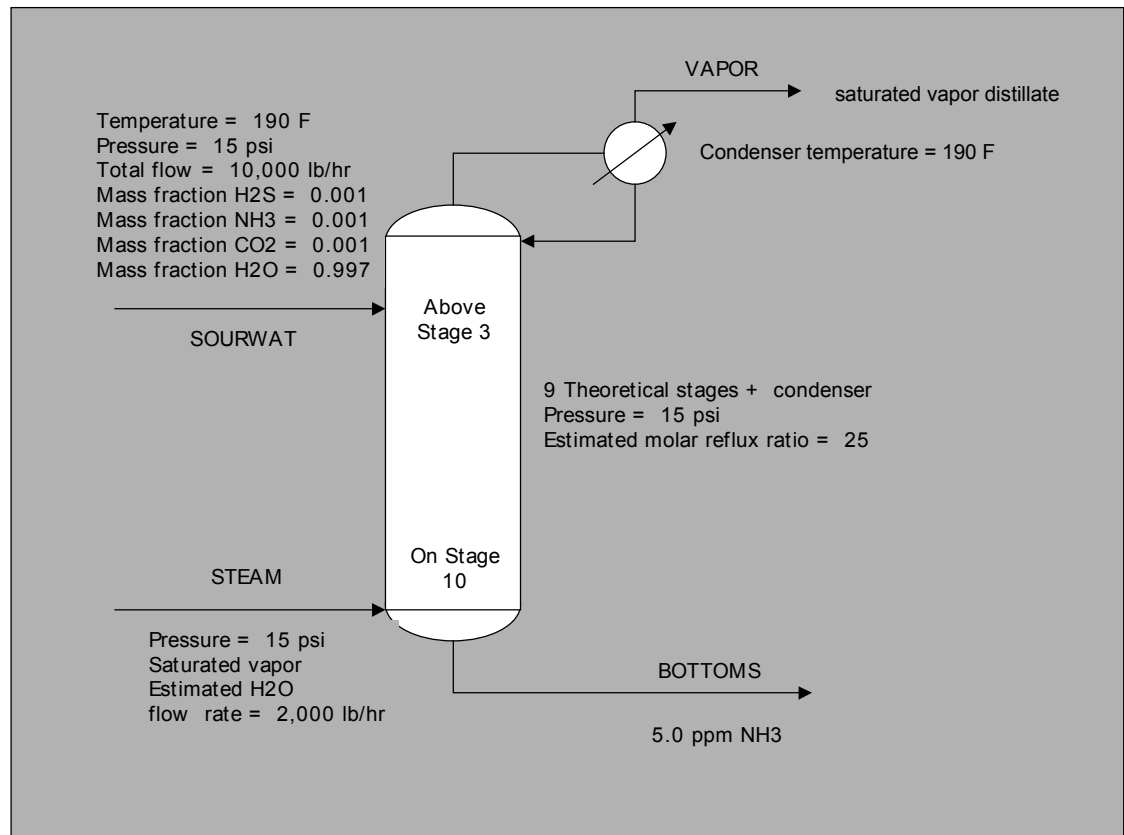
Process Diagram: Sour Water Stripper

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:

1. From your desktop, select Start and then select Programs.

2. Select AspenTech, then Aspen Plus 10.2, 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, use an Aspen Plus template.

To select the Template option:

1. Select the Template radio button and click [OK] .

    The **New** dialog box appears.

    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:

1. Select the Electrolytes with English Units template.

    Note   The default Run Type, Flowsheet, is appropriate for this
             simulation.

2. Click [OK] to apply these options.
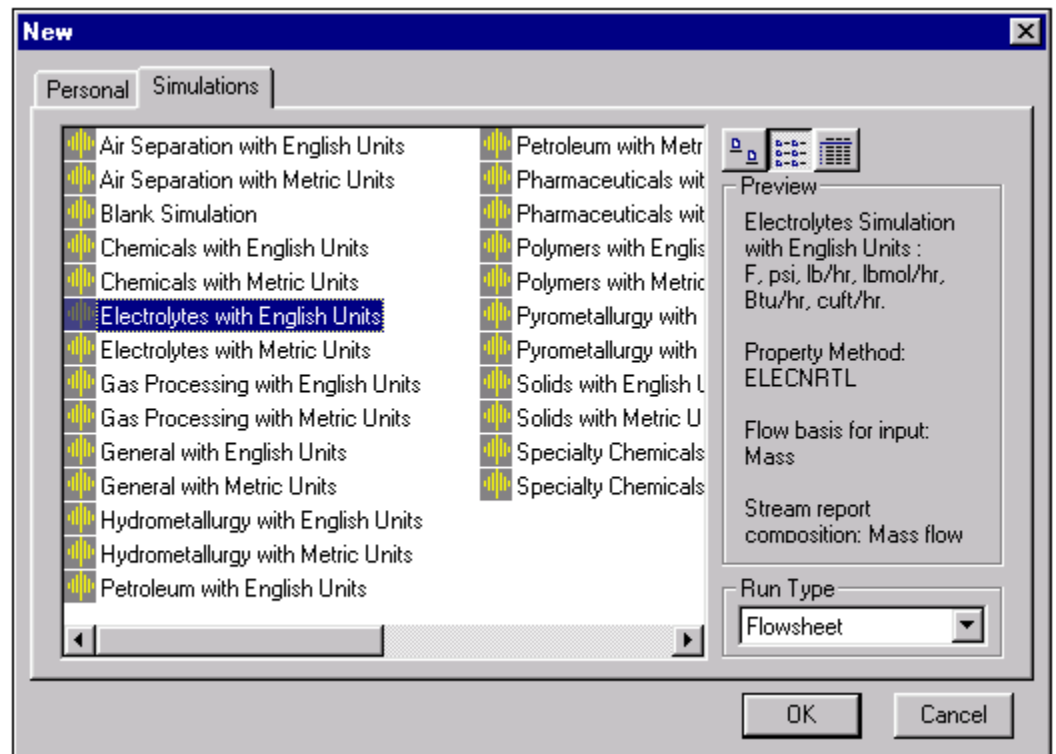
It will take a few seconds for Aspen Plus to apply these options.

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

The **Aspen Plus** window is now active.

Drawing the Graphical Simulation Flowsheet

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

1. From the Aspen Plus toolbar, select Tools and then select Options.

   The **Options** dialog box appears.

2. Select the **Flowsheet** tab.

3. Deselect the Automatically Assign Block Name with Prefix and the Automatically Assign Stream Name with Prefix options.
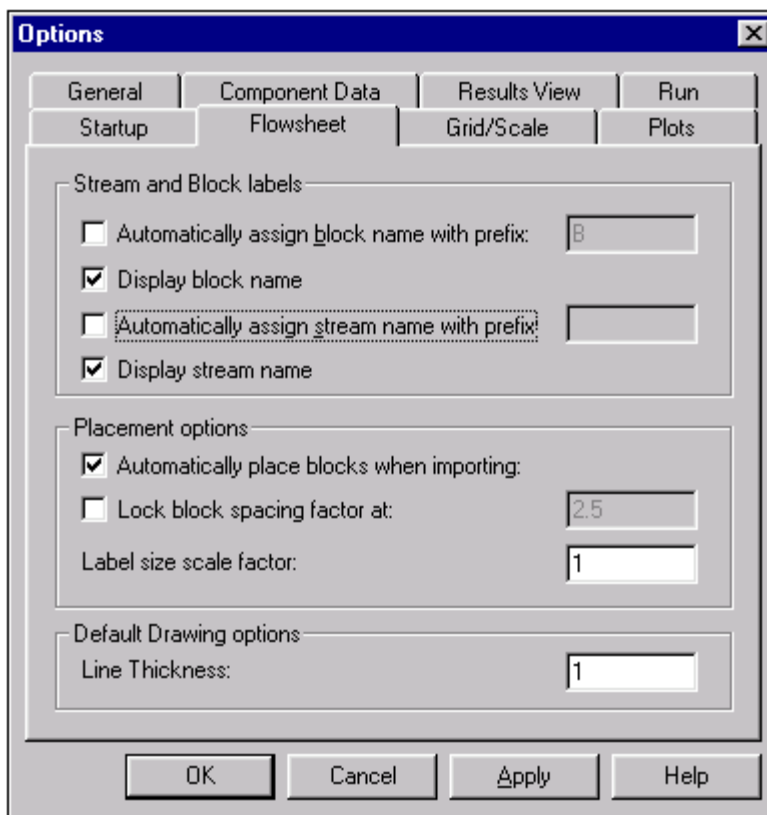
4. Click [OK] to close the **Options** dialog box and apply the changes.

