Aspen Plus

Getting Started Modeling Processes with Solids

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Who Should Read this Guide

This guide is suitable for Aspen Plus users who want to model processes containing solids. Users should be familiar with the procedures covered in *Aspen Plus Getting Started Building and Running a Process Model* before starting these examples.

Introducing Aspen Plus

Aspen Plus can be used to model many processes involving solids. Some of the solids processing applications that have been modeled with Aspen Plus include:

- Bayer process
- Cement kiln
- Coal gasification.
- Hazardous waste incineration
- Iron ore reduction
- Zinc smelting/roasting

All of the unit operation models (except Extract) and flowsheeting tools are available for use in modeling solids processing applications.

This book guides you in introducing solids to a simulation in Aspen Plus. The four sessions demonstrate the following concepts:

- Defining solid components
- Changing the global stream class
- Defining physical property methods for solid components
- Defining component attributes for solid components
- Defining a particle size distribution
- Modifying the default particle size distribution
- Accessing component attributes in a Fortran block
- Modifying component attributes in a block
- Using solids unit operation models

Getting Started Modeling Processes with Solids assumes that you have an installed copy of the Aspen Plus software, and that you have done the sessions in *Getting Started Building and Running a Process Model* so that you are familiar with the basics of how to use Aspen Plus.

Why Use Solids Simulation

The introduction of solids to a chemical process can affect the process in many ways. In all cases, the heat and mass balances of the process are changed, even if the solid essentially passes through the process as an inert component.

Simulation of the heat and mass balances of a solids process requires physical property models suitable for solid components. The physical property models used to characterize a liquid may not be relevant for solids.

In addition to specialized physical property models for solid components, accurate representation of the solids particle size distribution is required for some processes. For example, the separation efficiency of a cyclone is highly dependent on the size of the particles entrained in the feed gas.

Sessions in this Book

The sessions in this book guide you in building a flowsheet that uses solids.

This book includes the following hands-on sessions:

Follow the steps in this chapter	To learn how to
1 Modeling Coal Drying	Change the global stream class, define nonconventional solid components, specify physical properties for nonconventional solid components, specify streams with nonconventional solid components, and modify component attributes in a unit operation block.
2 Modeling Coal Combustion	Define conventional solid components, define a Fortran block to control solid decomposition.
3 Modeling Gas-Solid Separators	Modify the default particle size intervals; use solids-handling unit operation models.
4 Modeling Polymer Recovery	Use the component attribute GENANAL to characterize a nonconventional component, use the hydrocyclone model, the counter-current decanter model and the cyclone model.

Using Backup Files

We recommend that you perform all sessions sequentially in order to build the entire model. However, you can skip chapters and work on the session of your choice, using backup files containing simulation data.

Aspen Plus provides backup files containing all problem specifications and results for each tutorial session. In some cases, if you skip a session, you need to load a backup file to supply missing data. The chapter describes how to do this. If you perform each tutorial session in order, you can use backup files to compare your results.

Related Documentation

Title	Content
Aspen Plus Getting Started Building and Running a Process Model	Tutorials covering basic use of Aspen Plus. A prerequisite for the other Getting Started guides
Aspen Plus Getting Started Using Equation Oriented Modeling	Tutorials covering the use of equation-oriented models in Aspen Plus
Aspen Plus Getting Started Customizing Unit Operation Models	Tutorials covering the development of custom unit operation models in Aspen Plus
Aspen Plus Getting Started Modeling Processes with Electrolytes	Tutorials covering the Aspen Plus features designed to handle electrolytes
Aspen Engineering Suite Installation Manual	Instructions for installing Aspen Plus and other Aspen Engineering Suite products
Aspen Plus Help	Procedures for using Aspen Plus

Technical Support

AspenTech customers with a valid license and software maintenance agreement can register to access the online AspenTech 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
- Search for and download service packs and product updates
- 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 alert users to important technical support information such as:

- Technical advisories
- Product updates and releases

Customer support is also available by phone, fax, and email. The most up-to-date contact information is available at the AspenTech Support Center at **http://support.aspentech.com**.

1 Modeling Coal Drying

In this simulation you will simulate a coal drying process.

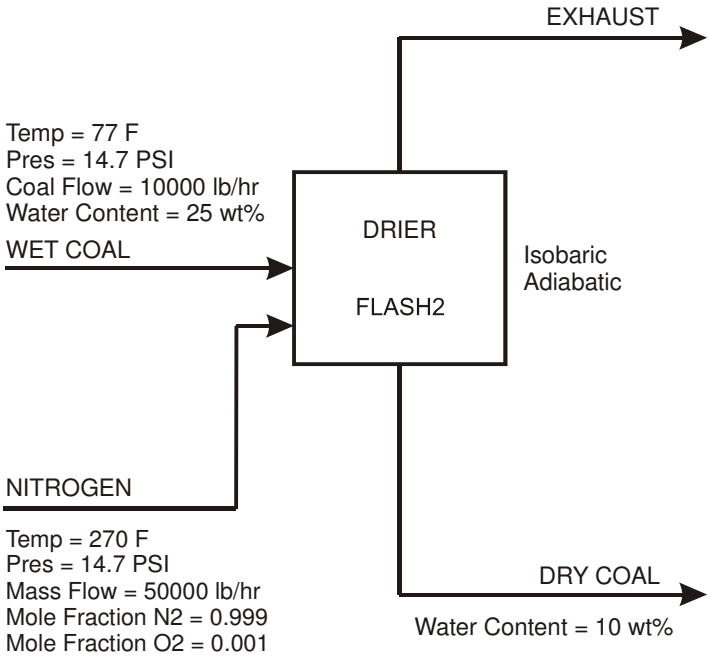
You will:

- Define nonconventional solid components.
- Specify physical properties for nonconventional solid components.
- Change the global stream class.
- Specify streams with nonconventional solid components.
- Modify component attributes in a unit operation block.
- Analyze the results.

Allow about 30 minutes to complete this simulation.

Coal Drying Flowsheet

The process flow diagram and operating conditions for this simulation are shown in the following figure. A wet coal stream and a nitrogen stream are fed to a drier. There are two products from the drier: a stream of dried coal and a stream of moist nitrogen.



To Start Aspen Plus

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

2 Select **AspenTech | Process Modeling <version> | Aspen Plus | Aspen Plus <version>**. The **Start Using Aspen Plus** window appears within the Aspen Plus main window.

On this window, Aspen Plus displays links for commands and cases so that you can quickly enter information or make a selection before proceeding. In this simulation, start a new case using an Aspen Plus template.

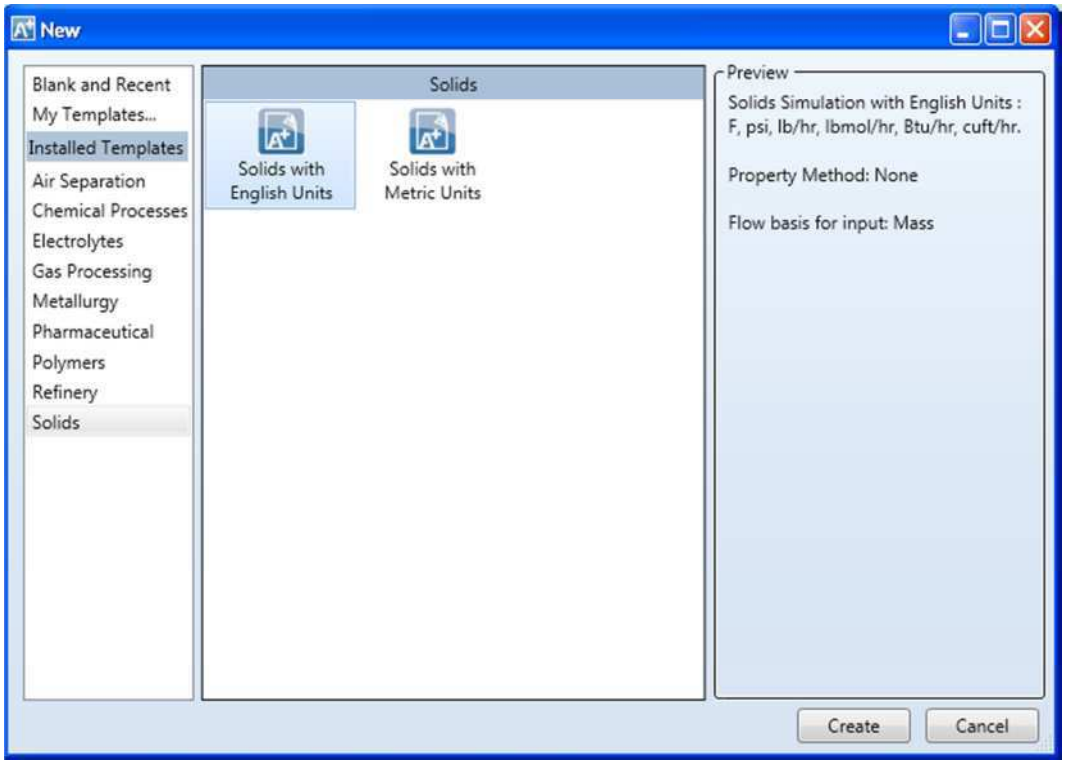
3 Click **New** on the **Start Using Aspen Plus** window.

The **New** dialog box appears. Use this dialog box to specify the template for the new run. With the template, Aspen Plus automatically sets various defaults appropriate to your application.

To Specify the Template for the New Run

1 Under **Installed Templates** in the panel on the left side of the **New** dialog box, click **Solids**, then click the **Solids with English Units** template.

Information for unit sets, property method, etc. that were pre-defined in the template is shown on the right side, in the **Preview** field.



2 Click **Create** to apply this template.

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

Specifying Components

The **Components - Specifications | Selection** sheet is used to enter the components present in the simulation. The components in this simulation are H_2O, N_2, O_2, and coal.

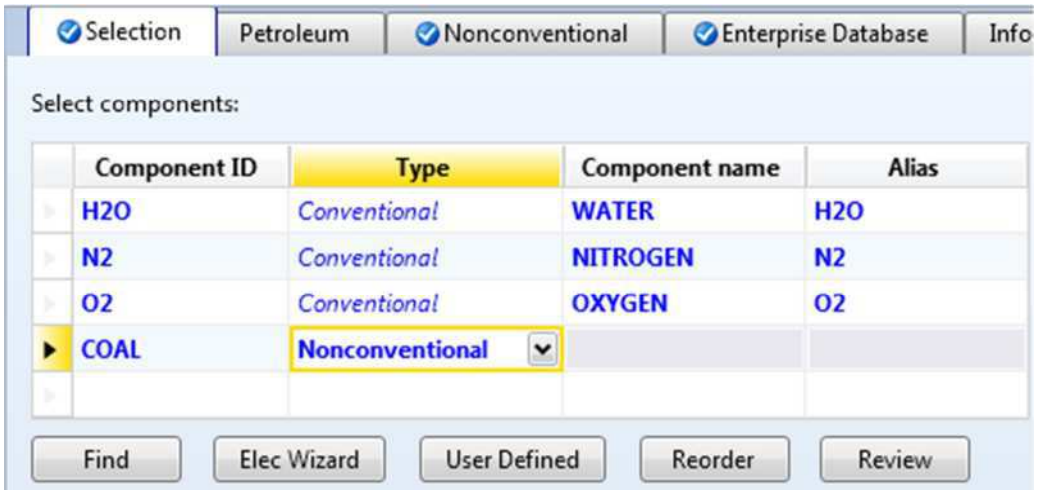
1 In the first four **Component ID** fields, enter **H2O**, **N2**, **O2**, and **COAL**.

Because H2O, N2, and O2 are present in the databanks, WATER, NITROGEN, and OXYGEN appear in the **Component name** field. Aspen Plus does not recognize COAL. Coal is actually a mixture of different compounds, but for this simulation it will be treated as a single component.

By default, Aspen Plus assumes all components are of the type **Conventional**, indicating that they participate in phase equilibrium calculations. However, in this simulation, coal will be modeled as a nonconventional solid.

2 From the COAL **Type** field, click  and select **Nonconventional**.

The **Components - Specifications | Selection** sheet is now complete:



3 From the Navigation Pane, select **Methods | Specifications**.
The **Methods - Specifications | Global** sheet appears.

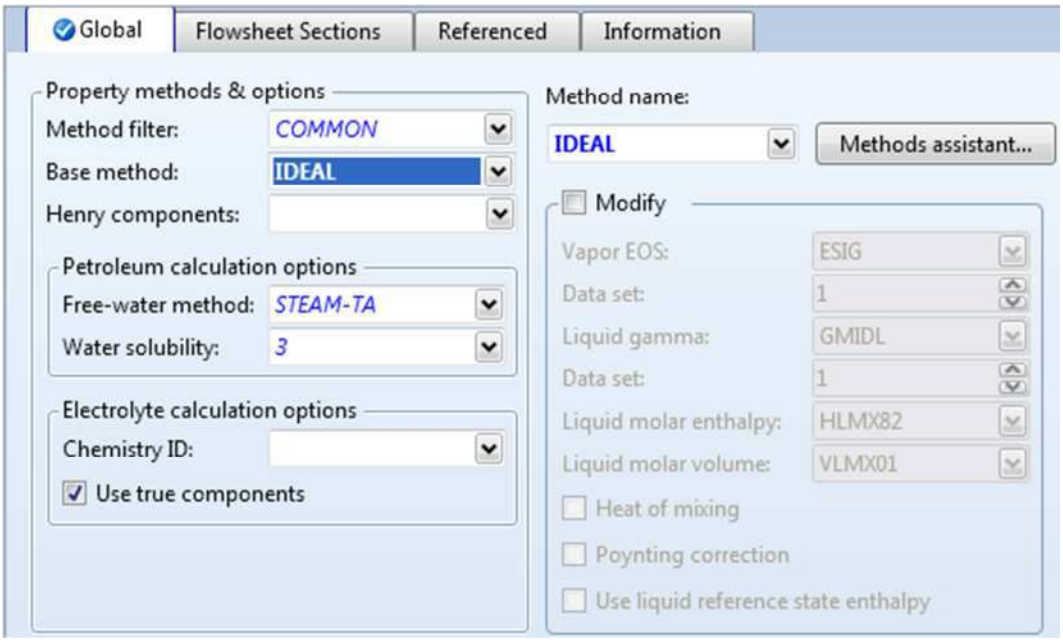
Defining Properties

The **Methods - Specifications | Global** sheet is used to select the thermodynamic methods used to calculate properties such as K-values, enthalpy, and density. Property methods in Aspen Plus are categorized into various process types.

Because the physical property methods for solid components are the same for all property methods, select a property method based on the conventional components in the simulation.

The **IDEAL** property method (Ideal gas and Raoult's Law, as the prompt indicates) is a good choice for this simulation, since the process involves the conventional components H_2O, N_2, and O_2, at low pressure.

1 In the **Base method** field, click  and select **IDEAL**.



2 Click to continue.

The **Methods - NC Props | Property Methods** sheet appears.

Specifying Nonconventional Solid Physical Property Models

The **Methods - NC Props | Property Methods** sheet is used to specify the models used to calculate the nonconventional solid properties. Because nonconventional components are heterogeneous solids that do not participate in chemical or phase equilibrium, the only physical properties that are calculated for nonconventional components are enthalpy and density.

In this simulation, use the **HCOALGEN** and the **DCOALIGT** models to calculate the enthalpy and density of coal.

1 In the **Model name** field for **Enthalpy**, click and select **HCOALGEN**.

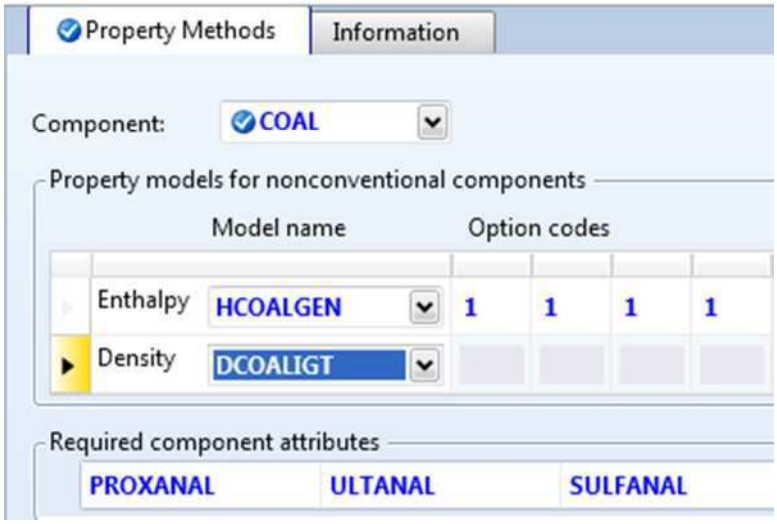
The component attributes **PROXANAL**, **ULTANAL**, and **SULFANAL** are automatically included in the **Required component attributes** field for COAL when you select HCOALGEN. Also, four **Option Codes** fields with values of **1** appear.

Aspen Plus uses component attributes to represent nonconventional components in terms of a set of identifiable constituents needed to calculate physical properties. HCOALGEN uses the proximate analysis, ultimate analysis, and sulfur analysis to calculate the enthalpy of coal.

The Option Codes fields define how the HCOALGEN model calculates the heat of combustion, the standard heat of formation, the heat capacity, and the enthalpy basis for coal.

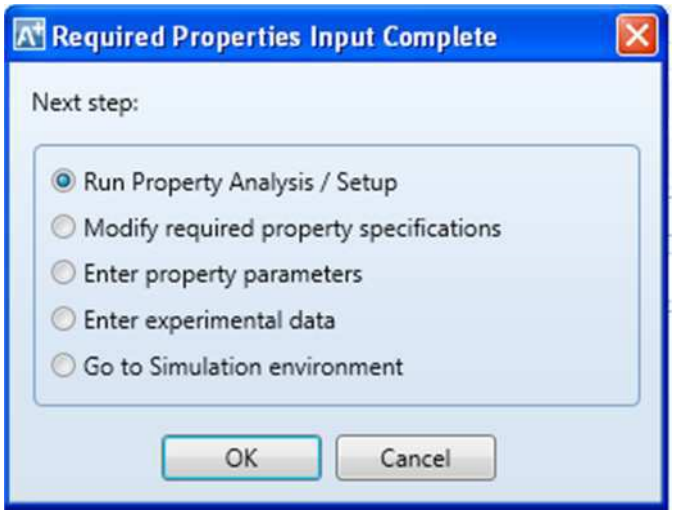
2 In the **Model name** field for **Density**, click and select **DCOALIGT**.

The **Property Methods** sheet is complete:



3 Click to continue.

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



Correct representation of physical properties is an essential component of process modeling. For many simulations, the only physical property specification that you must provide is the selection of a property method. The **Required Properties Input Complete** dialog box shows that the Aspen Plus physical property system has many optional capabilities that you can use to increase the accuracy of physical property calculations.