5. Place the flowsheet blocks and streams to create the graphical simulation flowsheet as follows:
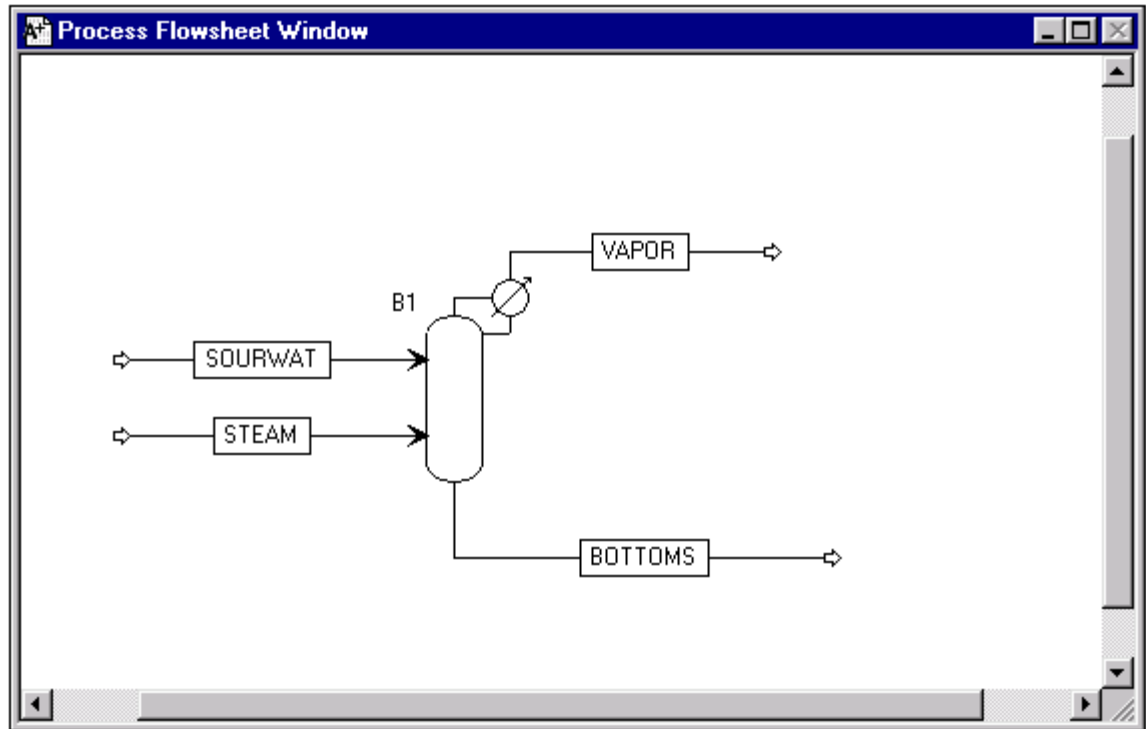
6. Click [N→] to guide you to the next required input.

The **Flowsheet Connectivity is Complete** dialog box appears.

7. 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 sheets.

Use this sheet 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.

Note   The Run type field displays Flowsheet, which is appropriate for this simulation.

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 enter a title for the simulation.

1. In the Title field, enter Getting Started with Electrolytes - Simulation 2.
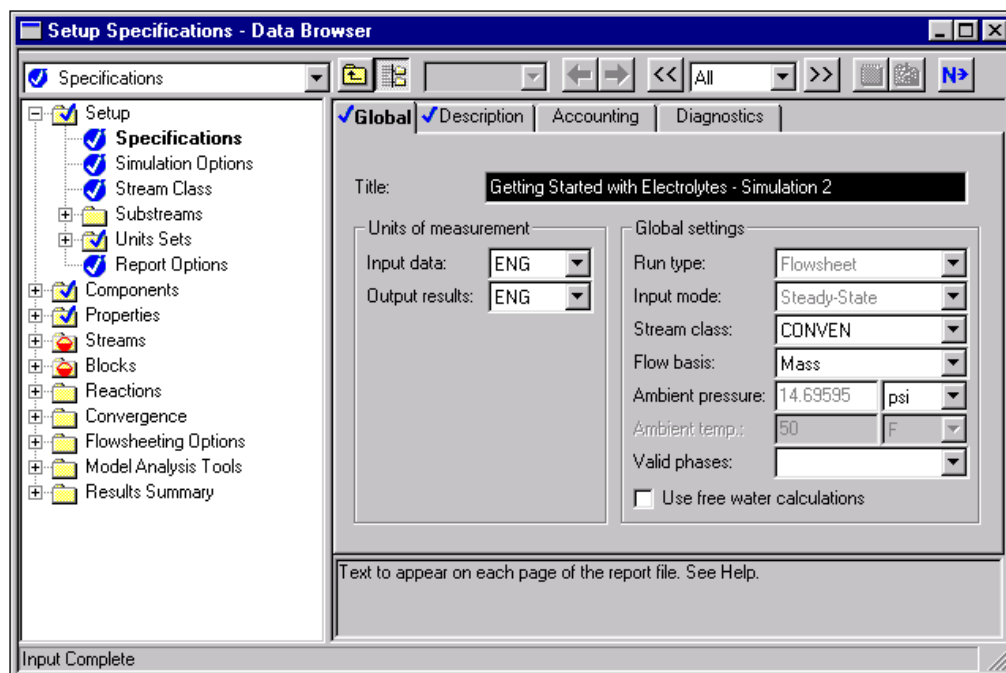
Based on the Electrolytes with Metric Units template, Aspen Plus displays the following defaults for calculating and reporting stream properties:

- Flow and Fraction Basis of Mass: Aspen Plus will report the component flow rates on a mass flow basis.

- ELEC_E Stream Sheetat: Aspen Plus sheetats the Stream Summary sheet for electrolytes.

To review the report options specified in the selected Template:

1. From the Data Browser, select the **Setup Report Options** sheet.

2. Select the **Stream** sheet.

To move to the next required input sheet:

1. From the Data Browser, select the **Components** folder and then select Specifications.

Specifying Components

The **Components Specifications Selection** sheet appears.

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

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

1. Enter the following components:

   H2O   Water
   NH3   Ammonia
   H2S   Hydrogen-Sulfide
   CO2   Carbon-Dioxide

2. Click Elec Wizard .

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

The Electrolytes Wizard

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 sheet, and to generate the reactions that occur among these components in the liquid phase.

1. On the **Electrolytes Wizard** dialog box, click Next > .

2. Click >> to move all components in the **Available components** column to the **Selected components** column.

3. Click Next > to continue.

The **Generated Species and Reaction** dialog box appears:
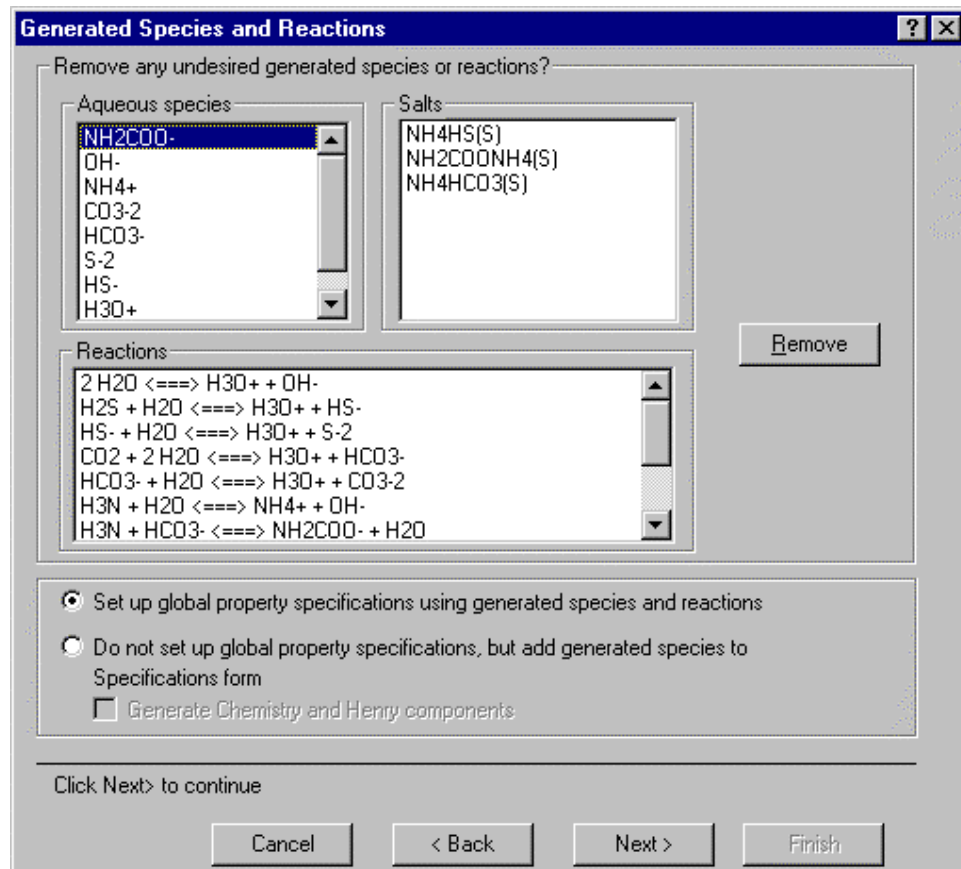
Aspen Plus generates all possible ionic species and reactions for the H2O-NH3-H2S-CO2 system.