4 Select **Go to Simulation environment** and click **OK** to continue.

Drawing the Graphical Simulation Flowsheet

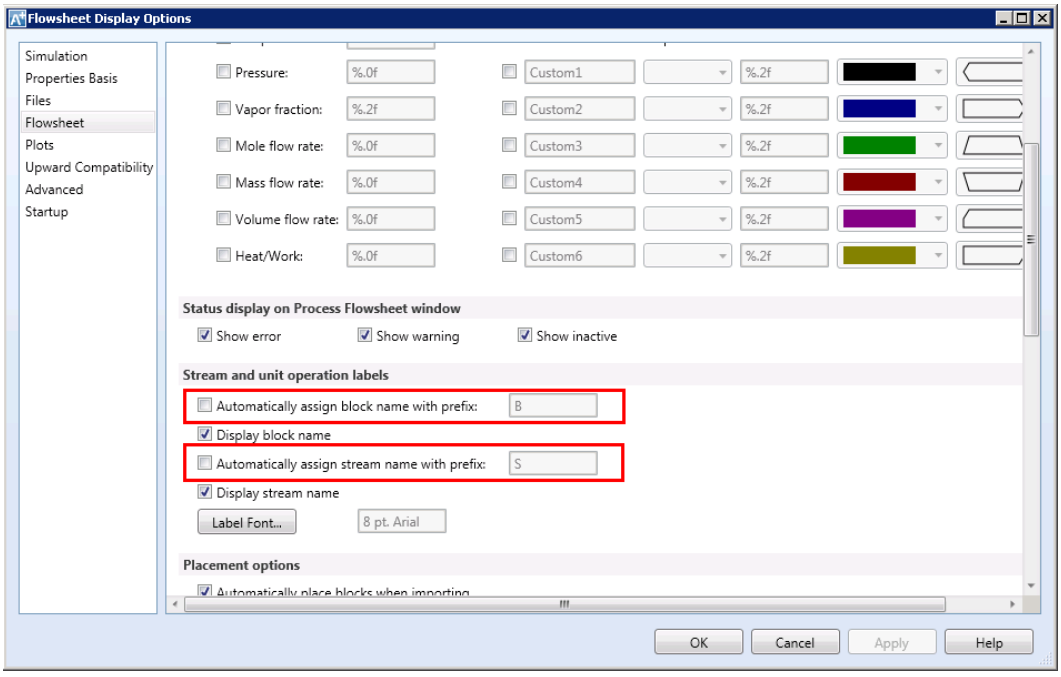
In this simulation, begin building the process flowsheet. Since you will enter your own block and stream IDs, turn off the automatic naming of blocks and streams, which provide these IDs automatically.

1 From the ribbon, click **File**. Click **Options**.

The **Options** dialog box appears.

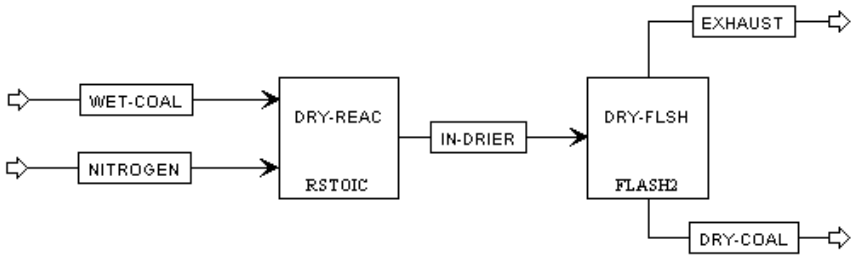
2 Select **Flowsheet** from the panel on the left side of the dialog box.

3 Clear the **Automatically assign block name with prefix** and **Automatically assign stream name with prefix** check boxes under **Stream and unit operation labels**.



4 Click **Apply** and then **OK** to apply the changes and close the dialog box.

The simulation flowsheet shown in the following figure feeds the WET-COAL stream and the NITROGEN stream to an RStoic model. In the RStoic block, a portion of the coal reacts to form water. Because the RStoic model has a single outlet stream, use a Flash2 model to separate the dried coal from the moist nitrogen.



5 Place the flowsheet blocks and streams to create the graphical simulation flowsheet as shown in the figure above. (See *Getting Started Building and Running a Process Model*, Chapter 2, if you need to review how to create a graphical simulation flowsheet.)

6 As you place blocks and streams, Aspen Plus prompts you to enter the IDs. Enter the block IDs and click **OK**.

The simulation flowsheet above appears different from the process diagram in the previous figure because the simulation flowsheet uses two unit operation models to simulate a single piece of equipment. Also, the simulation flowsheet defines an extra stream (IN-DRIER) to connect the two simulation unit operation models. There is no real stream that corresponds to the simulation stream IN-DRIER.

Specifying Title, Stream Properties, and Global Options

1 From the Navigation Pane, go to **Setup | Specifications**.

The **Setup - Specifications** form displays default settings Aspen Plus uses for other sheets. 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 Solids with English Units template.

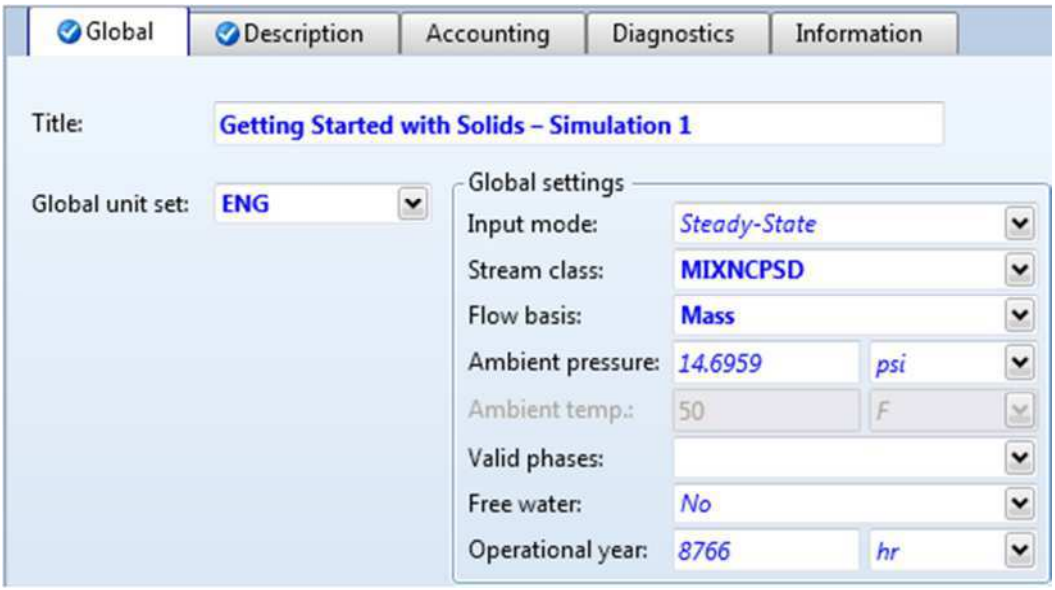
It is always good practice to describe your simulation by entering a title for the simulation.

2 In the **Title** field, enter the title **Getting Started with Solids – Simulation 1**.

In the Solids with English Units template, the following global defaults have been set for solids applications:

- **ENG** units (English Engineering Units)
- **Mass** Flow Basis for all flow inputs
- **MIXCISLD** for the global Stream class

3 In the **Stream class** field, click  and select **MIXNCPSD**.



Stream Classes and Substreams

Stream classes are used to define the structure of simulation streams when inert solids are present.

The default stream class for most simulations is CONVEN. The CONVEN stream class has a single substream: the MIXED substream. By definition, all components in the MIXED substream participate in phase equilibrium whenever flash calculations are performed.

To introduce inert solid components to a simulation, you must include one or more additional substreams. Aspen Plus has two other types of substreams available: the CISOLID substream type and the NC substream type.

The CISOLID substream (Conventional Inert Solid) is used for homogeneous solids that have a defined molecular weight. The NC substream (Nonconventional) is used for heterogeneous solids that have no defined molecular weight. Both the CISOLID substream and the NC substream give you the option of including a Particle Size Distribution (PSD) for the substream.

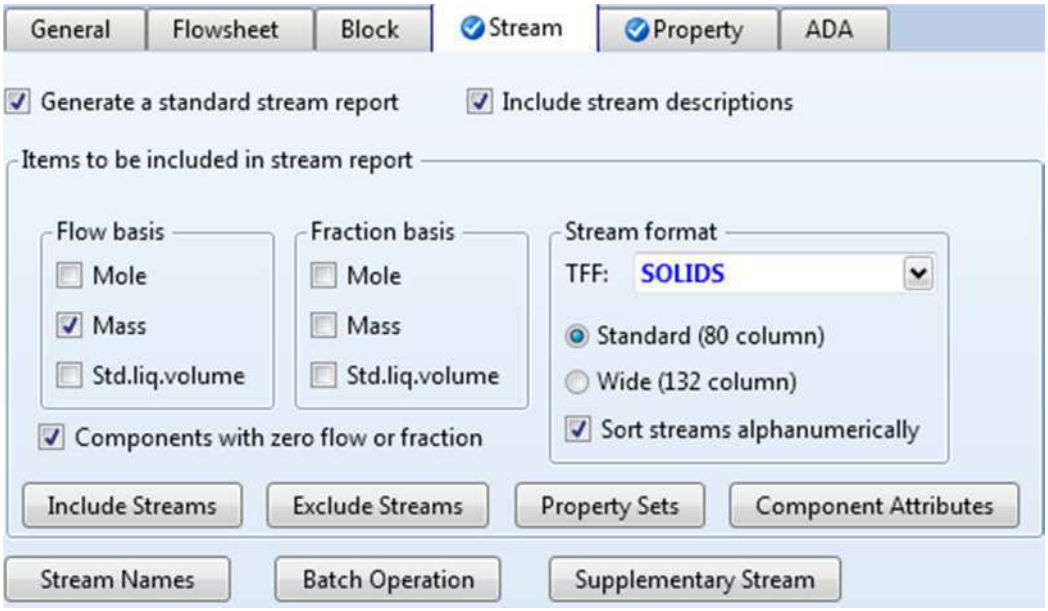
Substreams are combined in different ways to form different stream classes. The MIXNCPSD stream class contains two substreams: MIXED and NCPSD.

The default stream class of the Solids application type, MIXCISLD, is insufficient for this simulation since you will use an NC substream with a particle size distribution for the feed coal. In this simulation, use the MIXNCPSD stream class.

To Review the Report Options Specified in the Selected Template

4 From the Navigation Pane, click the **Setup | Report Options** form.

5 Click the **Stream** tab.



Since you chose the Solids with English Units template when you started this simulation, Aspen Plus has set the following defaults for calculating and reporting stream properties:

- The component mass flow rates will be included in the stream report.
- The stream results will be displayed using the **SOLIDS** stream format.
- Property set **ALL-SUBS** (properties for the entire stream, all substreams combined) will be reported for each stream.

6 Click **Property Sets** to view the selected property sets.

7 Click **Close** to return to the **Stream** sheet.

8 From the Quick Access Toolbar, click  to continue.

The **NITROGEN (MATERIAL) - Input | Mixed** sheet appears.

Entering Stream Data

To specify a stream, Aspen Plus requires two thermodynamic specifications, and enough information to calculate the flow rate of each component.

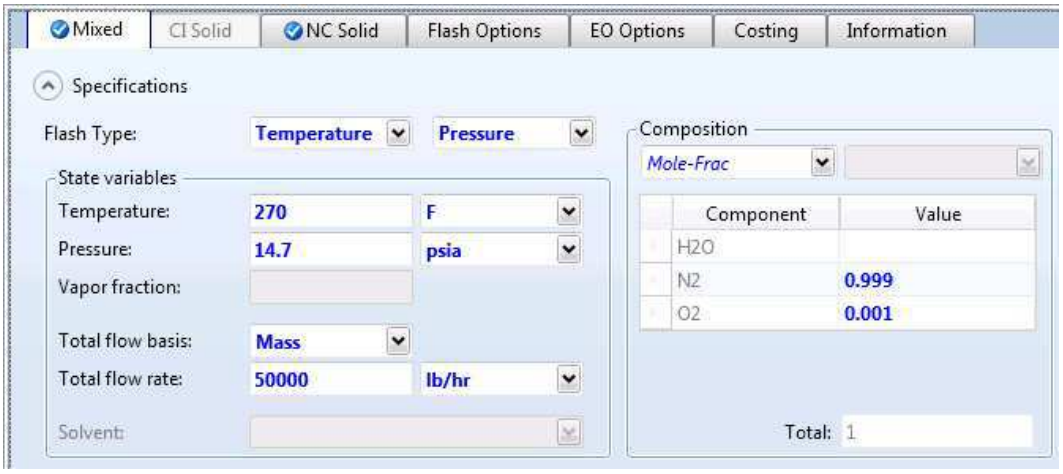
Specifying the Nitrogen Stream

1 On the **NITROGEN (MATERIAL) - Input | Mixed** sheet, enter the following specifications:

Parameter	Value
Temperature	270 F
Pressure	14.7 psia
Total flow	Mass 50000 lb/hr
Composition	Mole-Frac

2 Enter the following mole fractions:

Component	Value
N2	0.999
O2	0.001



3 Click to continue.

Specifying the Wet Coal Feed Stream

The **WET-COAL (MATERIAL) - Input | Mixed** sheet appears. Substream MIXED appears by default. To access the NCPSD substream:

4 Click the tab **NC Solid**. In the **Substream name** field, verify **NCPSD** has been selected.

5 For the NCPSD substream, enter the following specifications:

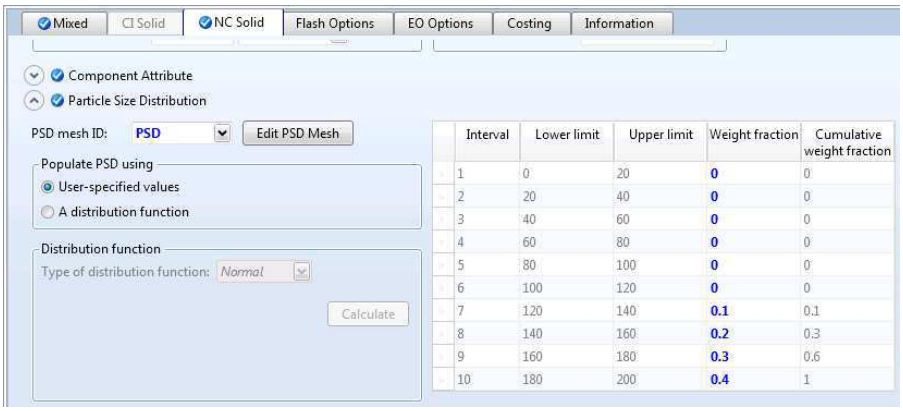
Parameter	Value
Temperature	77 F
Pressure	14.7 psia
COAL Mass flow	10000 lb/hr

6 Click **Particle Size Distribution** to display the PSD parameters.

By default, Aspen Plus uses a particle size distribution of 10 size ranges covering 20 microns each. The default size ranges are appropriate for this simulation. On this sheet, enter the weight fraction of coal in each size range.

7 On the last four **Weight fraction** fields, enter the following values:

Interval	Weight fraction
7	0.1
8	0.2
9	0.3
10	0.4

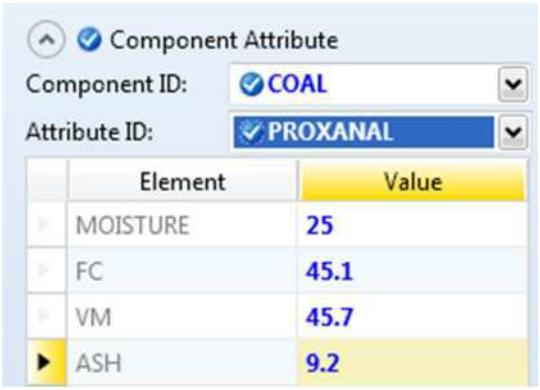


8 Click **Component Attribute**.

In this section, enter the component attributes for the component COAL in the NCPSD substream. The values in PROXANAL, ULTANAL, and SULFANAL are defined as weight % on a dry basis, except for Moisture in PROXANAL.

9 Enter the component attribute values for coal. For the attribute **PROXANAL**, enter these values:

Element	Value
Moisture	25
FC	45.1
VM	45.7
Ash	9.2



10 In the **Attribute ID** field, click  and select **ULTANAL**.

11 For the attribute ULTANAL, enter these values:

Element	Value
Ash	9.2
Carbon	67.1
Hydrogen	4.8
Nitrogen	1.1
Chlorine	0.1
Sulfur	1.3
Oxygen	16.4

12 In the **Attribute ID** field, click and select **SULFANAL**.

13 For the attribute SULFANAL, enter these values:

Element	Value
Pyritic	0.6
Sulfate	0.1
Organic	0.6

The values meet the following consistency requirements:

- SULFANAL values sum to the ULTANAL value for sulfur.
- ULTANAL value for ash equals the PROXANAL value for ash.
- ULTANAL values sum to 100.
- PROXANAL values for FC, VM, and ASH sum to 100.

14 Click to continue.

The **DRY-FLSH (Flash2) - Input | Specifications** sheet appears.

Specifying Blocks

The unit operation models RStoic and Flash2 simulate a single piece of plant equipment for drying coal. Nitrogen provides the heat for coal drying. Both the RStoic and Flash2 models are isobaric and adiabatic.

Specifying the Flash2 Block

On the **DRY-FLSH (Flash2) - Input | Specifications** sheet:

1 In the **Flash Type** fields, where **Temperature** is selected, click and change it to **Duty**.

2 In the **Pressure** field, enter **14.7** psia.

3 In the **Duty** field, enter **0** Btu/hr.

4 Click to continue.

Specifying the RStoic Block

The **DRY-REAC (RStoic) - Setup | Specifications** sheet appears.

1 In the **Pressure** field, enter **14.7** psia.

2 In the **Flash Type** fields, where **Temperature** is selected, click and change it to **Duty**.

3 In the **Heat duty** field, enter **0** Btu/hr.

4 Click to continue.

The **DRY-REAC (RStoic) - Setup | Reactions** sheet appears.

This RStoic block models the drying of coal. Although coal drying is not normally considered a chemical reaction, you are using an RStoic block to convert a portion of the coal to form water. The following equation is the chemical reaction for coal drying:

$$COAL(wet) \rightarrow 0.0555084\ H_2O$$

Aspen Plus treats all nonconventional components as if they have a molecular weight of 1.0. The reaction indicates that 1 mole (or 1 lb.) of coal reacts to form 0.0555084 mole (or 1 lb.) of water.

To Enter the Reaction Stoichiometry

1 Click **New**.

The **Edit Stoichiometry** dialog box appears. A reaction number of 1 is automatically chosen.

2 In the **Reactants | Component** field, click and select **COAL**.

3 In the **Reactants | Coefficient** field, enter **1**.

Note that the stoichiometric coefficient for reactants is displayed as negative, **-1**.

4 In the **Products | Component** field, click and select **H2O**.

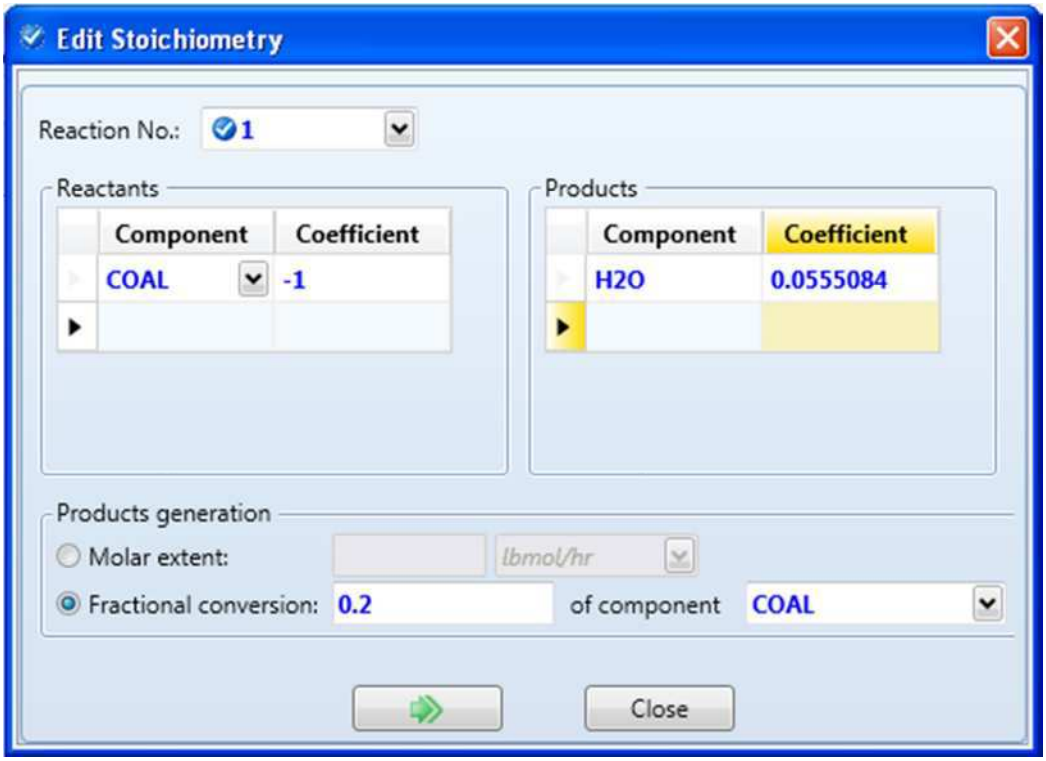
5 In the **Products | Coefficient** field, enter **0.0555084**.

The conversion for this reaction must be set to achieve the proper amount of drying.

6 Select the **Fractional conversion** option.

7 In the **Products generation** section, for the **Fractional conversion** field, enter **0.2**; in the **of component** field, click and select **COAL**.

The fraction conversion of Coal of 0.2 is a temporary value that you will override later with a Calculator block.



8 Click **Close** to return to the **DRY-REAC (RStoic) - Setup | Reactions** sheet.

Updating the Moisture Content

Drying the coal changes its component attribute for moisture in the Proximate Analysis. Since the other elements of PROXANAL, ULTANAL, and SULFANAL are on a dry basis, drying the coal does not change these attributes.

1 Click the **Component Attr.** tab. Click at the end of the row of tabs, if necessary, to access it.

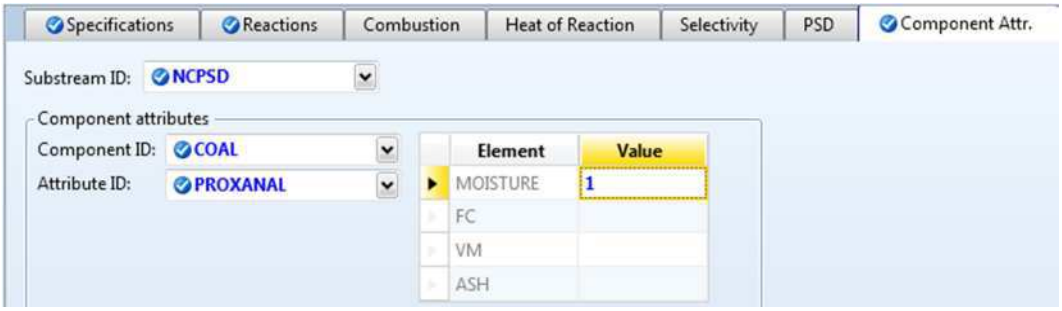
The **DRY-REAC (RStoic) - Setup | Component Attr.** sheet appears. On this sheet, enter the values for component attributes that change in this RStoic block. If you do not enter an attribute value, the attribute does not change.

2 In the **Substream ID** field, click and select **NCPSD**.

3 In the **Component ID** field, click and select **COAL**.

4 In the **Attribute ID** field, click and select **PROXANAL**.

5 In the **Moisture** field, enter a value of **1**. (The moisture content of 1 is a temporary value that you will override later with a Calculator block.)



6 Click to continue.

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

Although you could run your simulation now, you have not yet created the Calculator block to control the drying.

7 Click **Cancel**.

Using a Calculator Block to Control Drying

The material balance equations for this process define relations between the following quantities:

- Water content of the feed coal.
- Fractional conversion of coal to water.
- Water content of the dried coal.

$$COALIN \times \frac{H2OIN}{100} = COALOUT \times \frac{H2OOUT}{100} + COALIN \times CONV \quad (1)$$

$$COALIN = COALOUT + COALIN \times CONV \quad (2)$$

Where:

COALIN	=	Mass flow rate of coal in stream WET-COAL
COALOUT	=	Mass flow rate of coal in stream IN-DRIER
H2OIN	=	Percent moisture in the coal in stream WET-COAL
H2ODRY	=	Percent moisture in the coal in stream IN-DRIER
CONV	=	Fractional conversion of coal to H_2O in the block DRY-REAC

Equation 1 is the material balance for water, and equation 2 is the overall material balance. These equations can be combined to yield equation 3:

$$CONV = \frac{(H2OIN - H2OOUT)}{(100 - H2OOUT)} \quad (3)$$

Use equation 3 in a Calculator block to ensure these three specifications are consistent.

The Calculator block specifies the moisture content of the dried coal and calculates the corresponding conversion of coal to water.

Using a Calculator block to set specifications allows you to run different cases easily.

1 From the Navigation Pane, select **Flowsheeting Options | Calculator**.

The **Calculator** object manager appears.

2 Click **New** to create a new Calculator block.

The **Create New ID** dialog box appears, displaying an automatically generated Calculator ID, C-1.

3 Delete the ID **C-1** and enter the ID **WATER** and click **OK**.

The **WATER | Define** sheet appears.

4 Ensure that the **Active** checkbox is checked.

Use this sheet to access the flowsheet variables you want to use in the Calculator block. Define the three Calculator variables from equation 3: H2OIN, H2ODRY, and CONV.

H2OIN is the water content of the feed coal. The H2OIN variable accesses the first element (percent moisture) of the component attribute PROXANAL for component COAL in the NCPSD substream of stream WET-COAL.

Creating the H2OIN Variable

1 Click **New**.

The **Create new variable** dialog box appears.

2 In the **Variable name** field, enter **H2OIN** and click **OK**.

3 Click **H2OIN** in the grid. It appears in the **Edit selected variable** section.

4 In the **Category** frame, click **Streams**.

5 In the **Reference** frame, in the **Type** field, click and select **Compattr-Var** since the variable is a component attribute.

When you are specifying variables, Aspen Plus displays the other fields necessary to complete the variable definition. In this case, the **Stream** field appears.

6 In the **Stream** field, click and select **WET-COAL**.

The **Substream** and **Component** fields appear. In this example, do not modify the default choice of **NCPSD** in the **Substream** field.

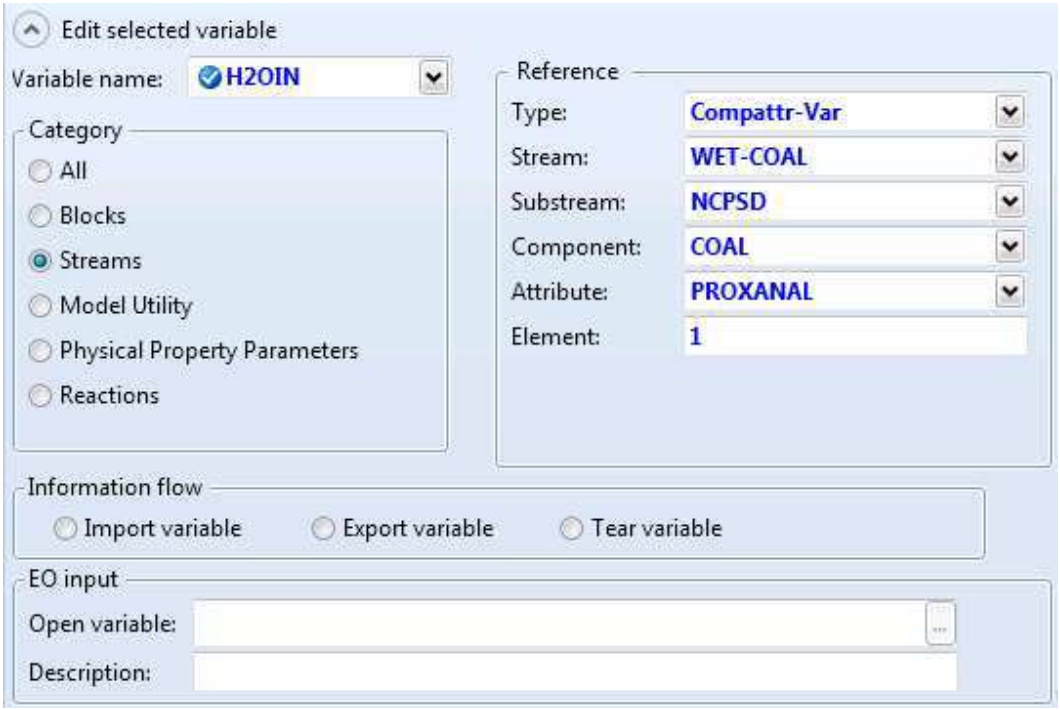
7 In the **Component** field, click and select **COAL**.

The **Attribute** field appears.

8 In the **Attribute** field, click and select **PROXANAL**.

9 In the **Element** field, enter **1**. Press **Enter**.

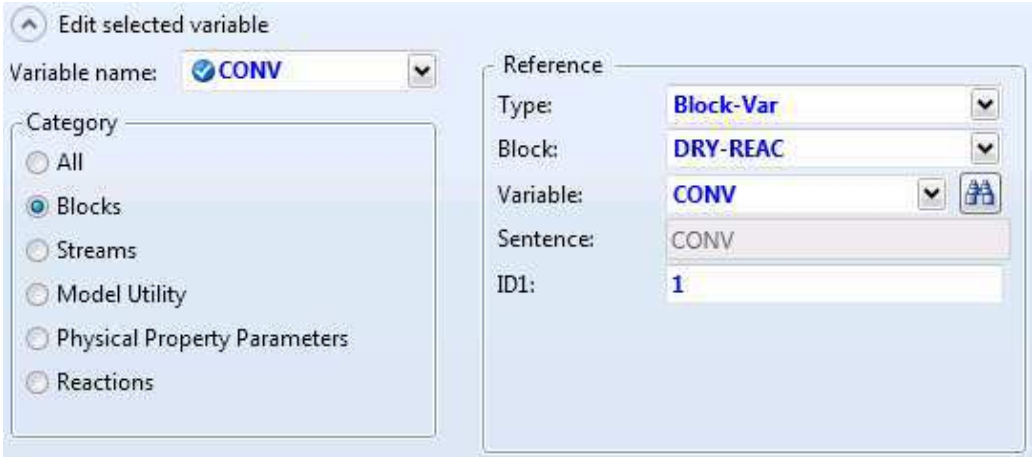
The blue check mark next to H2OIN in the **Variable name** field indicates that the definition of variable H2OIN is complete:

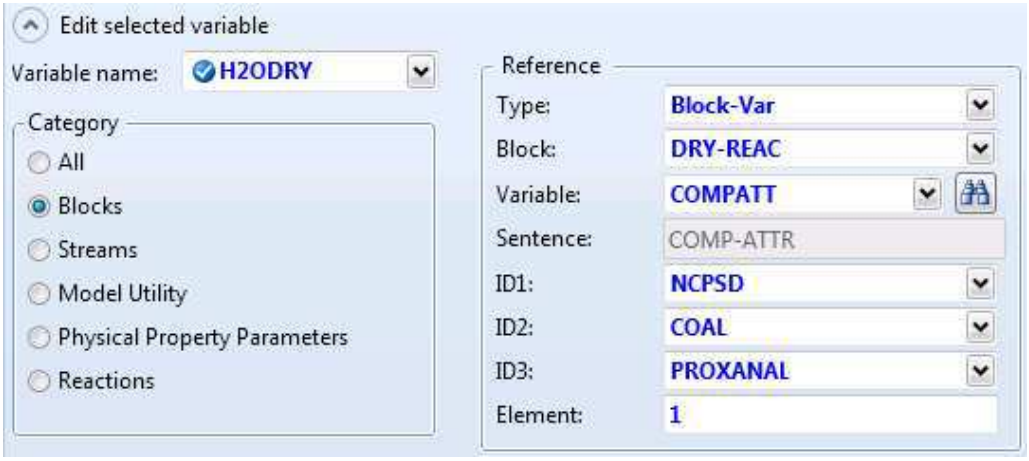


Creating the Other Variables

CONV and H2ODRY are block variables in the DRY-REAC block. CONV is the fractional conversion of the first (and only) reaction. H2ODRY is the moisture content of the coal leaving the RStoic block.

1 Click **New** to create another variable, **CONV**. Create the new **CONV** and **H2ODRY** variables as shown:





2 Click Next to continue.

Calculating the Conversion Variable

The **WATER | Calculate** sheet appears. Use this sheet to enter the Fortran statements you want Aspen Plus to execute to set H2ODRY and to calculate CONV from equation 3.

1 Enter the following Fortran statements:

```
H2ODRY = 10.0
CONV = (H2OIN - H2ODRY) / (100 - H2ODRY)
```

Note: Ensure that there are 6 spaces at the beginning of each line of the Fortran statements.

2 Click Next to continue.

Specifying When the Calculator Block Should Run

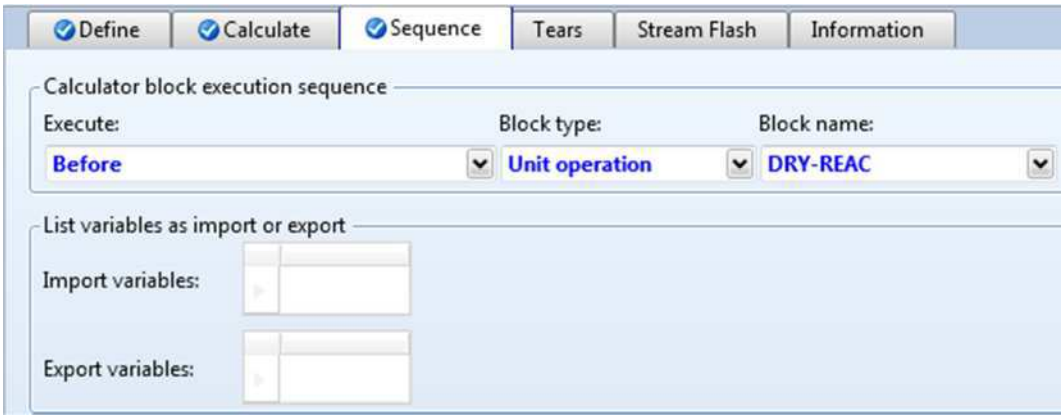
The **WATER | Sequence** sheet appears. Use this sheet to specify when Aspen Plus should execute this Calculator block. Since you have used inline

Fortran to modify the specifications for the RStoic block DRY-REAC, this Calculator block should execute immediately prior to DRY-REAC.

1 In the **Execute** field, click and select **Before**.

2 In the **Block type** field, click and select **Unit operation**.

3 In the **Block name** field, click and select **DRY-REAC**.



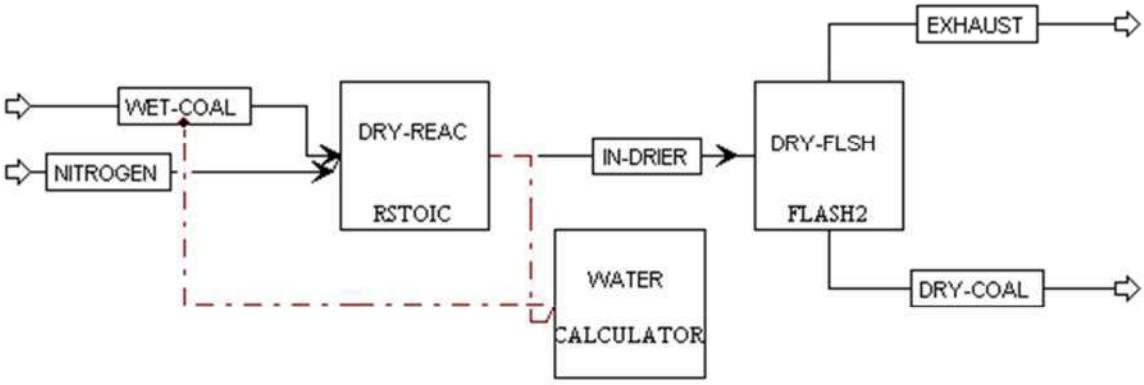
4 Click to continue.
The **Required Input Complete** dialog box appears.

5 Click **Cancel**.

Viewing the Calculator Block on the Flowsheet

Go to the Flowsheet to verify that the Calculator block **WATER** has been placed. If it does not appear, on the **Flowsheet | Modify** tab of the ribbon, click **Display Options** and click the **Calculators** and **Calculator Connections** options to make sure that check marks appear in front of these items.

The Flowsheet with the Calculator block added looks like this:



The connections between the WATER block and the block DRY-REAC and stream WET-COAL appear as red dashed lines.

Running the Simulation

1 Click and click **OK** to run the simulation.

The **Control Panel** window appears, allowing you to monitor and interact with the Aspen Plus simulation calculations.

As Aspen Plus performs the analysis, status messages display in the Control Panel.

The simulation completes without warnings or errors.

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

2 Examine the results of your simulation.

Examining Simulation Results

To View the Stream Results

1 In the Control Panel, click **Check Status**.

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

2 On the **Home** tab of the ribbon, in **Summary**, click **Stream Summary**.

The **Results Summary - Streams | Material** sheet appears.