In the Generated Reactions list, different-style arrows denote the following reaction types:

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

--->>   Denotes complete dissociation

For this simulation, you know that ammonium carbamate sheetation can be neglected.

To remove ammonium carbamate sheetation from the solution chemistry:

1. Select NH2COO- aqueous species.

2. Click ⬚Remove .

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:

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

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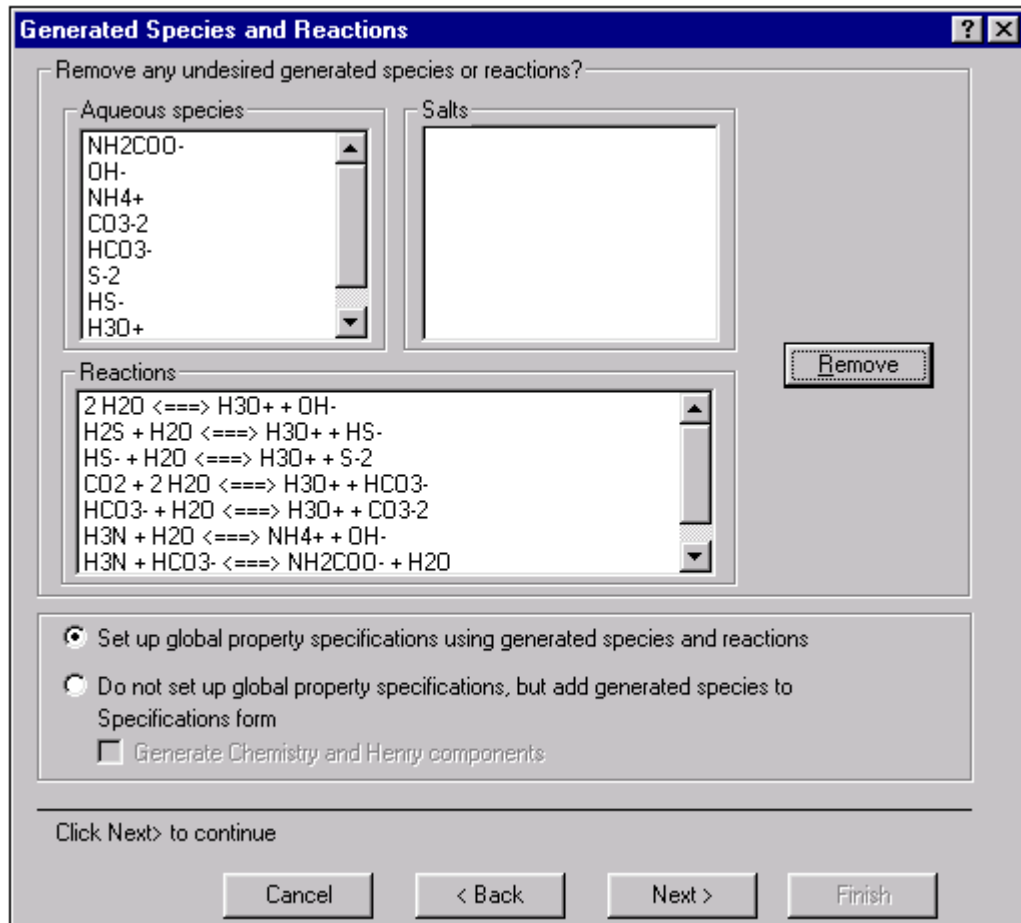
Note Any time you know that a reaction can be neglected because of expected process conditions, remove it from the solution chemistry, to decrease the execution time required for your simulation.

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^+.

3. On the **Generated Species and Reactions** dialog box click [Next >] 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 simulation, 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 H_2S that includes molecular H_2S, HS^-, and S^{-2}.

4. Select the radio button next to Apparent component approach.

5. Click [Next >] to move to the next dialog box.

The **Summary** dialog box appears, providing Aspen Plus electrolytes expert system information.

6. Click [Finish] to close the dialog box.

On the **Components Specifications** sheet, Aspen Plus has now added the generated electrolyte components. Since all components are databank components, Aspen Plus automatically retrieves all relevant physical property parameters.
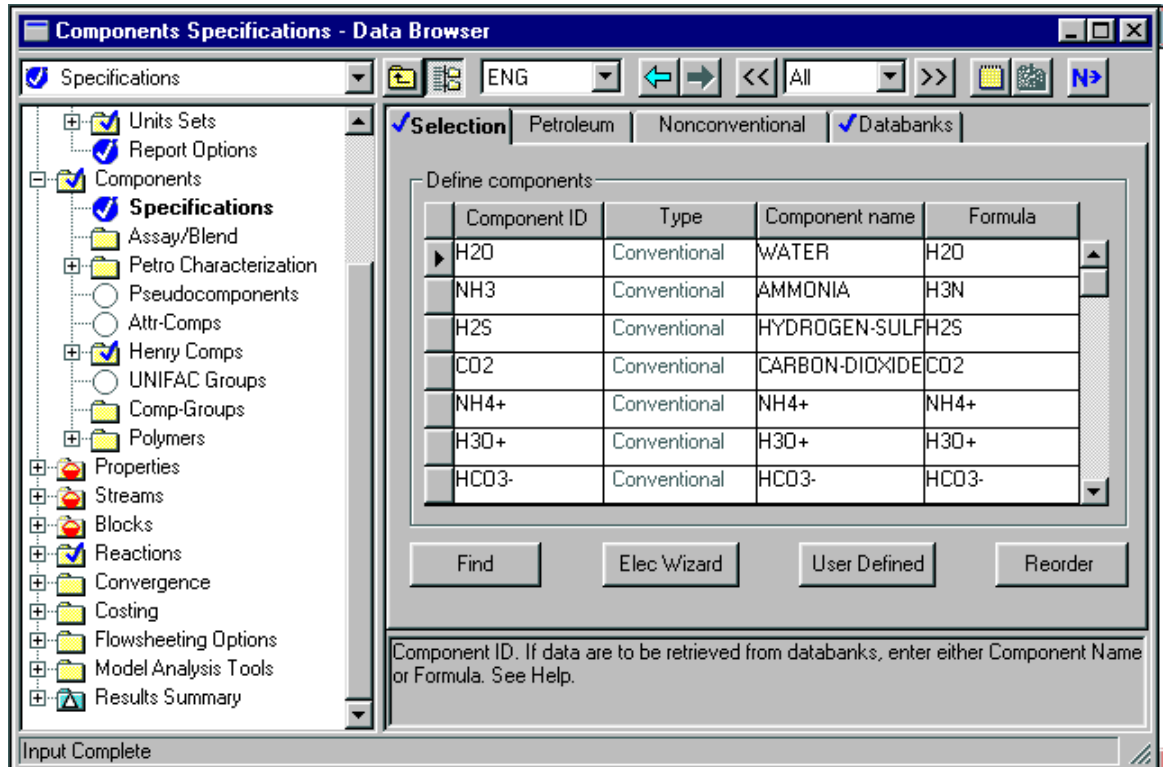
7. Click to continue.

The **Components Henry Comps Global** sheet appears for the Henry
Comps group GLOBAL, which was defined by the electrolytes expert
system. Use this sheet to 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 sheet.

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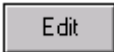
In the previous step, the Aspen Plus Electrolytes Wizard automatically generated the chemistry definition for your simulation and named it GLOBAL.

To examine the generated Chemistry:

1. From the Data Browser, select the **Reactions** folder.

2. From the **Reactions** folder, select the **Chemistry** folder and then select Global.

   The **Reactions Chemistry Global** sheet appears.