Material | Heat | Load | Work | Vol.% Curves | Wt. % Curves | Petro. Curves | Poly. Curves

Display: All streams Format: SOLIDS Stream Table

	DRY-COAL	EXHAUST	IN-DRIER	NITROGEN	WET-COAL
Temperature F	116.6	116.6	116.6	270	77
Pressure psia	14.7	14.7	14.7	14.7	14.7
Mass VFrac	0	1	0.861	1	0
Mass SFrac	1	0	0.139	0	1
*** ALL PHASES ***					
Mass Flow lb/hr	8333.33	51666.7	60000	50000	10000
Volume Flow cuft/hr	96.255	789719	789816	950620	115.506
Enthalpy Btu/hr	-1.145e+07	-9.0964e+06	-2.0546e+07	2.40049e+06	-2.2947e+07
Density lb/cuft	86.576	0.065	0.076	0.053	86.576
Mass Flow lb/hr					
H2O		1666.67	1666.67		

3 Review the results on this sheet. Since this is a scrolling sheet, use the scrollbars to review results that are off the screen.

Aspen Plus populates the **Results Summary - Streams | Material** sheet using the **SOLIDS** format. The SOLIDS format reports results in three sections.

The top section reports the thermodynamic variables temperature pressure, vapor fraction, and solid fraction for the stream.

The second section, beginning with ***ALL PHASES***, reports properties and component mass flow rates summed over all substreams. Examination of the component mass flow rates indicates that 1667 lb/hr of H2O are removed from the coal by the drying process.

The third section, beginning with *** SUBSTREAM NCPSD ***, displays information that is appropriate only for the NCPSD substream. In this case, it displays the component attributes for coal, and the overall particle size distribution for the NCPSD substream. Note that the moisture in the PROXANAL is different for stream DRY-COAL and stream WET-COAL.

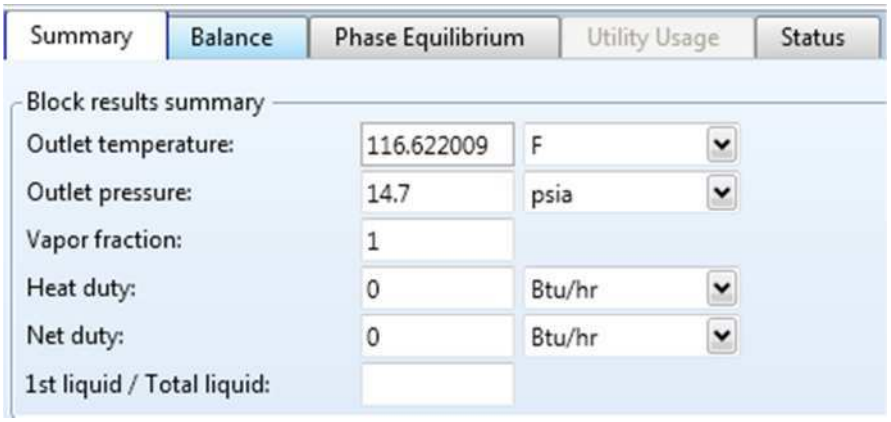
Stream summary results can also be displayed one substream at a time, by using the FULL format.

4 In the **Format** field, click and select **FULL**.

5 Examine the results reported for the MIXED and NCPSD substreams. When you are done, return to the SOLIDS Format.

6 From the Navigation Pane, expand the **Blocks** folder and select the **DRY-FLSH** folder. Click **Results**.

The **DRY-FLSH (Flash2) - Results | Summary** sheet appears. This sheet reports mixture thermodynamic properties for the block, such as outlet temperature.



To View the Block Results

7 Click the **Balance** tab.

The **DRY-FLSH (Flash2) - Results | Balance** sheet appears. This sheet is used to report the overall mass and energy balance for the block.

8 Click the **Phase Equilibrium** tab.

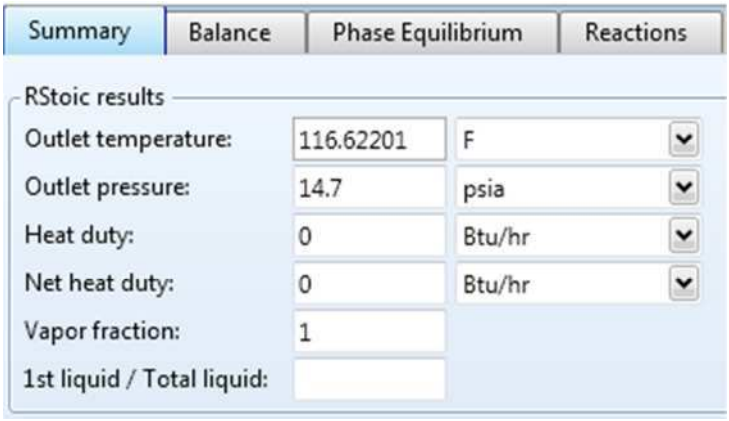
The **DRY-FLSH (Flash2) - Results | Phase Equilibrium** sheet appears. On this sheet, Aspen Plus reports the total molar flow rate, liquid mole fractions, vapor mole fractions and K-values. In this block, there is no liquid phase, so the liquid mole fractions and K-values refer to a hypothetical liquid phase.

9 Click **Blocks | DRY-FLSH | Stream Results** from the Navigation Pane.

The **DRY-FLSH (Flash2) - Stream Results | Material** sheet appears. This is similar to the **Results Summary - Streams | Material** sheet, but only lists streams entering or leaving this block.

10 Click **Blocks | DRY-REAC | Results** to move to the **DRY-REAC (RStoic) - Results | Summary** sheet.

This sheet, like the **DRY-FLSH (Flash2) - Results | Summary** sheet, displays the mixture thermodynamic results for the block, such as temperature.



11 Click the **Balance** tab to move to the next sheet with results.

The **DRY-REAC (RStoic) - Results | Balance** sheet appears. This sheet displays the mass and energy balance for the block. Because this block contains a reaction between the NCPSD substream and the MIXED substream, neither the conventional components nor the nonconventional are in mass balance. The total mass balance for the stream shows a very small relative difference.

12 Click the **Phase Equilibrium** tab to move to the next sheet with results.

The **DRY-REAC (RStoic) - Results | Phase Equilibrium** sheet appears. This sheet serves the same function as the **DRY-FLSH (Flash2) - Results | Phase Equilibrium** sheet.

Exiting Aspen Plus

When you are finished working with this model, save your simulation and exit Aspen Plus as follows:

1 From the ribbon, select **File | Save as | Aspen Plus Document**.

The **Save as** dialog box appears.

2 In the **File name** field, enter **Solid1**.

3 Click **Save**.

Aspen Plus saves the simulation as the Aspen Plus Document file, Solid1.apw, in your default working directory (displayed in the **Save in** field).

4 From the ribbon, select **File | Exit**.

Note: The chapter 2 simulation uses this run as the starting point.

2 Modeling Coal Combustion

In this simulation, you will simulate a coal combustion process.

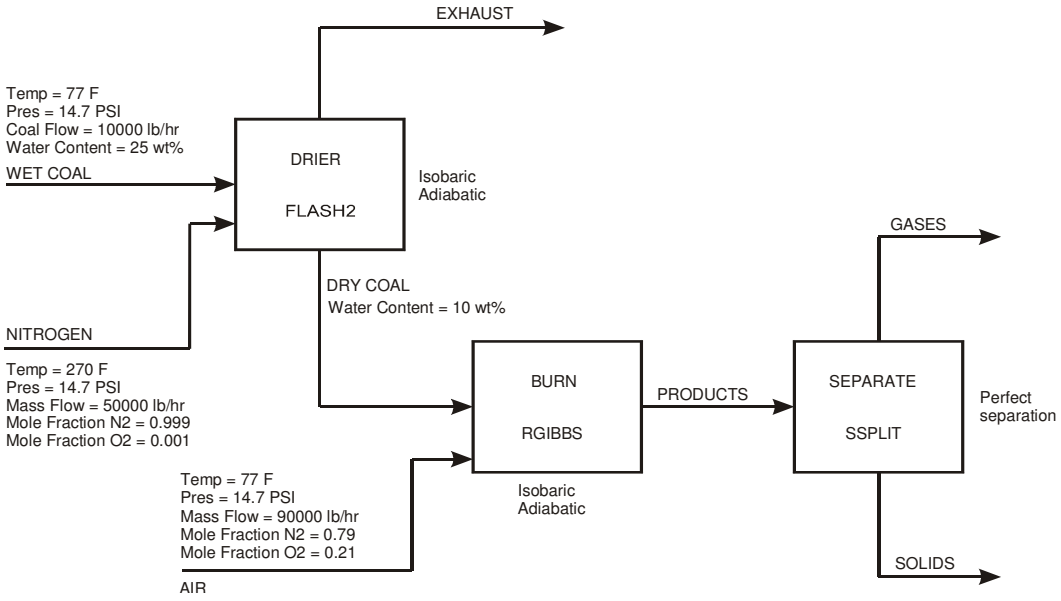
You will:

- Start with the simulation you created in chapter 1.
- Modify the flowsheet.
- Change the stream class.
- Add the components needed for combustion.
- Specify the unit operation models.
- Define a Fortran block to control the decomposition of coal.
- Analyze the results.

Allow about 45 minutes to complete this simulation.

Coal Combustion Flowsheet

The process flow diagram, operating conditions and problem definition for this simulation are shown in the following figure. The feed to the furnace is the dried coal stream from chapter 1. After combustion, the ash is separated from the gaseous combustion products.



Starting Aspen Plus

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

2 Select **AspenTech | Process Modeling <version> | Aspen Plus | Aspen Plus <version>**.

Opening an Existing Run

If You Completed the Simulation in Chapter 1 and Saved the Simulation

On the **Start Using Aspen Plus** window, click **Solid1.apw** in **Recent Models**.

If Your Saved File Solid1.apw is Not Displayed

1 Click **Open**.

The **Open** dialog box appears.

2 Navigate to the directory that contains your saved file Solid1.apw.

3 Select **Solid1.apw** in the list of files and click **Open**.

Note: If you did not create the simulation in chapter 1, open the backup file solid1.bkp from the **Examples** folder.

To Access the Examples Folder

1 Click **Open File**.

The **Open** dialog box appears.

2 At the left, under **Favorites**, click **Aspen Plus** <*version*> **Examples**.

By default, this folder contains folders that are provided with Aspen Plus.

3 Double-click the **Examples** folder, then the **GSG_Solids** folder.

4 Select **Solid1.bkp** and click **Open**.

Saving a Run Under a New Name

Before creating a new run, create and save a copy of Solid1 with a new Run ID, Solid2. Then you can make modifications under this new Run ID.

1 From the ribbon, select **File | Save As | Aspen Plus Document**.

2 In the **Save As** dialog box, choose the directory where you want to save the simulation.

3 In the **File name** field, enter **Solid2**.

4 Click **Save** to save the simulation and continue.

Aspen Plus creates a new simulation model, Solid2, which is a copy of the base case simulation, Solid1.

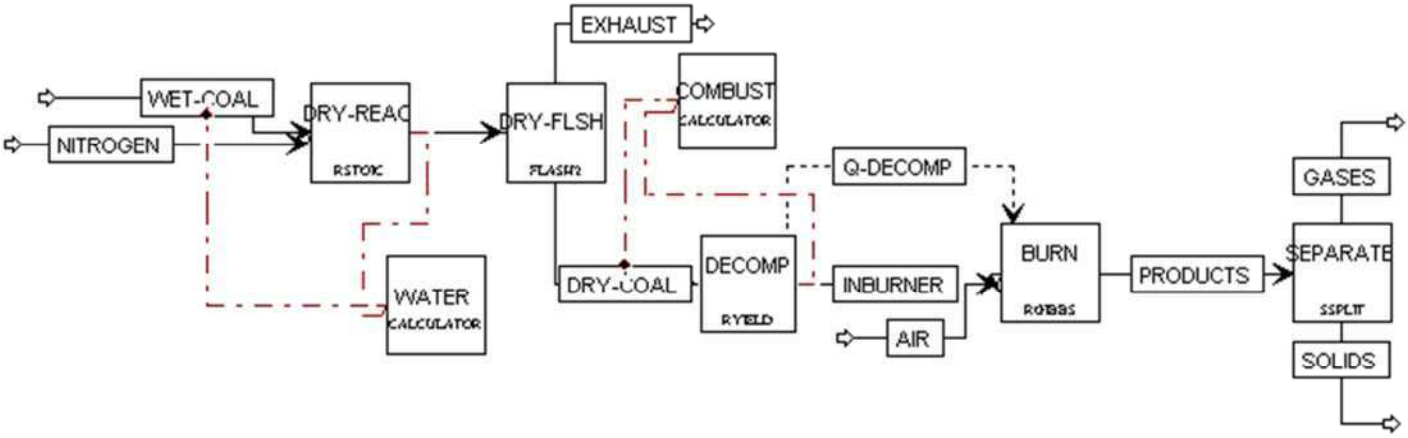
Modifying the Flowsheet

Use the RGibbs model to simulate combustion of the dry coal. RGibbs models chemical equilibrium by minimizing Gibbs free energy. However, the Gibbs free energy of coal cannot be calculated because it is a nonconventional component.

Before feeding the dried coal to the RGibbs block, decompose the coal into its constituent elements. This is done in the RYield block, DECOMP. The heat of reaction associated with the decomposition of coal must be considered in the coal combustion. Use a heat stream to carry this heat of reaction from the RYield block to the RGibbs block.

Finally, separate the combustion gases from the ash using the Aspen Plus model SSplit for this separation.

Modify the flowsheet to include the additional unit operation models and streams, as shown below. (See *Getting Started Building and Running a Process Model*, Chapter 2, if you need to review how to create a graphical simulation flowsheet.) You will add three unit operation models (an RYield, an RGibbs, and an SSplit), a calculator block (its connections, shown in red, will be created in the steps that follow), five material streams, and one heat stream.



The simulation flowsheet appears different from the process diagram in the previous figure because the simulation flowsheet uses two unit operation models to simulate a single piece of equipment. An extra stream (INBURNER) is defined to connect the two simulation unit operation models. There is no real stream that corresponds with the simulation stream INBURNER.

Changing the Stream Class

Because the decomposition of coal forms carbon, you must use a stream class that includes conventional solids. Use the **MCINCPSD** stream class. MCINCPSD contains the following substreams:

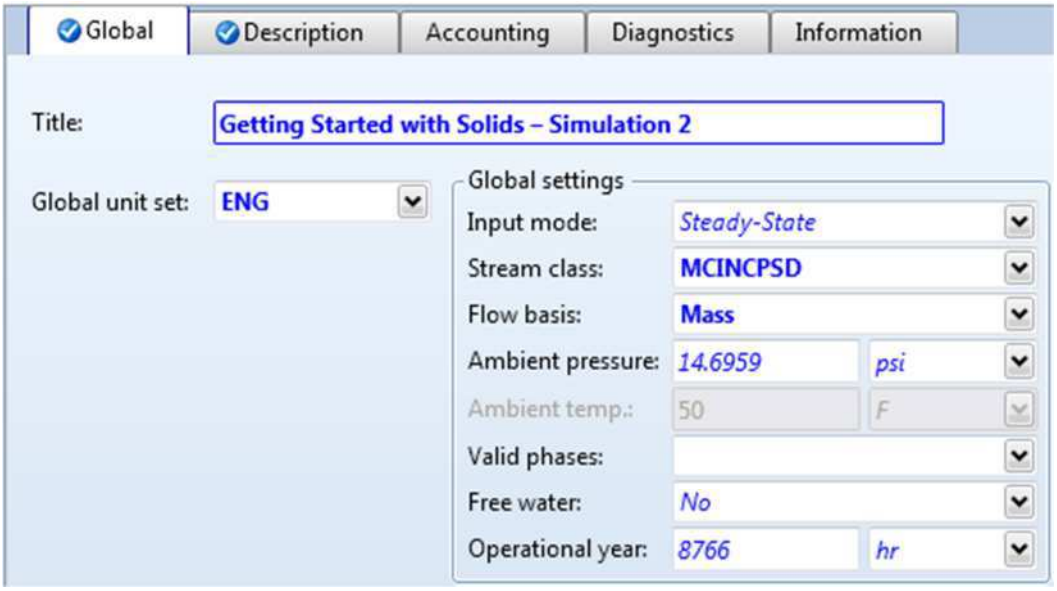
- MIXED
- CIPSD
- NCPSD

To Change the Global Stream Class

1 From the Navigation Pane, go to **Setup | Specifications**.
The **Setup - Specifications | Global** sheet appears.

2 In the **Stream class** field, click  and select **MCINCPSD**.

3 In the **Title** field, enter **Getting Started with Solids – Simulation 2**.



Adding Components to the Model

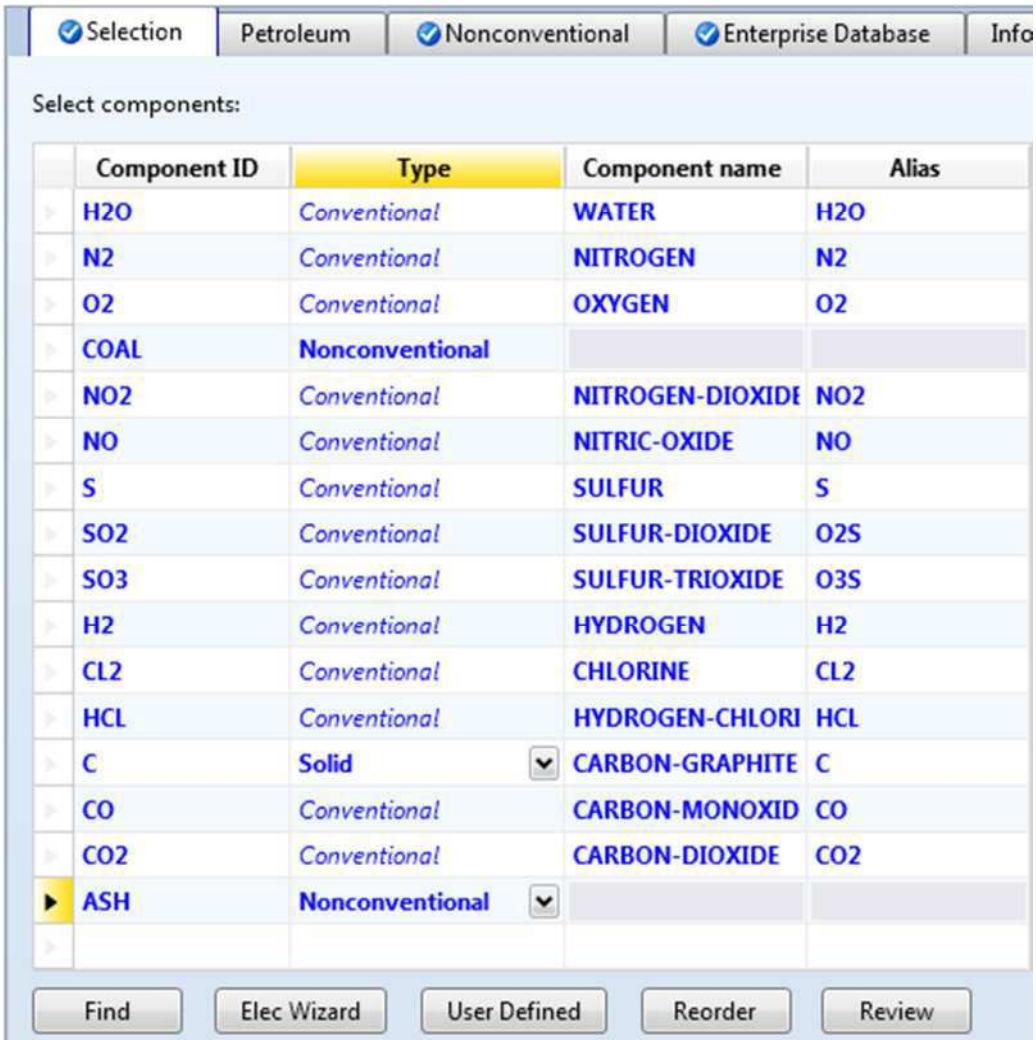
Simulation 1 had four components: H2O, N2, O2, and COAL. Add the components that are formed by decomposing and combusting coal.

First of all, you need to enter the **Properties** environment.

1 Click the **Properties** bar on the Navigation Pane.

2 Go to the **Components - Specifications | Selection** sheet. Add the components listed below:

Component ID	Type	Component Name
NO2	Conventional	NITROGEN DIOXIDE
NO	Conventional	NITRIC OXIDE
S	Conventional	SULFUR
SO2	Conventional	SULFUR-DIOXIDE
SO3	Conventional	SULFUR-TRIOXIDE
H2	Conventional	HYDROGEN
CL2	Conventional	CHLORINE
HCL	Conventional	HYDROGEN-CHLORIDE
C	Solid	CARBON-GRAPHITE
CO	Conventional	CARBON-MONOXIDE
CO2	Conventional	CARBON-DIOXIDE
ASH	Nonconventional	



Note that you assigned Carbon a **Type** of **Solid**. Specifying a component type of Solid allows that component to be placed in the CIPSD substream.

3 Click N to continue.

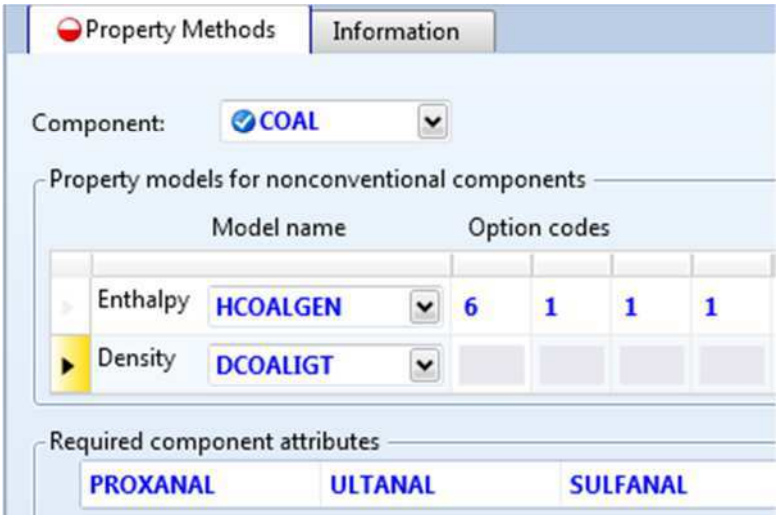
The **Methods - NC Props | Property Methods** sheet appears.

Defining Properties

Use the **Methods - NC Props | Property Methods** sheet to specify the models used to calculate the nonconventional solid properties. In Simulation 1, Aspen Plus estimates the heat of coal combustion based on its PROXANAL, ULTANAL, and SULFANAL. In this simulation, enter the heat of combustion directly.

Change the Heat of Combustion Method for Coal

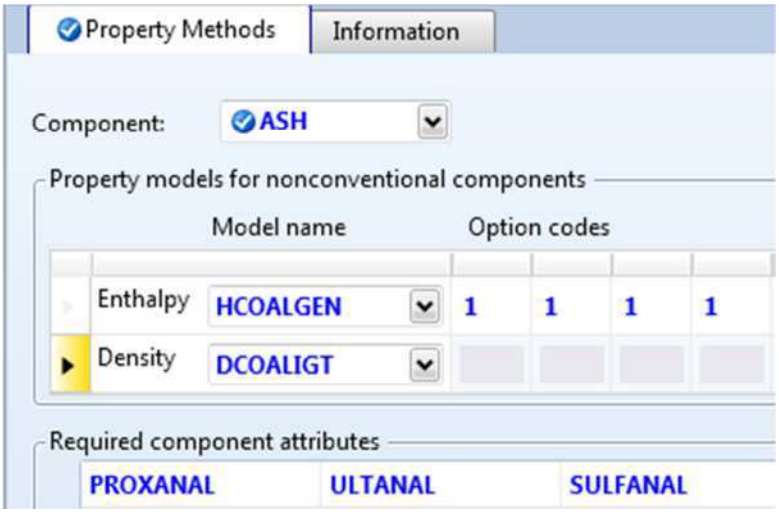
1 In the **Component** field, click and select **COAL**.
2 Change the first HCOALGEN **Option codes** field from **1** to **6**.



Specify Methods for Calculating Ash Properties

You must also specify how Aspen Plus calculates the enthalpy and density of ASH.

1 In the **Component** field, click and select **ASH**.
2 In the **Model name** field for **Enthalpy**, click and select **HCOALGEN**. The **Option codes** defaults of **1**, **1**, **1**, and **1** are acceptable for ASH.
3 In the **Model name** field for **Density**, click and select **DCOALIGT**.



Specify the Heat of Combustion for Coal

You just specified that Aspen Plus will use a user-specified value for the heat of combustion of coal. Now you must specify that value.

1 From the Navigation Pane, select **Methods | Parameters | Pure Components**.

The **Pure Components** object manager appears.

2 Click **New**.

The **New Pure Component Parameters** dialog box appears. The heat of combustion for coal is a Nonconventional type.

3 Select the **Nonconventional** option.

4 Delete the default name **NC-1** and enter **HEAT** as the new name in the **Enter new name or accept default** field.

5 Click **OK**.

The **Pure Components - HEAT | Input** sheet appears.

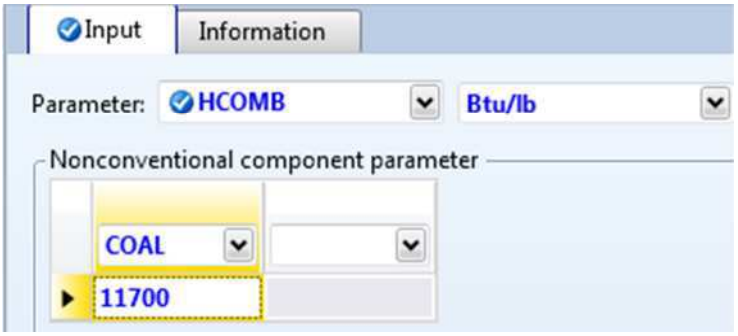
6 In the **Parameter** field, click and select **HCOMB**.

Note that HCOMB is the heat of combustion on a dry basis. Use the following equation to convert the heat of combustion on a wet basis to a dry basis:

$$\text{HCOMB} = \text{Heat of Combustion (wet)} * \frac{100}{100 - \%\ \text{Moisture}}$$

7 In the first line under the **Nonconventional component parameter** column, click and select **COAL**.

8 In the parameter value field directly below COAL, enter the heat of combustion on a dry basis: **11700** Btu/lb.



9 Click to continue.

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

10 Select **Go to Simulation environment** and click **OK** to access the next required input sheet in the Simulation Environment.

Specifying the Air Stream

Click **Streams | AIR | Input** from the Navigation Pane. The **AIR (MATERIAL) - Input | Mixed** sheet appears. Aspen Plus requires two

thermodynamic specifications, and enough information to calculate the flow rate of each component.

1 Enter the following thermodynamic specifications for the **MIXED** substream:

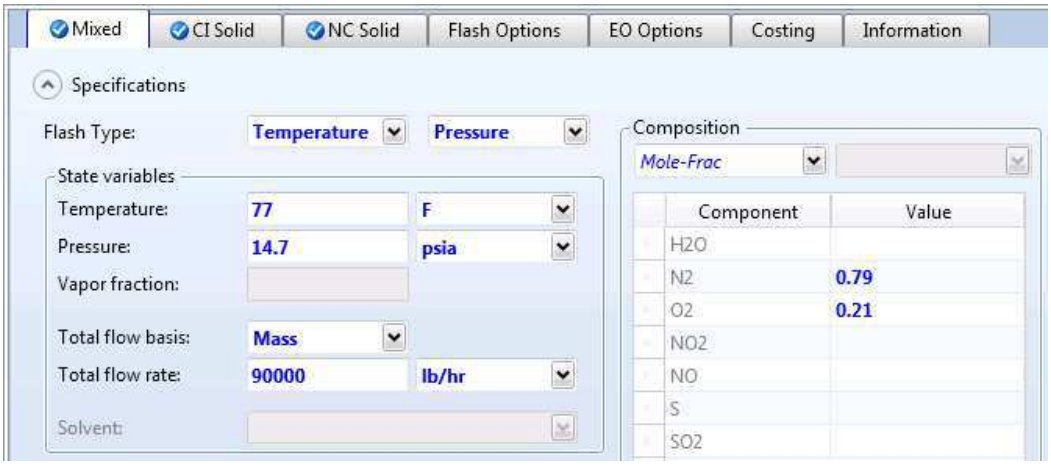
Parameter	Value
Temperature	77 F
Pressure	14.7 psia

2 In the **Composition** field, click and select **Mole-Frac**.

3 Enter the following mole fractions:

Component	Value
N2	0.79
O2	0.21

4 Enter a total mass flow of **90000** lb/hr.



5 Click to continue.

Specifying Unit Operation Models

The **BURN (RGibbs) - Setup | Specifications** sheet appears.

RGibbs is used to model reactions that come to chemical equilibrium. RGibbs calculates chemical equilibrium and phase equilibrium by minimizing the Gibbs free energy of the system. Therefore, you do not need to specify the reaction stoichiometry.

Specify the RGibbs Reactor Model

On the **BURN (RGibbs) - Setup | Specifications** sheet, enter your thermodynamic specifications. This reactor will be at atmospheric pressure.

1 In the **Pressure** field, enter **14.7** psia.

The heat duty for this reactor is specified by the heat stream Q-DECOMP.

2 In the **Calculation options** field, verify that **Calculate phase equilibrium and chemical equilibrium** has been selected.

3 Click the **Products** tab.

The **BURN (RGibbs) - Setup | Products** sheet appears. On this sheet, enter the list of products that may exist at equilibrium.

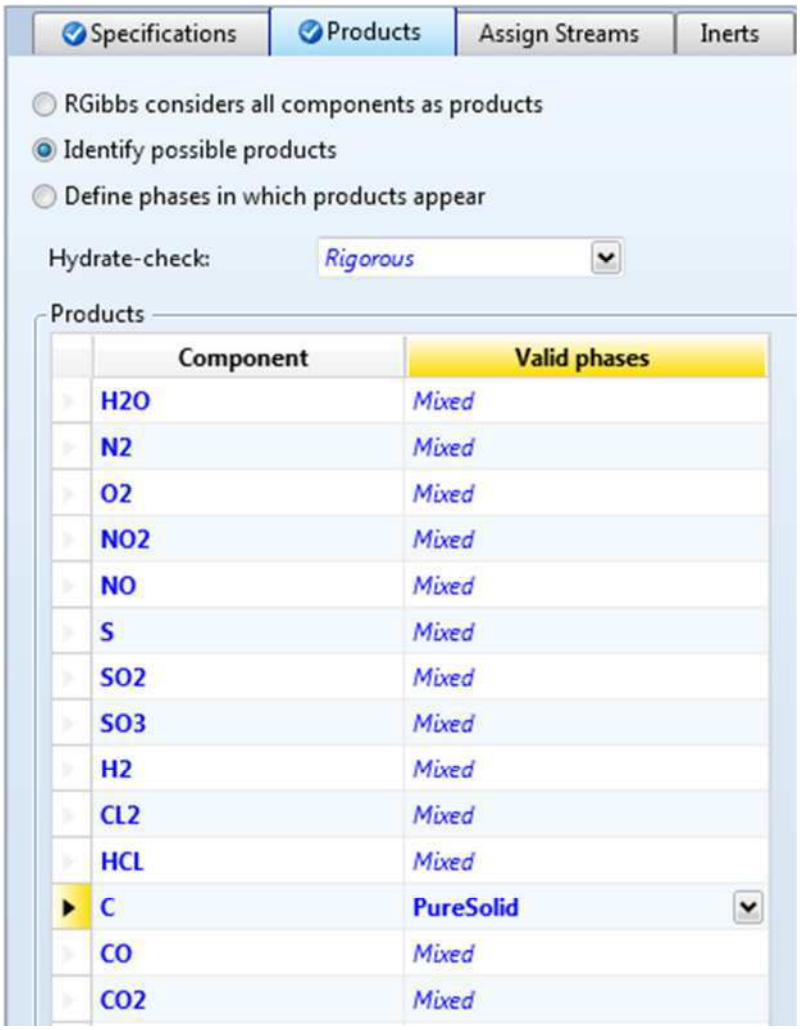
By default, RGibbs assumes that all of the components that are listed on the **Components - Specifications | Selection** sheet are potential products in the vapor phase or the liquid phase. This default is not appropriate for this simulation, since any carbon that remains after combustion would be solid.

4 Select **Identify possible products**.

The **Products** list appears. For this simulation, all components are potential MIXED substream products, except for carbon, which is a solid product. Carbon must be assigned a phase of Pure Solid. This means that any carbon that forms will be present as a pure, solid phase, not present as a solid solution or alloy.

5 In the products list, enter the component species and phases shown below: (Be sure to change the Phase for **C** to **PureSolid**.)

Component	Phase	Component	Phase
H2O	Mixed	SO3	Mixed
N2	Mixed	H2	Mixed
O2	Mixed	CL2	Mixed
NO2	Mixed	HCL	Mixed
NO	Mixed	C	PureSolid
S	Mixed	CO	Mixed
SO2	Mixed	CO2	Mixed



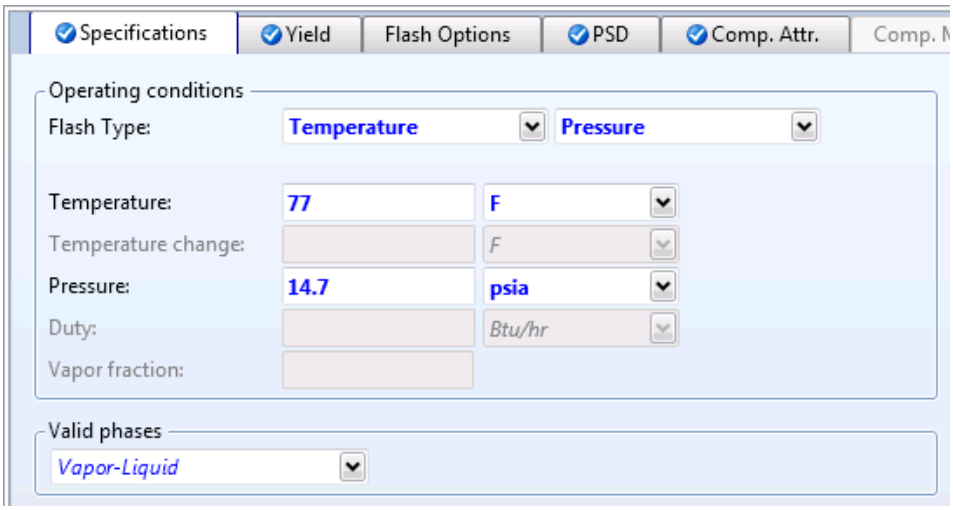
6 Click N to continue.

Specify the RYield Reactor Model

The **DECOMP (RYield) - Setup | Specifications** sheet appears. RYield is used to simulate a reactor with a known yield, and does not require reaction stoichiometry and kinetics.

1 On the **DECOMP (RYield) - Setup | Specifications** sheet, enter the pressure and temperature:

Parameter	Value
Pressure	14.7 psia
Temperature	77 F



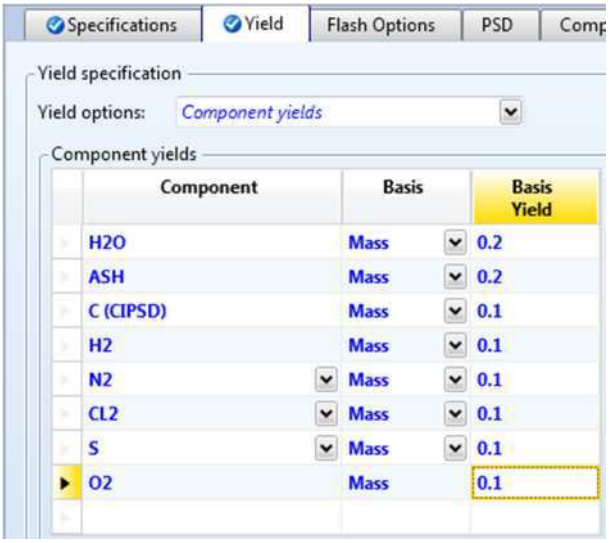
2 Click N to continue.

The **Yield** sheet appears.

For this simulation, the yield distribution you enter on this sheet is not the true yield distribution. Use a Calculator block to calculate the actual yield distribution from the component attributes for coal in the feed stream to the RYield model (stream DRY-COAL).

3 Enter the component yields as follows:

Component	Basis	Yield
H2O	Mass	0.2
ASH	Mass	0.2
C (CIPSD)	Mass	0.1
H2	Mass	0.1
N2	Mass	0.1
CL2	Mass	0.1
S	Mass	0.1
O2	Mass	0.1



In addition to the MIXED substream products, this RYield block forms carbon in the CIPSD substream and ash in the NCPSD substream. To fully specify the yield, specify the particle size distributions of the CIPSD and NCPSD substream and the component attributes of the ash that is formed.