To view the generated chemistry:

1. Select a Reaction and click [Edit].

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

2. Close the dialog box and view the other reactions using the same steps.

   Note   All six reactions have equilibrium constant that have been retrieved from the Aspen Plus reactions database.
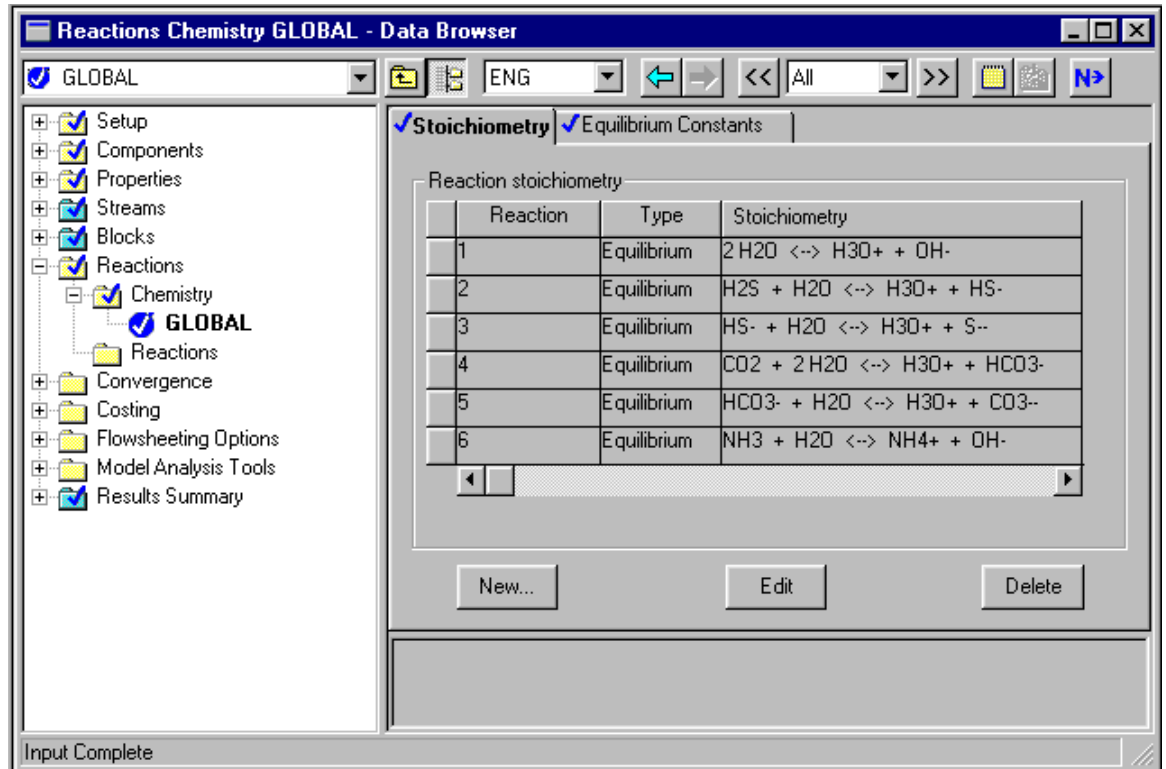
3. From the Data Browser, select the **Properties** folder and then select Specifications.

The **Properties Specifications** sheet appears. The Electrolytes Wizard has already completed this sheet:
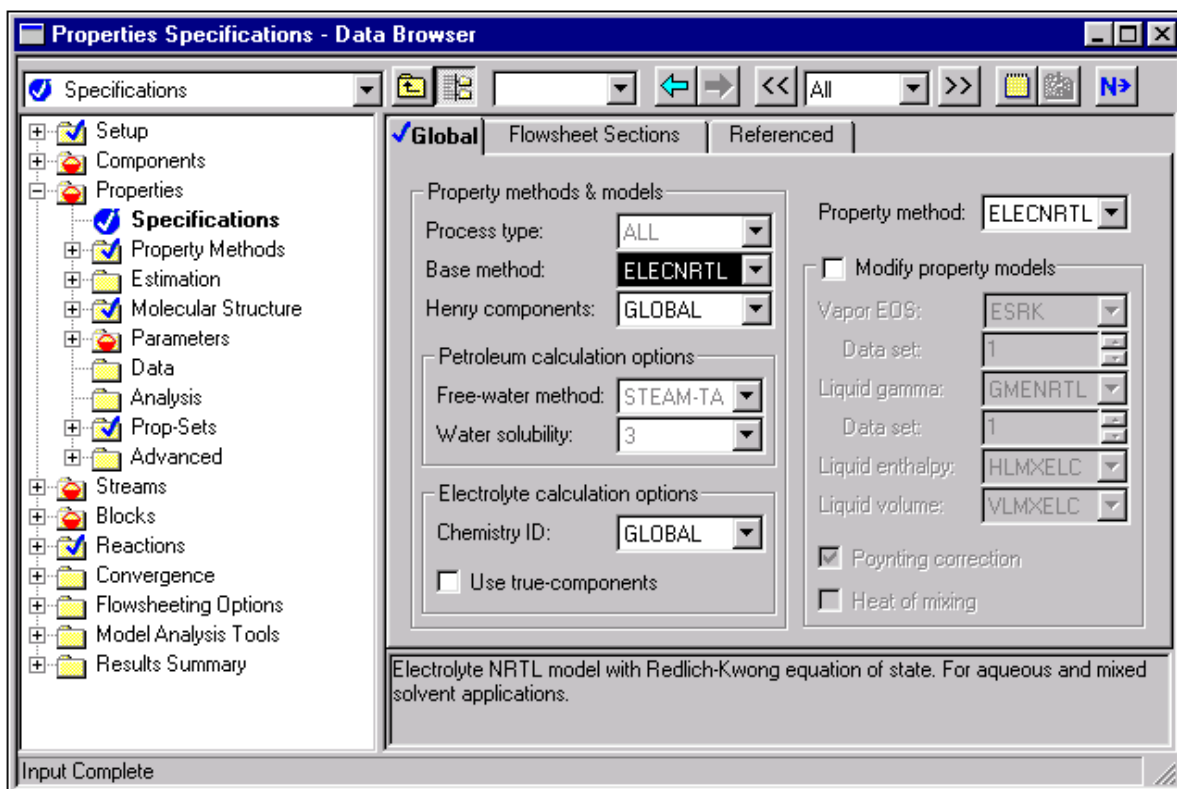
4. Select the checkbox next to Use True-Components.

5. Click ![N→] to continue.

The **Binary Interaction** sheet appears for the binary parameters HENRY-1. Use this sheet to view the Henry's Law parameters retrieved by the electrolytes expert system. If you had your own Henry's Law parameters, enter them on this sheet.

6. Click ![N→] to continue.

The **Binary Interaction** sheet appears for the binary parameters NRTL-1. Use this sheet to view the molecule-molecule interaction parameters retrieved by the electrolytes expert system. If you had your own molecule-molecule interaction parameters, enter them on this sheet.

7. From the Data Browser, select the **Properties** folder, then select the **Parameters** folder, and then select the **Electrolyte Pair** folder.

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

8. Click ![N→] to continue.

   The **Electrolyte Pair GMELCC-1 Input** sheet appears.

9. Click ![N→] to continue.

   The **Electrolyte Pair GMELCD-1 Input** sheet appears.

10. Click ![N→] to continue.

    The **Electrolyte Pair GMELCE-1 Input** sheet appears.

11. Click ![N→] to continue.

    The **Electrolyte Pair GMELCN-1 Input** sheet appears.

12. Click ![N→] 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 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, complete the rest of the flowsheet specifications in the same way as for nonelectrolytes. Use all Aspen Plus unit operation models in an electrolytes simulation.