Specify the Particle Size Distributions

1 Click the **PSD** tab.

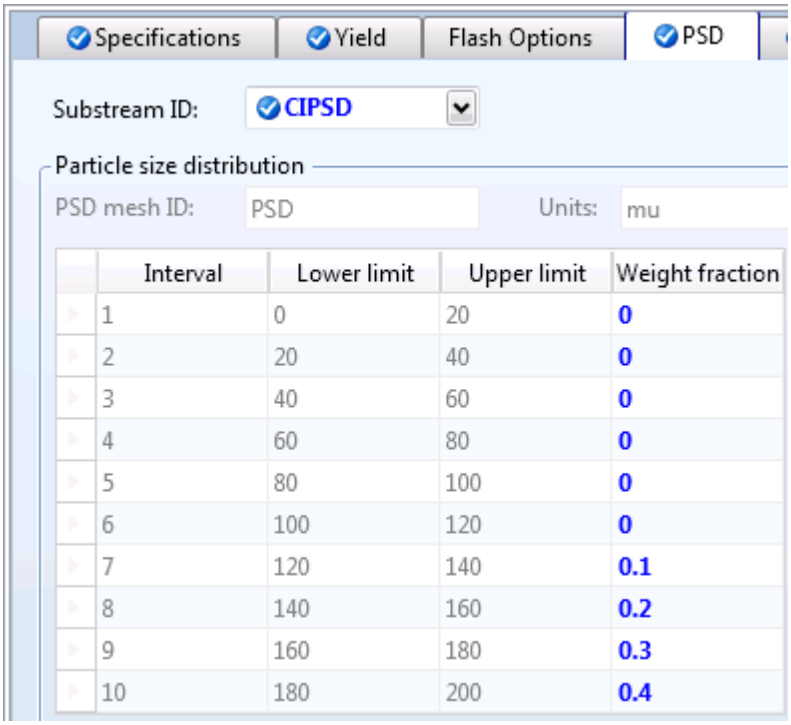
The **DECOMP (RYield) - Setup | PSD** sheet appears.

2 In the **Substream ID** field, click and select **CIPSD**.

3 Specify the weight fractions for the last four intervals of the particle size distribution for the carbon formed in the CIPSD substream:

Interval	Weight Fraction
7	0.1
8	0.2
9	0.3
10	0.4

It is not necessary to enter zero for intervals 1 through 6.



You must also define the particle size distribution for the NCPSD substream.

4 In the **Substream ID** field, click and select **NCPSD**.

5 Enter the same weight fractions for the particle size distribution for the NCPSD substream that you entered for the CIPSD substream above.

Specify the Component Attributes for Ash

1 Click the **Comp. Attr.** tab.

The attributes PROXANAL, ULTANAL, and SULFANAL are required for RYield to calculate the enthalpy and density of ash.

2 In the **Substream ID** field, click and select **NCPSD**.

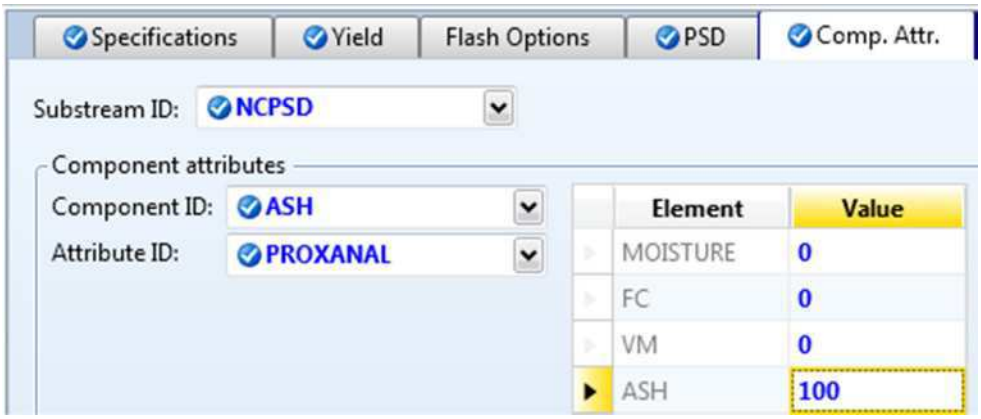
3 In the **Component ID** field, click and select **ASH**.

ASH has the attributes PROXANAL, ULTANAL, and SULFANAL.

4 In the **Attribute ID** field, click and select **PROXANAL**.

5 For the attribute PROXANAL, enter these values:

Element	Value
Moisture	0
FC	0
VM	0
Ash	100



6 In the **Attribute ID** field, click and select **ULTANAL**.

7 For the attribute ULTANAL, enter these values:

Element	Value
Ash	100
Carbon	0
Hydrogen	0
Nitrogen	0
Chlorine	0
Sulfur	0
Oxygen	0

8 In the **Attribute ID** field, click and select **SULFANAL**.

9 For the attribute SULFANAL, enter these values:

Element	Value
Pyritic	0

Element	Value
Sulfate	0
Organic	0

10 Click to continue.

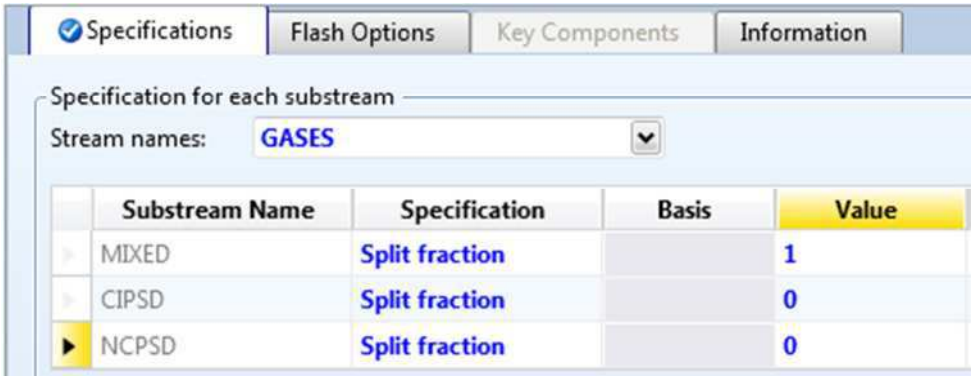
Specify the Splits for the SSplit Block

The **SEPARATE (SSplit) - Input | Specifications** sheet appears. SSplit mixes all of its feed streams, then splits the resulting mixture into two or more streams according to substream specifications. SSplit operates on substreams the same way a Sep block operates on components.

In this simulation, the SSplit block provides perfect separation between the gaseous products of combustion (MIXED substream) and the solid products of combustion (CIPSD and NCPSD substreams).

1 Enter the following split fraction values for the **GASES** outlet stream:

Substream Name	Value
MIXED	1
CIPSD	0
NCPSD	0



Defining a Calculator Block

You have completed enough specifications to run the simulation. However, the yields you specified in the RYield block were only temporary placeholders. You could directly enter the correct yields on the **DECOMP (RYield) - Setup | Yield** sheet. However, by defining a Calculator block to calculate the yields based on the component attributes of the feed coal, you will be easily able to run different cases (such as different feed coals).

Create the Calculator Block

1 From the Navigation Pane, select **Flowsheeting Options | Calculator**. The **Calculator** object manager appears.

2 Click **New** to create a new Calculator block.

The **Create New ID** dialog box appears with an automatically generated ID, C-1.

3 In the **Create New ID** dialog box, enter **COMBUST** as the ID and click **OK**.

Define the Calculator Variables

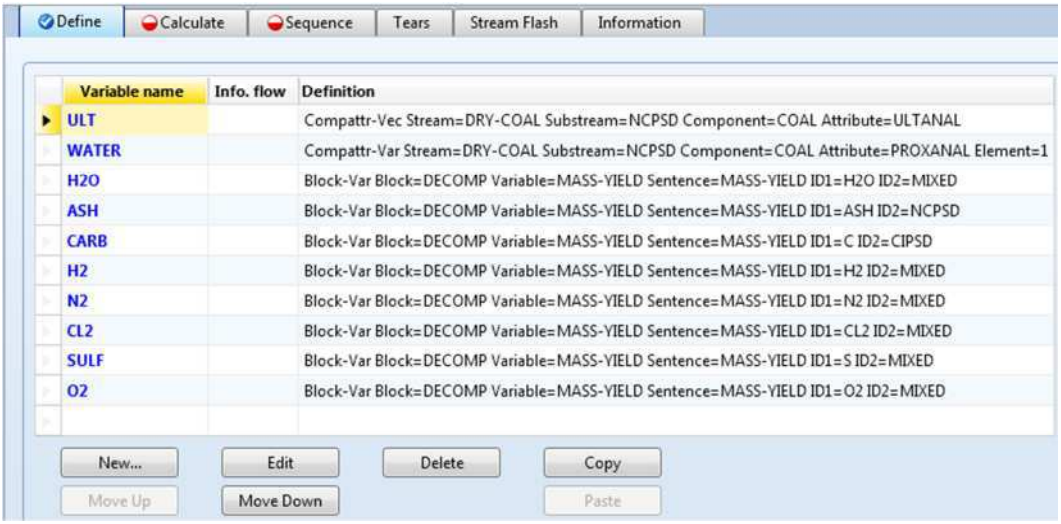
The **COMBUST | Define** sheet appears. Use this sheet to access the flowsheet variables you want to use in the Fortran block. In the simulation in chapter 1, you accessed individual elements of component attributes. You can also access component attributes as a vector. In this simulation, access the ultimate analysis of coal in stream DRY-COAL as a component attribute vector; also, define variables to access the moisture content of coal and the yield of each component in the DECOMP block.

4 Create and define the following two variables using category **Streams**:

Variable Name	Type	Stream	Substream	Component	Attribute	Element
ULT	Compattr-Vec	DRY-COAL	NCPSD	COAL	ULTANAL	
WATER	Compattr-Var	DRY-COAL	NCPSD	COAL	PROXANAL	1

5 Also define the following eight mass yield variables using category **Blocks**.

Variable Name		ID1	ID2
H2O	Type **Block-Var** Block **DECOMP** Variable **MASS-YIELD** for all eight variables.	H2O	MIXED
ASH		ASH	NCPSD
CARB		C	CIPSD
H2		H2	MIXED
N2		N2	MIXED
CL2		CL2	MIXED
SULF		S	MIXED
O2		O2	MIXED



6 Click the **Calculate** tab.

Specify the Calculations to be Performed

The **COMBUST | Calculate** sheet appears. ULTANAL is defined as the ultimate analysis on a dry basis. The variable WATER, defined as the percent H2O in the PROXANAL for coal, is used to convert the ultimate analysis to a wet basis. The remaining eight variables (H2O through O2) are defined as the individual component yields of various species in the RYield block. ULT and WATER can then be used to calculate the yield of the individual species in the RYield block.

7 Enter the following Fortran statements:

```
C      FACT IS THE FACTOR TO CONVERT THE ULTIMATE ANALYSIS TO
C      A WET BASIS.
       FACT = (100 - WATER) / 100
       H2O = WATER / 100
       ASH = ULT(1) / 100 * FACT
       CARB = ULT(2) / 100 * FACT
       H2 = ULT(3) / 100 * FACT
       N2 = ULT(4) / 100 * FACT
       CL2 = ULT(5) / 100 * FACT
       SULF = ULT(6) / 100 * FACT
       O2 = ULT(7) / 100 * FACT
```

Note: These calculations assume that the inlet stream consists entirely of coal. That is true for this problem, but may not be true in other problems you work with. A good way of handling the multi-component case is to insert a Sep before the RYield and a Mixer after it, allowing all non-coal components to bypass the RYield block.

8 Click the **Sequence** tab.

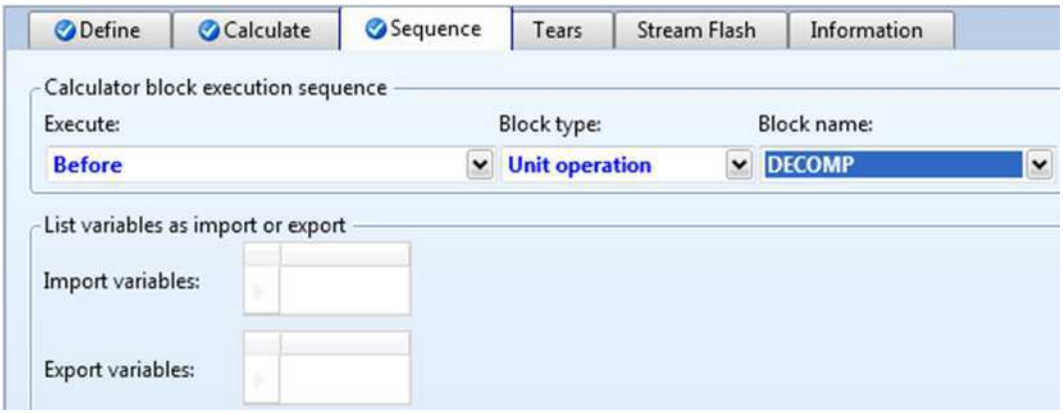
Specify When the Calculator Block Should be Run

The **COMBUST | Sequence** sheet appears. Since this Calculator block sets values in block DECOMP, the Calculator block must execute before DECOMP.

9 In the **Execute** field, click  and select **Before**.

10 In the **Block type** field, click  and select **Unit operation**.

11 In the **Block name** field, click  and select **DECOMP**.



12 Click to continue.

Running the Simulation

1 In the **Required Input Complete** dialog box, click **OK** to run the simulation.

The **Control Panel** window appears, allowing you to monitor and interact with the Aspen Plus simulation calculations.

Aspen Plus issues warnings while processing input specifications. The warnings report that a certain physical property parameter for carbon is outside the range considered normal by Aspen Plus.

Aspen Plus uses warnings to alert you that it has encountered some unexpected or possibly ambiguous situation. In this case, you can safely ignore the warnings because the simulation is specified exactly as you intended.

As Aspen Plus performs the analysis, you will see status messages displayed in the Control Panel. No further warnings are generated.

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

2 Examine the results of your simulation.

Examining Results

View the Stream Results

1 In the Control Panel, click **Check Status**.

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

2 On the **Home** tab of the ribbon, in **Summary**, click **Stream Summary** to access the streams results sheet.

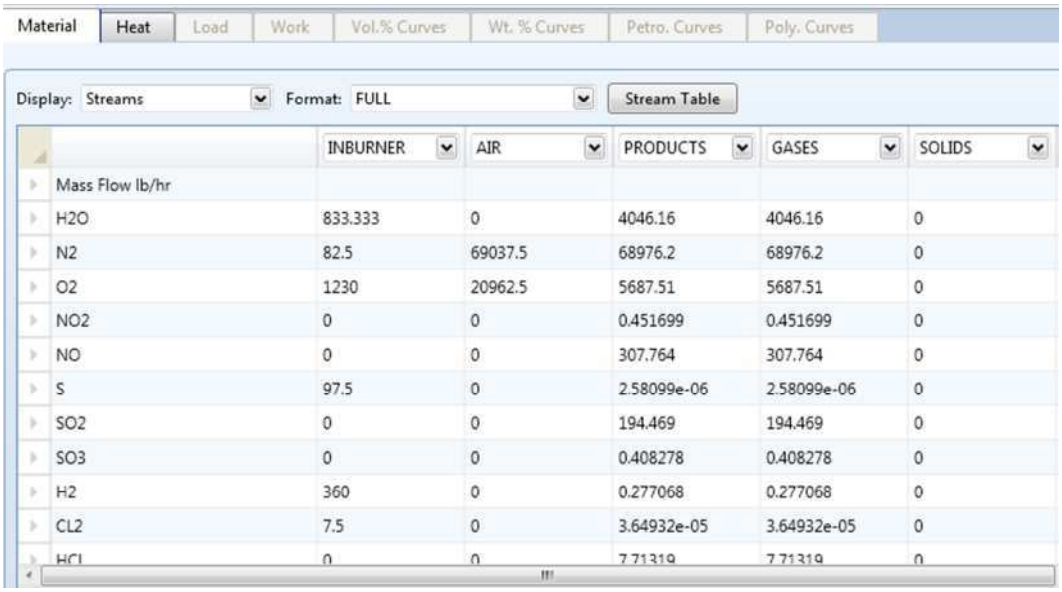
The **Results Summary - Streams | Material** sheet appears.

3 Review the results on this sheet. Use the horizontal scrollbar to review results that are off the screen.

4 In the Display field, click and select **Streams**.

5 At the top of each column, click and select **INBURNER**, **AIR**, **PRODUCTS**, **GASES**, and **SOLIDS**.

Results are filled in for each stream as it is specified.



	INBURNER	AIR	PRODUCTS	GASES	SOLIDS
Mass Flow lb/hr					
H2O	833.333	0	4046.16	4046.16	0
N2	82.5	69037.5	68976.2	68976.2	0
O2	1230	20962.5	5687.51	5687.51	0
NO2	0	0	0.451699	0.451699	0
NO	0	0	307.764	307.764	0
S	97.5	0	2.58099e-06	2.58099e-06	0
SO2	0	0	194.469	194.469	0
SO3	0	0	0.408278	0.408278	0
H2	360	0	0.277068	0.277068	0
CL2	7.5	0	3.64932e-05	3.64932e-05	0
HCL	0	0	7.71319	7.71319	0

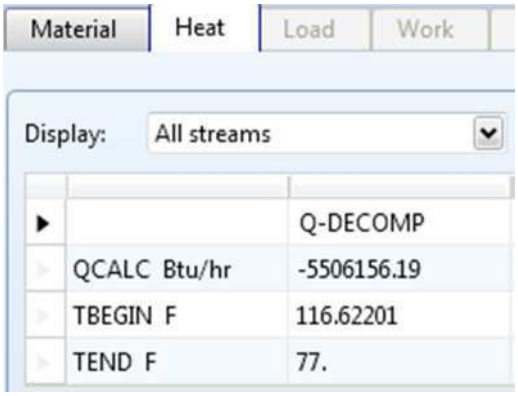
6 Review the results on this sheet. Use the scrollbars to review results that are off the screen.

Stream PRODUCTS is the outlet of the RGibbs equilibrium reactor that models the combustion process. Since oxygen appears in stream PRODUCTS, the combustion process has excess air. An examination of stream PRODUCTS enables you to determine the most stable products for each atom in the combustion process:

- SO2 is favored over SO3 and S.
- N2 is favored over NO and NO2.
- CO2 is favored over CO and C (solid).
- HCL is favored over CL2.

7 Click the **Heat** tab to access the next results sheet.

The **Results Summary - Streams | Heat** sheet appears. This sheet is displays the results for heat streams. Examine the results for Q-DECOMP. The heating value of Q-DECOMP represents the enthalpy change in breaking down the coal in stream DRY-COAL into its constituent elements.



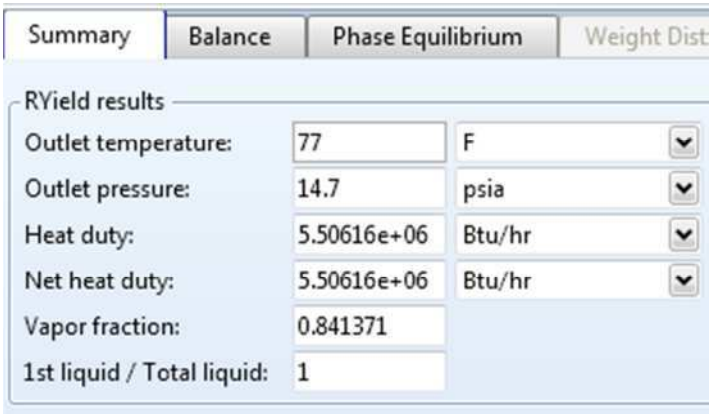
View the Block Results

You do not need to view the results for Blocks DRY-REAC and DRY-FLSH, since they are unchanged from Simulation 1. View the results for blocks DECOMP, BURN, and SEPARATE.

1 In the Flowsheet, select the DECOMP block.

2 Right-click DECOMP and select **Results** from the menu.

The **DECOMP (RYield) - Results | Summary** sheet appears. This sheet reports the outlet thermodynamic conditions for the block.



3 Click the **Balance** tab to access the next results sheet.

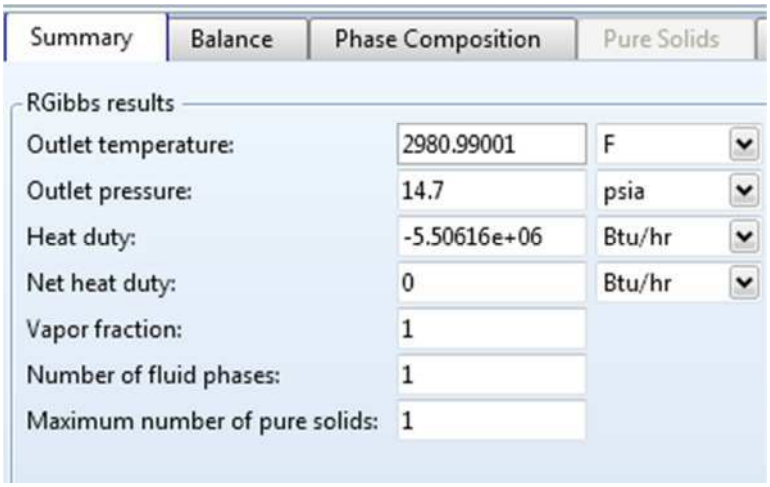
The **DECOMP (RYield) - Results | Balance** sheet appears. Use this sheet to report the mass and energy balance for the block. Because RYield has a net reaction from nonconventional components to conventional components, the mass balance for both conventional components and nonconventional components is out of balance. However, the total mass balance is in balance.

4 Click the **Phase Equilibrium** tab to access the next results sheet.

The **DECOMP (RYield) - Results | Phase Equilibrium** sheet appears. This sheet indicates that the liquid from the RYield block is a solution of water and sulfur. In actuality, the sulfur would form a solid at this temperature. However, this fact does not matter for this simulation, because the stream (coal broken down into its constituents) does not exist in a real combustion process. This stream exists only as a mathematical construct to simplify the specification of the combustion process.

5 In the Navigation Pane, expand the list of forms for the **BURN** block and select **Results**.

The **BURN (RGibbs) - Results | Summary** sheet appears. This sheet reports the outlet thermodynamic conditions of the RGibbs block. The outlet temperature is the adiabatic flame temperature of the coal with a fixed amount of excess air.



6 Click the **Balance** tab to access the next results sheet.

The **BURN (RGibbs) - Results | Balance** sheet appears.

7 Click the **Phase Equilibrium** tab to access the next results sheet.

The **BURN (RGibbs) - Results | Phase Composition** sheet appears. This sheet displays the mole fraction of components in all phases. In this case, there is only a vapor phase.

8 Click the **Atom Matrix** tab to access the next results sheet.

The **BURN (RGibbs) - Results | Atom Matrix** sheet appears. This sheet reports the atomic composition for each component.

9 In the Navigation Pane, expand the list of forms for the **SEPARATE** block and select **Results**.

The **SEPARATE (SSplit) - Results | Summary** sheet appears. This sheet reports the split fraction for each substream.

Exiting Aspen Plus

When finished working with this model, exit Aspen Plus as follows:

1 From the ribbon, select **File | Exit**.

The **Aspen Plus** dialog box appears.

2 Click **Yes** to save the simulation.

Aspen Plus saves the simulation as the Aspen Plus Document file, Solid2.apw, in your default working directory (displayed in the **Save in** field).

Note: The chapter 3 simulation uses this run as the starting point.

3 Modeling Gas-Solid Separators

In this simulation, start with the simulation developed in chapter 2, and add a rigorous gas-solid separation train to separate the ash from the combustion gases.

You will:

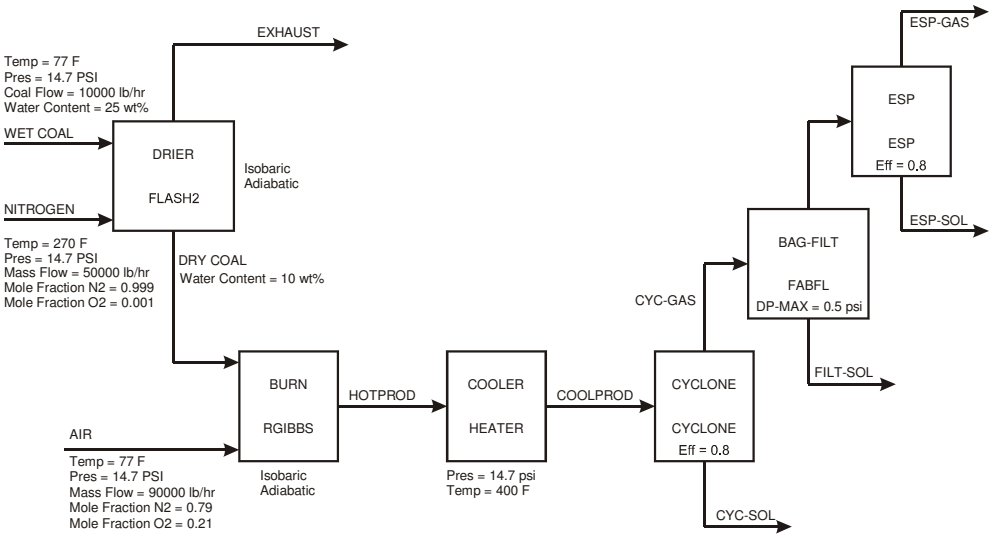
- Modify the flowsheet.
- Modify the default particle size intervals.
- Use solids-handling unit operation models.

Allow about 20 minutes to do this simulation.

Gas-Solid Separation Flowsheet

The process flow diagram and operating conditions for this simulation are shown in the following figure.

The combustion products from Simulation 2 are fed to a rigorous gas-solid separation train. Once the products are cooled, solids are removed from the gases by a cyclone, a fabric filter, and an electrostatic precipitator in series.



Starting Aspen Plus

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

2 Select **AspenTech | Process Modeling <version> | Aspen Plus | Aspen Plus <version>**.

Opening an Existing Run

If You Completed the Simulation in Chapter 2 and Saved the Simulation

In the **Start Using Aspen Plus** window, click the link to **Solid2.apw** under **Recent Models**.

If Your Saved File Solid2.apw is Not Displayed

1 Click **Open**.

The **Open** dialog box appears.

2 Navigate to the directory that contains your saved file Solid2.apw.

3 Select **Solid2.apw** in the list of files and click **Open**.

Note: If you did not create the simulation in Chapter 2, open the backup file Solid2.bkp in the Examples folder.

To Access the Examples Folder

1 Click **Open File**.

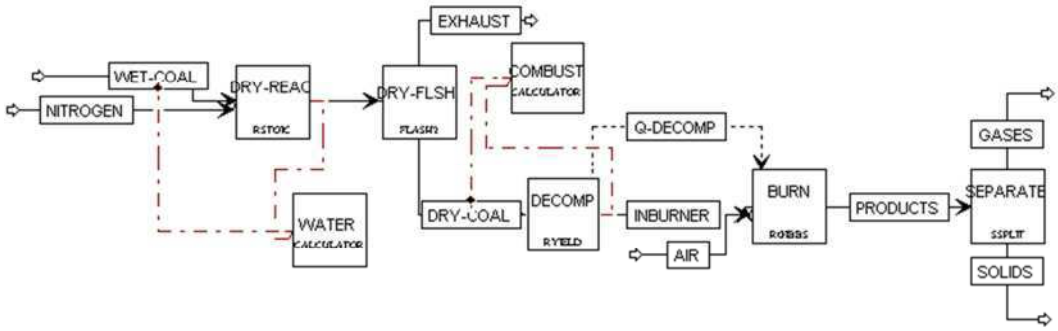
The **Open** dialog box appears.

2 At the left, under **Favorites**, click **Aspen Plus** <*version*> **Examples**.
By default, this folder contains folders that are provided with Aspen Plus.

3 Double-click the **Examples** folder, then the **GSG_Solids** folder.

4 Select **Solid2.bkp** and click **OK**.

The process flowsheet from chapter 2 appears:



Saving a Run Under a New Name

Before creating a new run, create and save a copy of Solid2 with a new Run ID, Solid3. Then you can make modifications under this new Run ID.

1 From the ribbon, select **File | Save As | Aspen Plus Document**.

2 In the **Save As** dialog box, choose the directory where you want to save the simulation.

3 In the **File name** field, enter **Solid3**.

4 Click **Save** to save the simulation and continue.
Aspen Plus creates a new simulation model, Solid3, which is a copy of the base case simulation, Solid2.

Modifying the Flowsheet

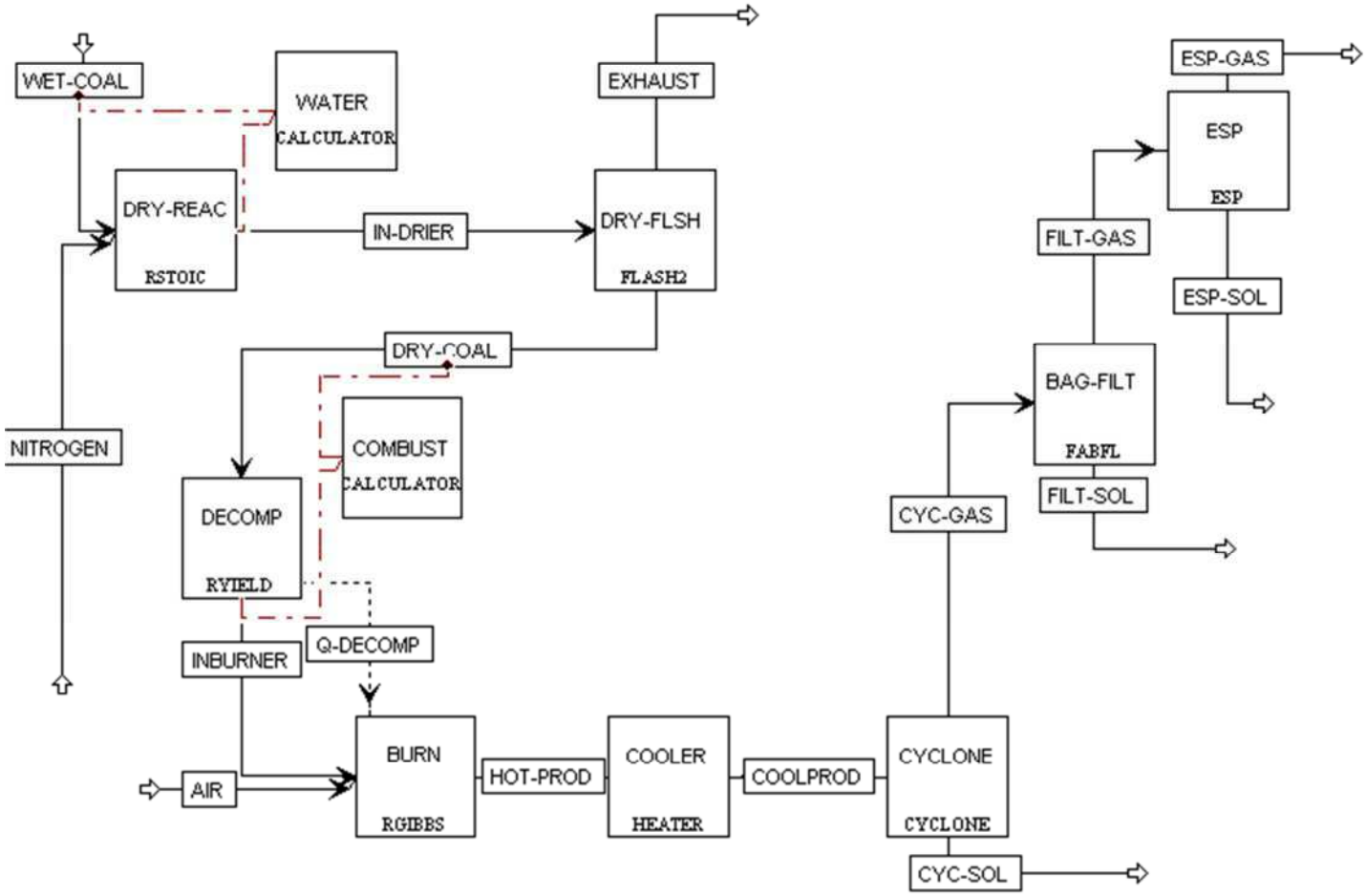
In the previous simulation, the SSplit block after combustion assumed perfect separation of the ash from the combustion gases. In the simulation in this chapter, replace the SSplit block with the following blocks in series: Heater, Cyclone, FabFl, and ESP.

1 Click and drag a region around the SSplit block and its product streams.

2 Press **Delete** on the keyboard.

3 In the **Confirm Delete** dialog box, click **OK** to delete the group.

4 Draw the flowsheet shown below. (See *Getting Started Building and Running a Process Model*, chapter 2, if you need to review how to create a graphical simulation flowsheet.) Change the name of the product stream of the RGibbs block and connect it to the new Heater block.



Changing the Default Particle Size Distribution

To Update the Title for This Simulation

1 From the Navigation Pane, select **Setup | Specifications**.
The **Setup - Specifications | Global** sheet appears.
2 Enter the new title **Getting Started with Solids - Simulation 3**.

Next, modify the system defaults for the size intervals in a particle size distribution.

To Modify the Particle Size Distribution Intervals

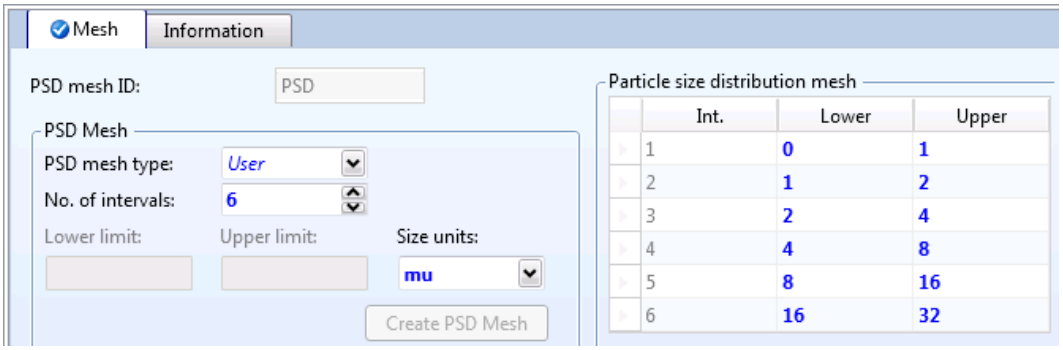
1 From the Navigation Pane, expand the **Setup | Solids** folder.
2 From the **Solids** folder, select **PSD**.

The **Solids - PSD | Mesh** sheet appears. Use this sheet to modify the default particle size distribution.

3 In the **No. of intervals** field, enter **6**.

4 Enter the following six intervals to describe the particle size distribution. Each **Upper** value is automatically copied to the next **Lower** value.

Interval	Lower [mu]	Upper [mu]
1	0	1
2	1	2
3	2	4
4	4	8
5	8	16
6	16	32



Updating Particle Size Distributions Previously Entered

Changing the intervals of the particle size distribution (PSD) modifies the particle size distributions you entered in the previous simulations.

1 In the Navigation Pane, select the **Streams | WET-COAL | Input** form.

2 Click the **NC Solid** tab.

The **WET-COAL (MATERIAL) - Input | NC Solid** sheet appears.

3 Click the arrow in front of **Particle Size Distribution** to display the data sheet for PSD.

The original PSD for this stream used size intervals 7 through 10. Since you just deleted intervals 7 through 10, the PSD is now empty and you must provide a new PSD. Because the coal is combusted before it reaches any of the solids-handling unit operation models, an accurate PSD for coal is not necessary.

4 Enter a value of **1** for the **Weight Fraction** between 16 and 32 microns.

You must also modify the particle size distribution you specified in the RYield block DECOMP.

5 In the Navigation Pane, select the **Blocks | DECOMP | Setup** form.

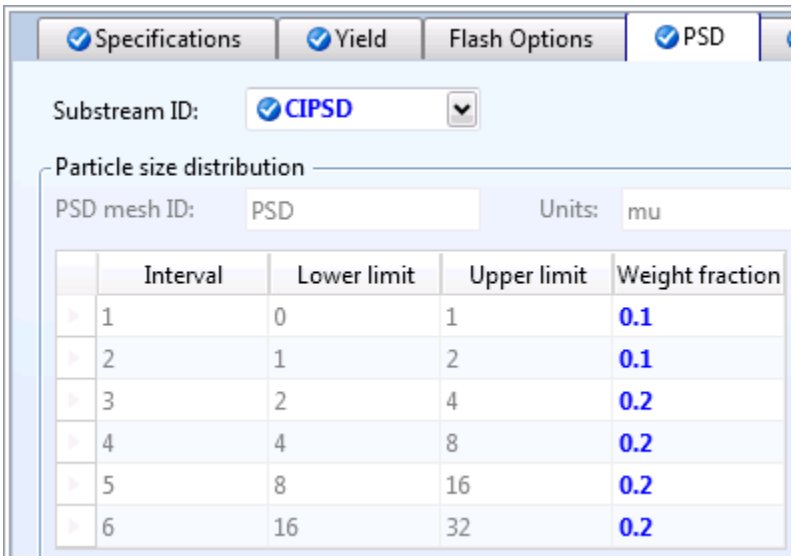
6 Click the **PSD** tab.

The **DECOMP (RYield) - Setup | PSD** sheet appears.

7 In the **Substream** field, click and select **CIPSD**.

8 Enter the following values of **Weight fraction** for the CIPSD substream. These particle size distributions are chosen for illustrative purposes only and are not meant to be typical of an industrial application.