13. Click OK to move to the next required input.

Entering Stream Data

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

1. On the **Streams SOURWAT Input Specifications** sheet, enter the following:

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

2. In the Composition field, click ▼ and select Mass-Frac.

3. Enter the following mass fraction values:

H2O	0.997
NH3	0.001
H2S	0.001
CO2	0.001

Getting Started Modeling Processes with Electrolytes
Version 10.2
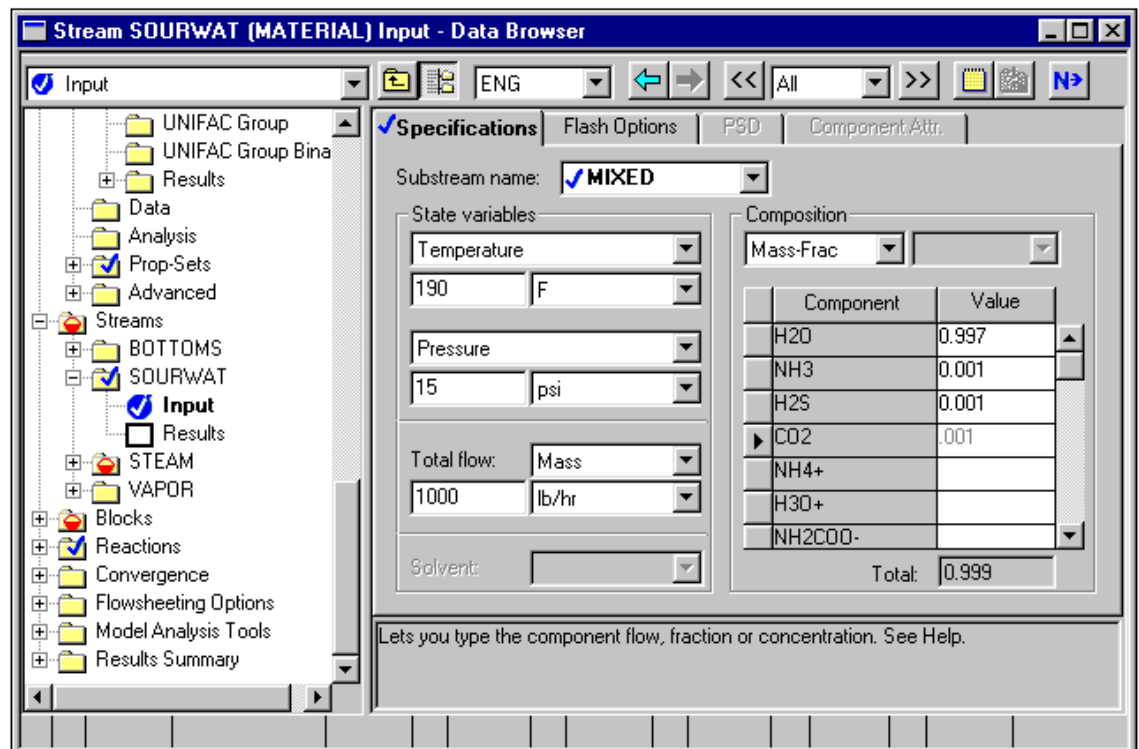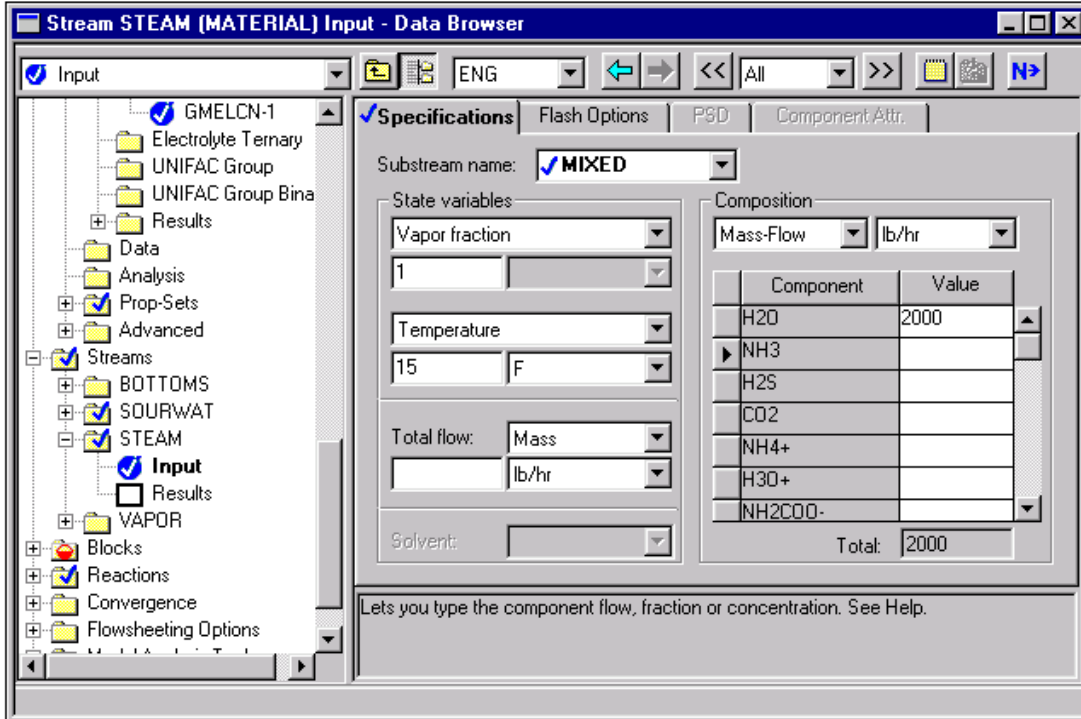
4. Click ![N→] to continue.

   The **Streams STEAM Input** sheet appears.

5. On the **Streams Steam Input Specifications** sheet, enter the following:

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

6. Click ![N→] to continue.

Specifying the RadFrac Block

The **Block B1 Setup** sheet appears.

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

1. Use Help on the **RadFrac Setup** sheet.

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

3. On the **Block B1 Setup Configuration** sheet, enter the following:

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

4. In the **Operating Specifications** section, at the Reflux Ratio field, select Mole and specify 25 as the initial estimate for reflux ratio.

The **Block B1 Setup Configuration** sheet is complete:
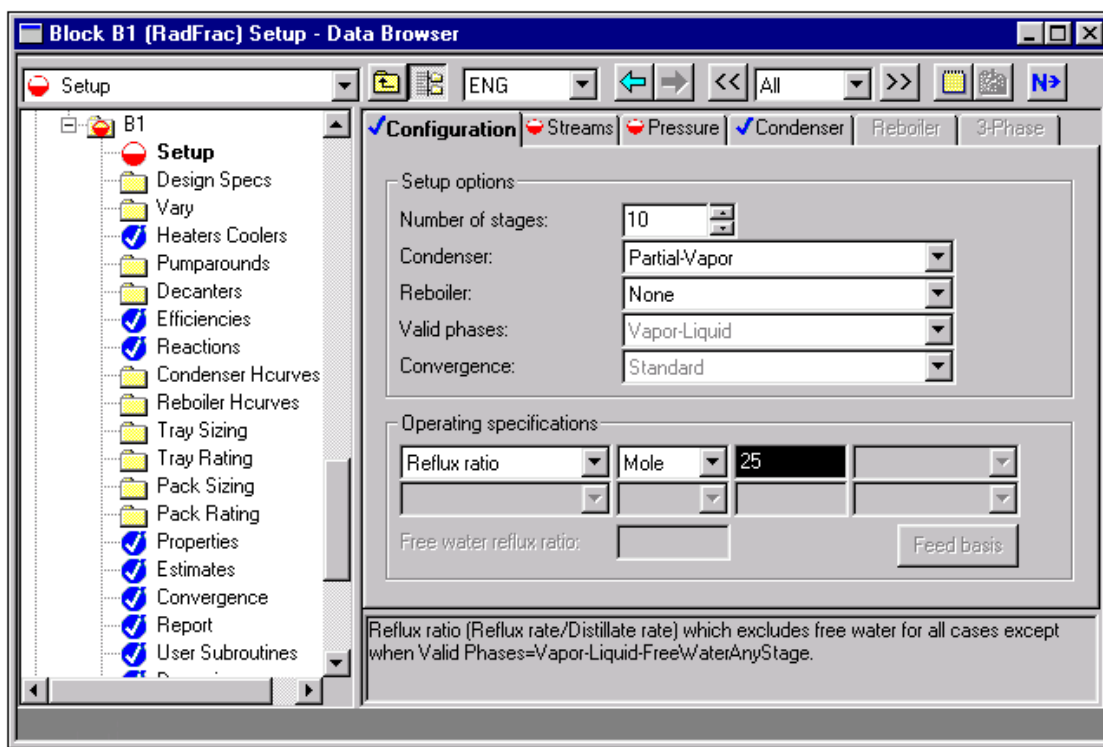
5. Click [N→] to continue.

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

6. For the SOURWAT feed stream, enter 3 in the Stage field and Above-Stage in the Convention field.

7. For the STEAM feed stream, enter 10 in the Stage field and On-Stage in the Convention field.

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.

8. Click [N→] to continue.

The **Setup Pressure** sheet appears.

To specify that this column operates isobarically at 15 psia:

1. In the Stage 1 / Condenser pressure field, enter 15 PSI.

2. Click to continue.

    The **Required Input Complete** dialog box appears, indicating that all
    required input specifications for RadFrac Block B1 have been entered:
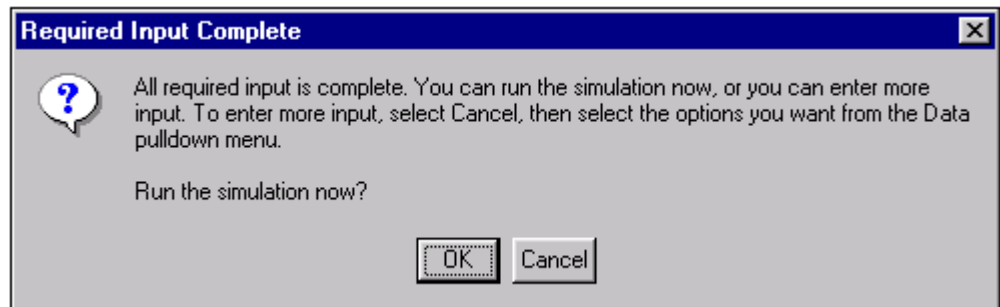
3. Click to close the dialog box.

    You can now enter optional specifications. These specifications include
    setting up two design specifications. The first will be a concentration of 50
    ppm NH3 in BOTTOMS, and the second will be a condenser temperature
    of 190°F.

To define the first design specification:

1. From the Data Browser, click the **Blocks B1 Design Specs** folder.

    The **Design Specs Object Manager** appears.

2. Click .

The **Create new ID** dialog box appears:
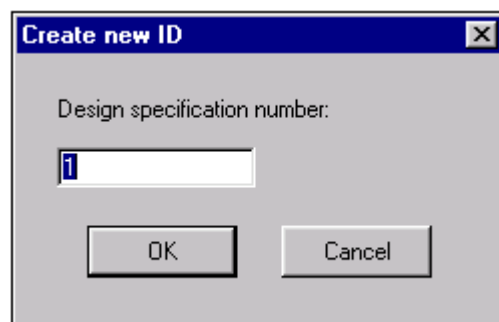
3. In the **Create new ID** dialog box , click [OK] to accept 1 (the default ID).

The **Design Specs 1** sheet appears.

4. In the Type field, click [▼] and select Mass purity.

5. In the Target field, enter the value 5.0E-5.

   Note   Specify where this specification is to be applied, and what component and phase it applies to.
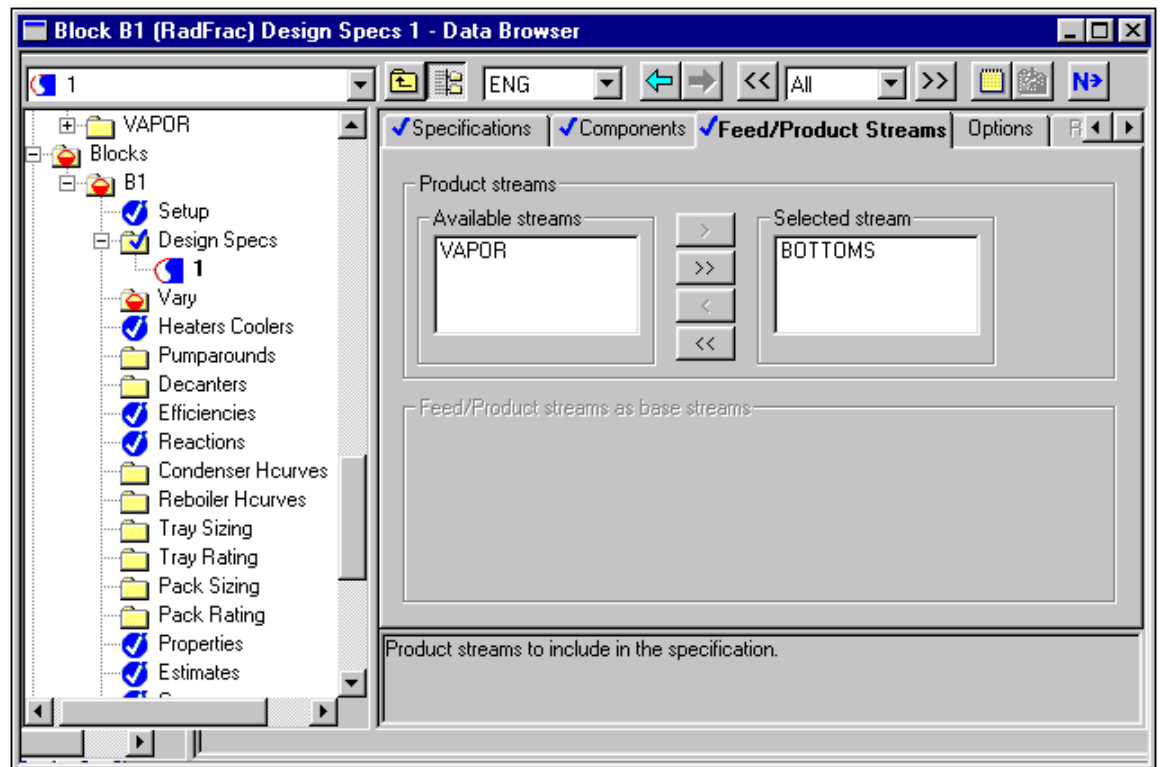
6. Click [N→] to continue.

The **Design Specs 1 Components** sheet appears.

7. From the **Available components** column, select NH3 (AMMONIA) and click [>].

8. Click [N→] to continue.

The **Design Specs 1 Feed/Product Streams** sheet appears.

9. From the **Available streams** column, select BOTTOMS and click [>].

The **Design Specs 1** sheet is complete:

To define another design specification:

1. From the Data Browser, select the **Design Specs** folder.

   The **Design Specs Object Manager** appears.

2. Click New... .

3. In the Create new ID dialog box , click OK to accept 2 (the default ID).

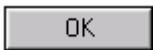   A new **Design Specs Specifications** sheet appears.

4. In the Type field, enter Stage temperature.

5. In the Target field, enter 190 F.

6. In the Stage field, enter 1.

7. Click to continue.

The **Vary Object Manager** appears.

Define two manipulated variables to meet the two design specifications. In this simulation keep free the steam feed rate and the reflux ratio specifications provided on the Blocks B1 Setup sheet. Aspen Plus adjusts 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:

1. Click and then click .

The **Vary 1 Specifications** sheet appears.

On this sheet, specify which input variables you want to keep free in order to meet the design specifications you provide.

2. In the Type field, enter Feed rate.

3. In the Stream name field, enter STEAM.

4. In the Lower bound field, enter 50 lbmol/hr.

5. In the Upper bound field, enter 200 lbmol/hr.

On the **Streams STEAM** sheet you specified a Mass-Flow for Stream STEAM. However, when you select the variable type Feed rate on the Vary 1 sheet, 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).
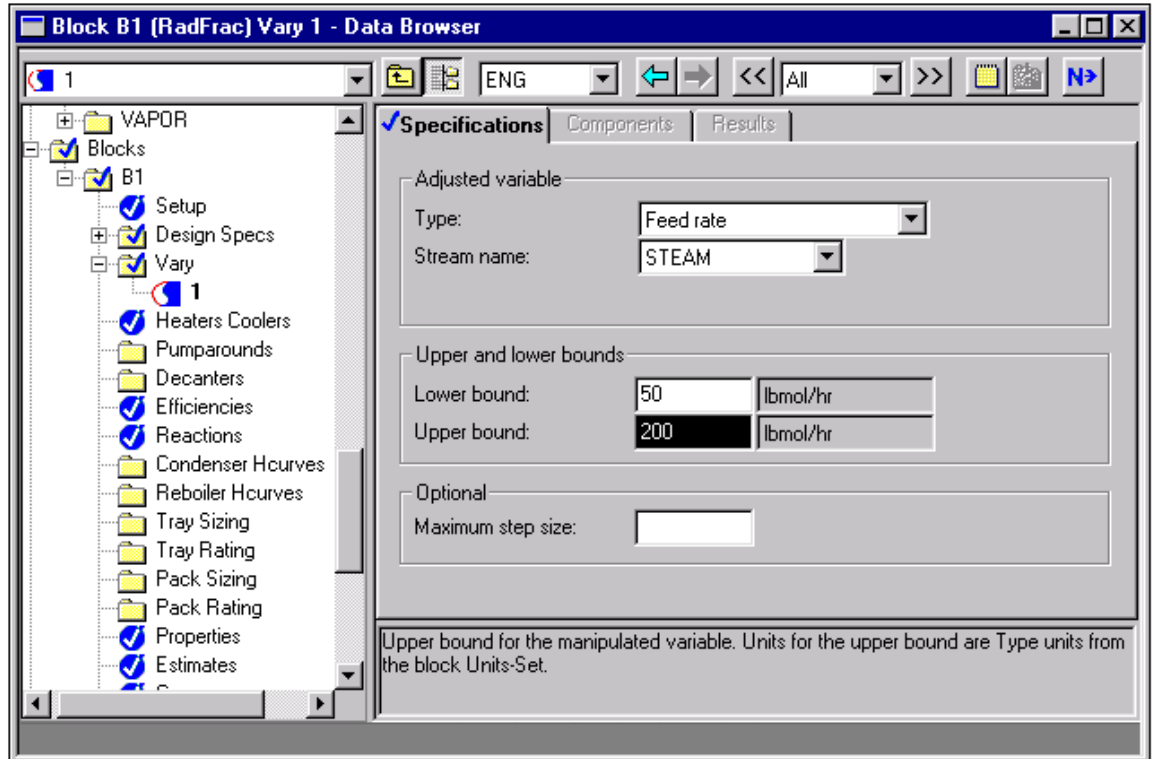
To define the second manipulated variable:

1. From the Data Browser, select the **Vary** folder.

2. Click [New...] and then click [OK].

3. In the Type field, enter Reflux ratio.

4. In the Lower bound field, enter 15.

5. In the Upper bound field, enter 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** sheet.

6. Click [N→] to continue.

   The **Required Input Complete** dialog box appears, indicating that all required specifications are complete.

7. 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. Modify the default stage report so that results are reported for all stages.

To change the report:

1. From the Data Browser, select the **Blocks** folder, then select the **B1** folder, and then select Report.

    The **Report Properties Options** sheet appears.

2. Select the **Report Profile Options** sheet.

3. On the **Report Profile Options** sheet, select the radio button next to the All Stages field.

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

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

4. Select the **Report Properties** sheet.

5. In the **Defined property sets** column, select PH and XTRUE and click > to move the selected property sets into the **Selected property sets** column.
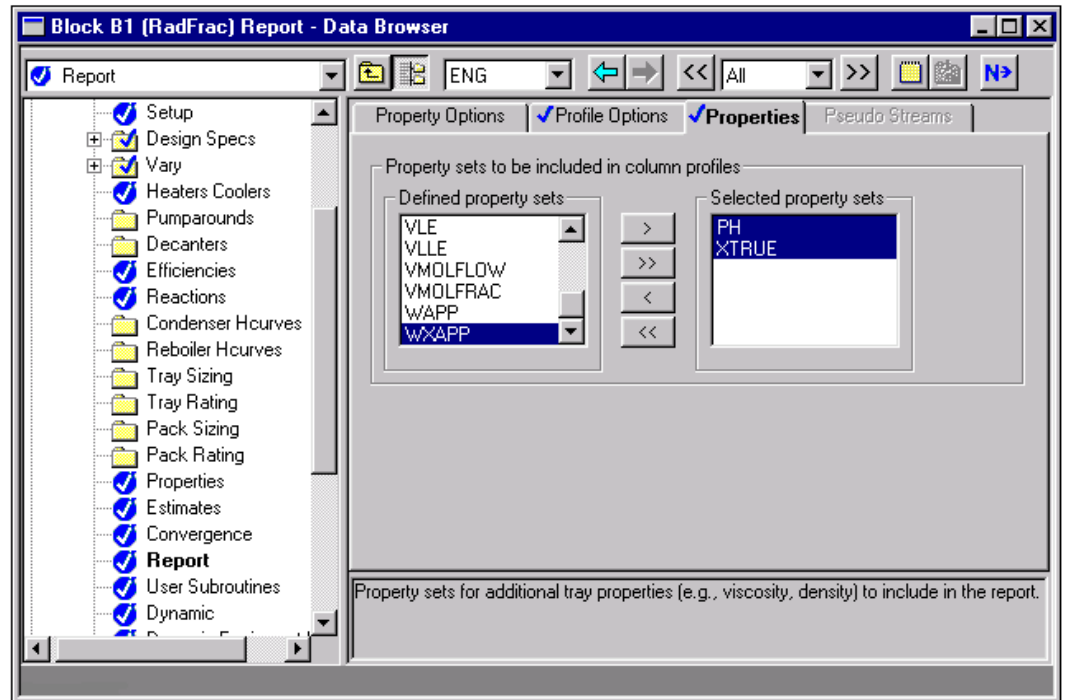
6. Click to continue.

Running the Simulation

The **Required Input Complete** dialog box appears.

1. 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 persheet the simulation.

   As in simulation 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.

2. When the message *Results Available* appears in the toolbar, click ⬜ to view the results of your run.

Examining Simulation Results

Aspen Plus generates many results for this simulation. Examine any results that are of interest to you. This simulation guides you through a review of some of the simulation results.

To view RadFrac results:

1. Select the **Process Flowsheet** tab at the bottom of the screen.

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

3. Right-click on the mouse and select Results.

   The **Blocks B1 Results Summary** sheet appears. This sheet reports the flows, temperatures, and duties for the top and bottom stage of the column.
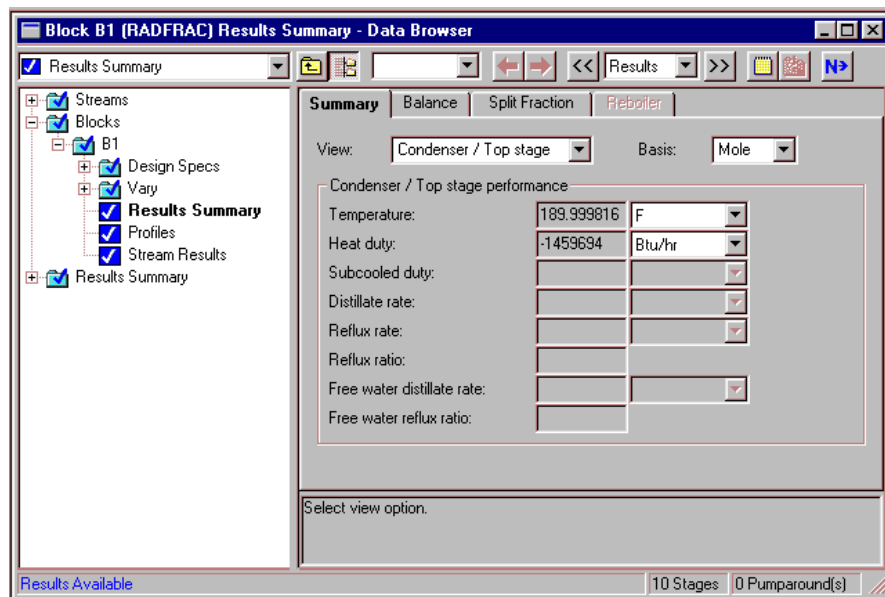
4. Click to move to the next results sheet.

   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.
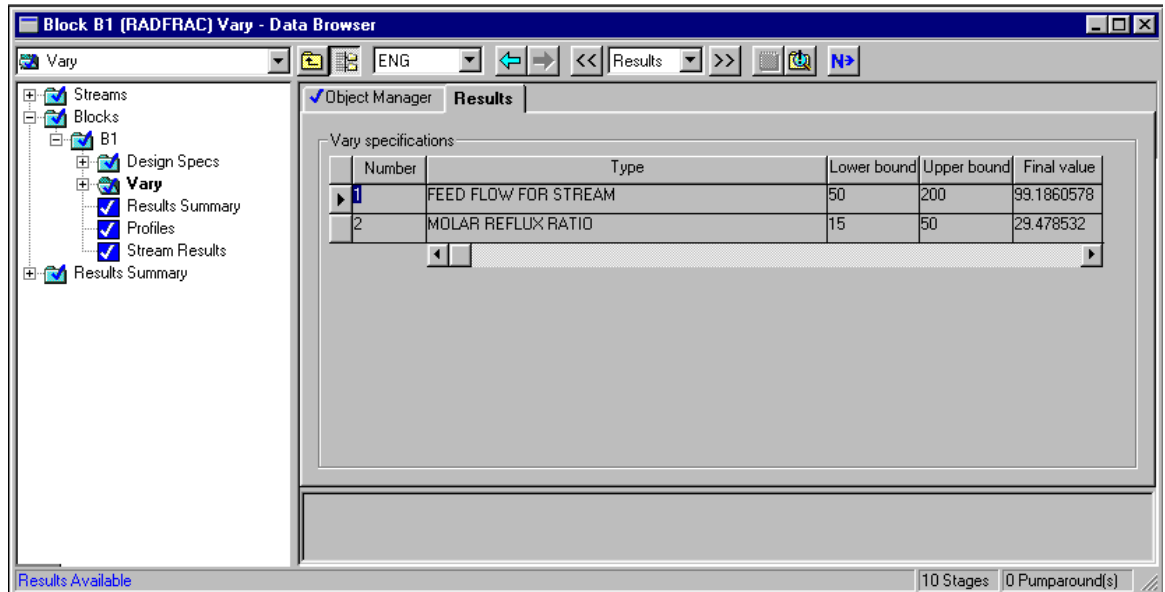
To view these results:

1. From the Data Browser, select the **Design Specs** folder.

2. Select the **Results** sheet to view the Design Specs results.
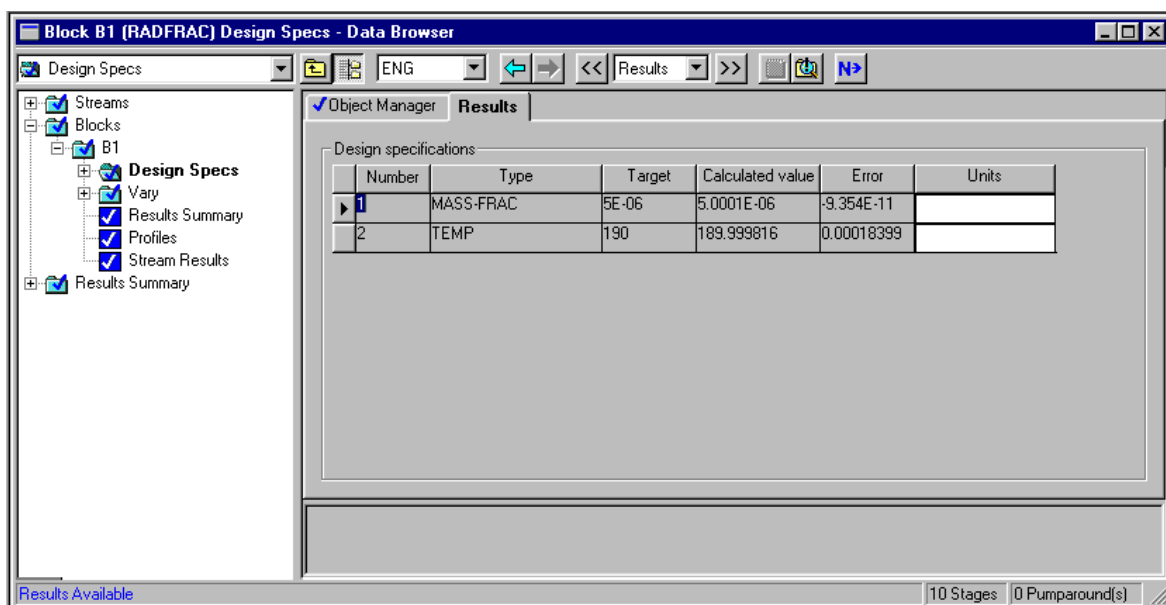
A summary of the results of the manipulated variables is located on the **Vary Results** sheet. This sheet reports the specified bounds and the final values for all of the manipulated variables.

To view these results:

1. From the Data Browser, select the **Vary** folder.

2. Select the **Results** sheet 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:

1. From the Data Browser, select the **Profiles** folder.

2. Select the **Compositions** sheet to view the results.

3. In the View field, click ▼ and select Liquid.

The **Profiles Properties** sheet reports the actual composition of molecular components and ions.

To view these results:

1. Select the **Properties** sheet.

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:

$CO_2 + 2H_2O <<===>> H_3O^+ + HCO_3^-$
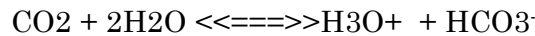
The total number moles on an apparent component basis will be different from the total number of moles on a true component basis. Thus X_{NH_3} (apparent basis) is not exactly equal to X_{NH_3} (true basis) + $X_{NH_4^+}$ (true basis).

The liquid composition of apparent NH3 on stage 1 is:

$X_{NH_3} = 0.0314$

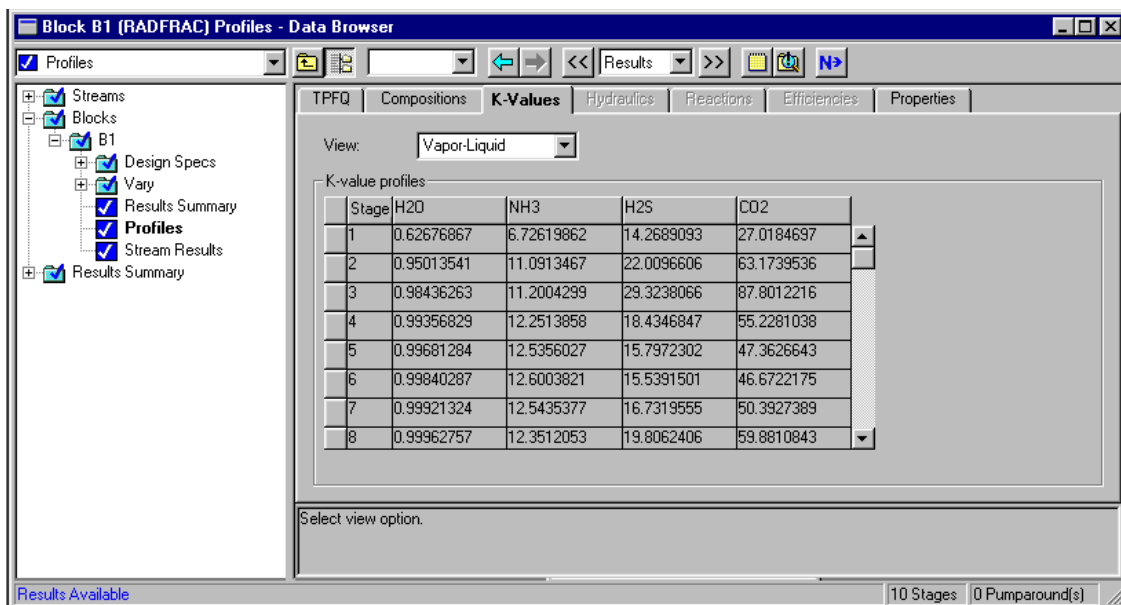2. Select the **Compositions** sheet.

3. In the View field, select Vapor.

The vapor composition of apparent NH3 on stage is:

$Y_{NH_3} = 0.2112$

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

$K = Y_{NH_3}/X_{NH_3} = 6.73$

4. Select the **K-Values** sheet.

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.

5. 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 simulations, 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:

1. From the Aspen Plus menu, select Data and then select Properties.

2. On the **Properties Specifications Global** sheet, select the checkbox next to True-Components.

    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:

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

2. Right-click inside the RadFrac block and select Input.

3. From the Data Browser, select the **Design Specs** folder.

    The **Design Spec Object Manager** appears.

4. Select Design Spec ID 1, and click Edit .

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

5. In the Type field, click and select Property value.
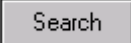
6. In the Target field, enter 5.0E-6.

7. In the Property set field, right-click the mouse and select New.

8. In the **Aspen Plus** dialog box, enter XNH3APP as the new property set.

9. Click [OK].

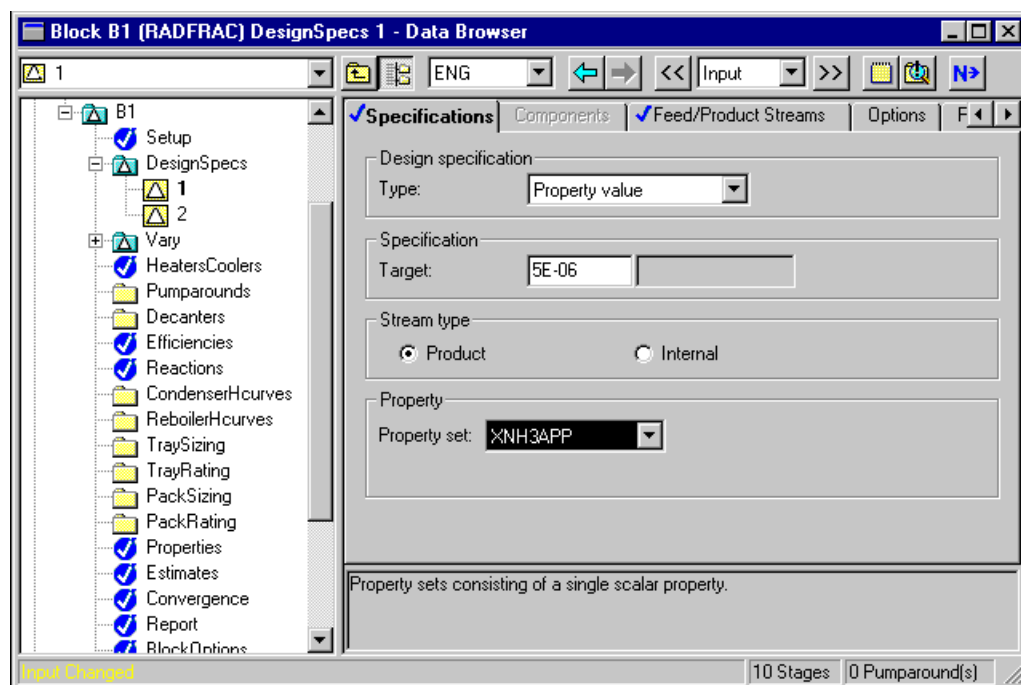10. Select the **Feed/Product Streams** sheet.

11. In the **Available streams** column, select Bottoms and click [>] to move the stream to the **Selected stream** column.

12. Click [N→] to continue.

   The **Properties Prop-Sets XNH3APP** sheet appears.

   Aspen Plus uses this property set to calculate the apparent mass fraction of NH3 in the liquid phase.

13. Click Search .

14. In the **Search Physical Properties** dialog box, enter apparent component mass fraction in the first field.

15. Click Search .

The system searches for valid physical properties and displays them in the second field of the **Search Physical Properties** dialog box.

16. Select **Apparent component mass fraction (alias WXAPP)** from the search results.

17. Click Add .

The system adds the selected physical property and displays it in the third field of the **Search Physical Properties** dialog box.

18. Click OK .

19. Select the **Qualifiers** sheet.

20. In the Phase field, click and select Liquid.

21. In the Component field, click and select NH3.

22. Click to continue.

The **Required Properties Input Complete** dialog box appears.

23. Click OK .

Running the True Component Simulation

The **Required Input Complete** dialog box appears insheeting you that all specifications are complete and the simulation can be run.

1. Click [OK] .

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

2. Close all open windows, and the Control Panel.

To view selected results of the true component simulation:

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

2. Right-click inside the RadFrac block and select Results.

3. From the Data Browser, select the **Profiles** folder.

4. Select the **Compositions** sheet to view the results.

5. In the View field, click [▼] and select Liquid.

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

   $X_{NH3} = 0.02093$

   $X_{NH4+} = 0.01054$

6. In the View field, click [▼] and select Vapor.

   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.

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

7. Select the **K-Values** sheet.

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:

1. From the Aspen Plus menu, select File and then select Exit.

   The **Aspen Plus** dialog box appears.

2. Click No.

   – or –

   Click 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. Use this backup file to check your results.

Modeling a
Sour Water
Stripper

❖   ❖   ❖   ❖

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.

1. In the Server type field, click 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.

2. Click to continue.

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

3. In the Node name field, enter the node name of the computer on which the Aspen Plus simulation engine will execute.

4. In the other fields, enter the following information:

    User name   Your user name for the specified
                         host/server.

    Password   Your password for the above user
                         name.

    Working directory   The associated working directory.

5. Click [OK] .

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

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.

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