Interval	Weight Fraction
1	0.1
2	0.1
3	0.2
4	0.2
5	0.2
6	0.2



9 In the **Substream** field, click and select **NCPSD**.

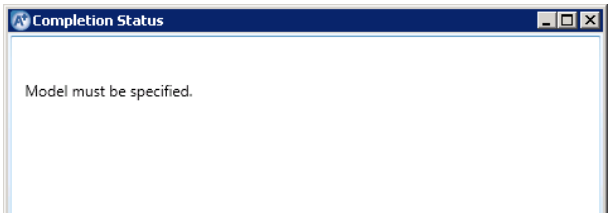
10 Enter the same weight fractions for the particle size distribution for the NCPSD substream that you entered for the CIPSD substream above.

11 Click to continue.

Specifying the Solids-Handling Blocks

The **BAG-FILT (FabFl) - Input | Specifications** sheet appears.

1 Click to find out what must be specified on this sheet.



2 Close the **Completion Status** window.

Use the design mode of the fabric filter model (FabFl), not the simulation mode. Simulation mode determines the capacity of an existing piece of equipment. Design mode determines the size of a new piece of equipment with a given capacity.

3 In the **Model** field, click and select **Fabric Filter**.

4 In the **Mode** field, click and select **Design**.

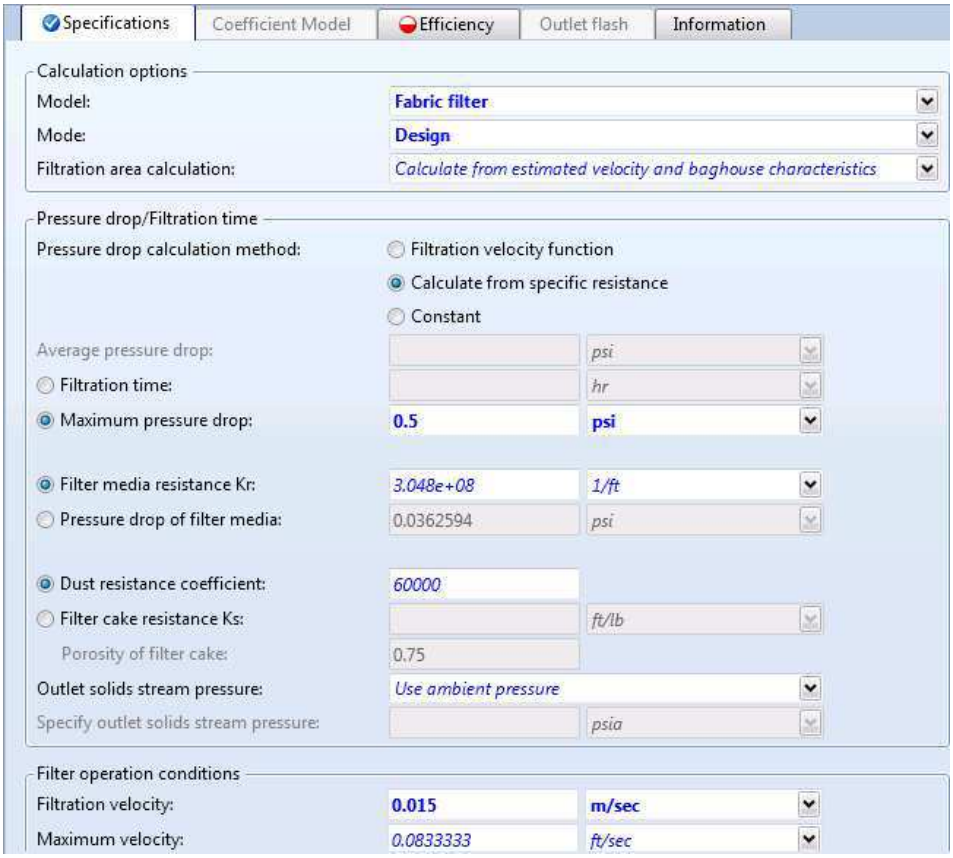
5 Click to determine what input is required for the FabFl model in design mode.

In Design mode, FabFl requires a specification for the maximum pressure drop and Filtration Velocity (the latter of which is an estimate in this case).

6 Close the **Completion Status** window.

7 In the **Maximum pressure drop** field, enter a value of **0.5** psi.

8 Scroll down to the **Filtration Velocity** field and enter a value of **0.015 m/sec**. Be sure to set the units.



9 Click to continue.

The **Efficiency** sheet appears.

10 In the **Separation Efficiency** field, click and select **Piecewise**.

11 Click to continue.

The **COOLER (Heater) - Input | Specifications** sheet appears. This block cools the gas after combustion, allowing the solid ash to be removed. The Heater block requires two thermodynamic specifications.

12 In the **Temperature** field, enter **400** F.

13 In the **Pressure** field, enter **14.7** psia.

14 Click to continue.

The **CYCLONE (Cyclone) - Input | Specifications** sheet appears.

To Learn About the Cyclone Model Using Help

1 Click anywhere in the **CYCLONE (Cyclone) - Input | Specifications** sheet.

2 Press **F1** on the keyboard. If a help topic without a blue heading bar appears, click the link for Sheet Help.

The help for the **Cyclone Input Specifications Sheet** appears.

3 In the **See Also** list at the end of the topic, click the Specifying Cyclone hypertext link.

4 Use the links, scrollbars, and arrow keys to move through the topics.

5 After reviewing the help, close the help window.

6 In the **Model** field, click and select **Cyclone**.

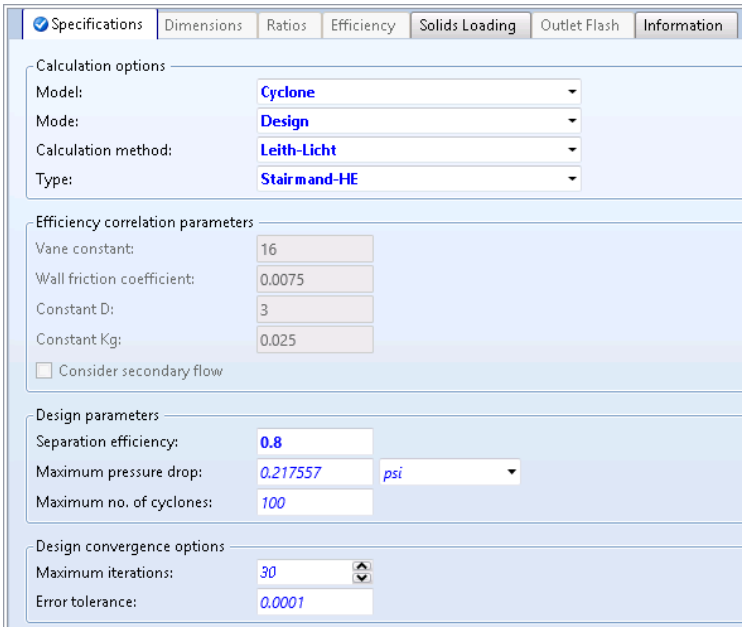
7 In the **Mode** field, click and select **Design**.

8 In the **Calculation method** field, click and select **Leith-Licht**.

9 In the **Type** field, click and select **Stairmand-HE**.

10 In the **Separation efficiency** field, enter a separation efficiency of **0.8**.

No further specifications are required for CYCLONE.



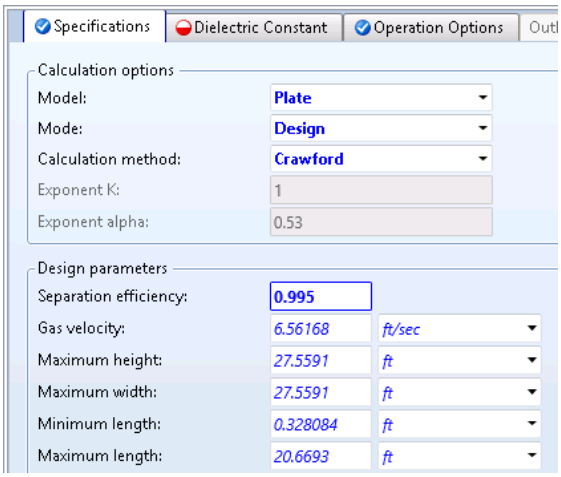
11 Click to continue.
The **ESP (ESP) - Input | Specifications** sheet appears.

12 In the **Model** field, click and select **Plate**.

13 In the **Mode** field, click and select **Design**.

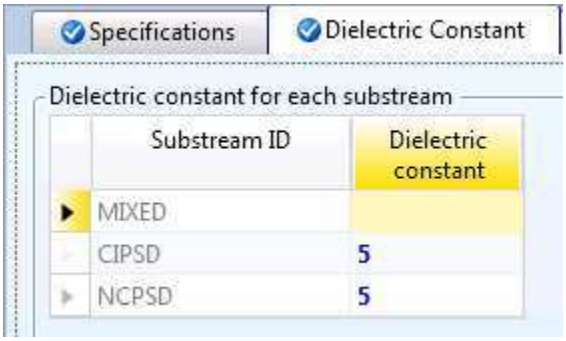
14 In the **Calculation Method** field, click and select **Crawford**.

15 In the **Separation efficiency** field, enter **0.995**.



16 Click the **Dielectric Constant** tab.

17 Specify a dielectric constant of **5** for both **CIPSD** and **NCPSD** substreams. Dielectric constant is not needed for the MIXED substream, as it does not contain solids. The value of the dielectric constant is for illustrative purposes only.



18 Click to continue.

Running the Simulation

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

1 Click **OK** to run the simulation.
The **Control Panel** allows you to monitor and interact with the Aspen Plus simulations calculations. As Aspen Plus performs the simulation, status messages display in the Control Panel.

Aspen Plus reports some warnings while processing input specifications. Ignore these warnings, which are the same warnings that were generated in Simulation 2. No further warnings are generated.

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

2 Use the vertical scrollbar to see the messages.

3 Examine the results of your run.

Examining Results

To View the Stream Results

1 In the Control Panel, click **Check Status**.

The **Results Summary - Run Status | Status** sheet appears, indicating the input warnings mentioned earlier.

2 Click the **Summary** sheet.

The **Summary** sheet indicates that the simulation completed normally.

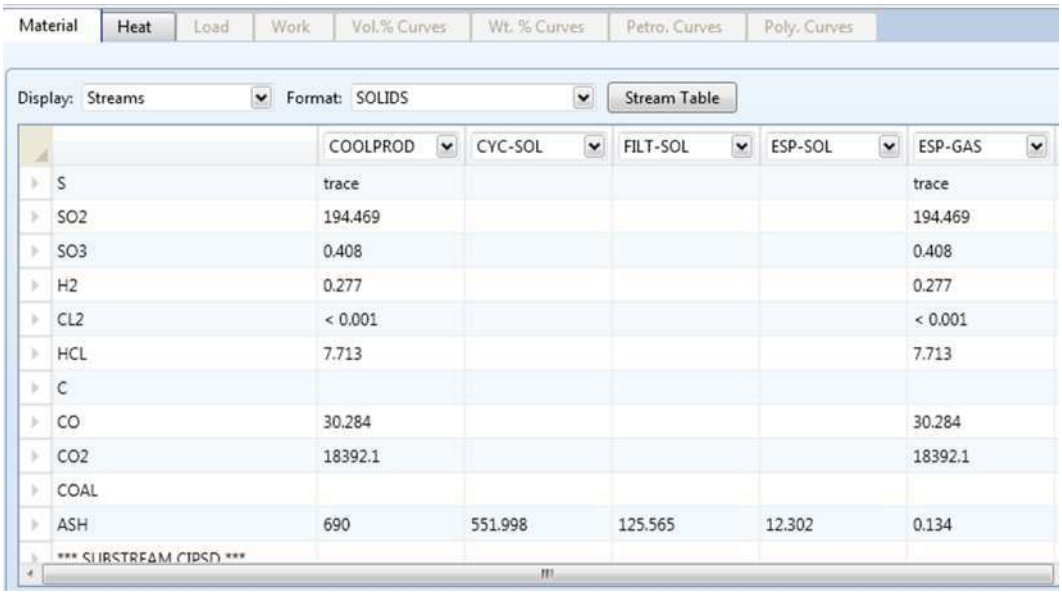
3 On the **Home** tab of the ribbon, in **Summary**, click **Stream Summary**.

The **Results Summary - Streams | Material** sheet appears.

4 Review the results on this sheet. Use the horizontal and vertical scrollbars to review results that are off the screen.

5 In the **Display** field, click and select **Streams**.

6 At the top of each column, click and select **COOLPROD**, **CYC-SOL**, **FILT-SOL**, **ESP-SOL**, and **ESP-GAS**.



	COOLPROD	CYC-SOL	FILT-SOL	ESP-SOL	ESP-GAS
S	trace				trace
SO2	194.469				194.469
SO3	0.408				0.408
H2	0.277				0.277
CL2	< 0.001				< 0.001
HCL	7.713				7.713
C					
CO	30.284				30.284
CO2	18392.1				18392.1
COAL					
ASH	690	551.998	125.565	12.302	0.134
*** SUBSTREAM CIPSD ***					

Compare the mass flow rate of ASH in the streams. The cyclone removes 80% of the ash in COOLPROD. The fabric filter removes 91% of the ash

not captured by the cyclone. Finally, the electrostatic precipitator captures virtually all of the remaining ash.

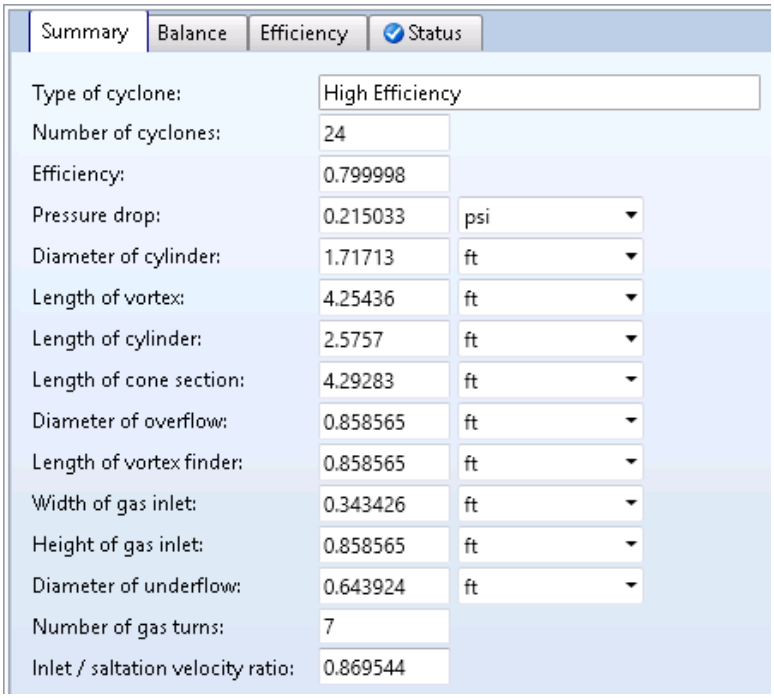
Compare the particle size distribution of the NCPSD substreams. The particle size distribution is a calculated result of the models. The cyclone removes the larger particles. The fabric filter removes the medium-size particles. The electrostatic precipitator removes the smaller particles.

To View the Block Results

There are many results forms for these blocks. You can now examine any results of interest to you. This example guides you through a review of some of the simulation results.

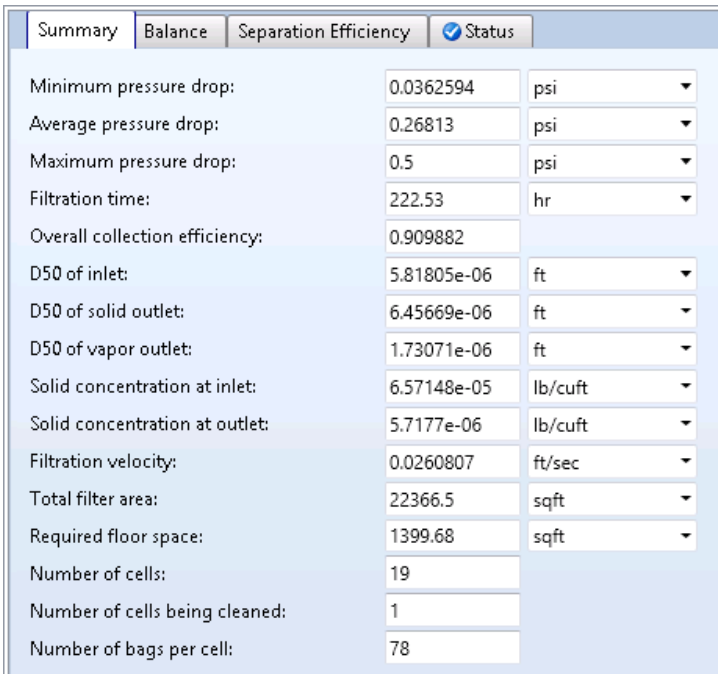
1 From the Flowsheet, right-click the CYCLONE block and from the shortcut menu, select **Results**.

The **CYCLONE (Cyclone) - Results | Summary** sheet appears. This sheet reports the calculated geometry for the cyclone.



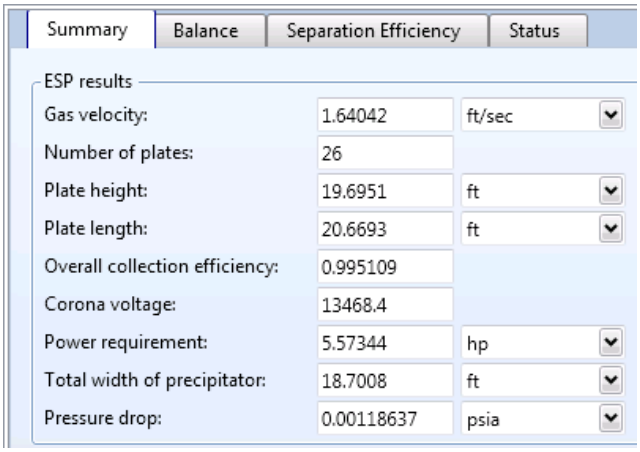
2 From the Flowsheet, right-click the **BAG-FILT** block and from the shortcut menu, select **Results**.

The **BAG-FILT (FabFl) - Results | Summary** sheet appears. This sheet displays results from the fabric filter calculations, including gas velocity and overall collection efficiency.



3 From the Flowsheet, right-click the **ESP** block and from the shortcut menu, select **Results**.

The **ESP (ESP) - Results | Summary** sheet appears. This sheet reports the geometry, the collection efficiency, and the power requirements of the electrostatic precipitator.



Exiting Aspen Plus

When finished working with this model, exit Aspen Plus as follows:

1 From the Navigation Pane, select **File | Exit**.

The **Aspen Plus** dialog box appears.

2 Click **Yes** to save the simulation.

Aspen Plus saves the simulation as the Aspen Plus Document file, Solid3.apw, in your default working directory (displayed in the **Save in** field).

4 Modeling Polymer Recovery

In this simulation you will model a simplified polymer washing and drying process.

You will use:

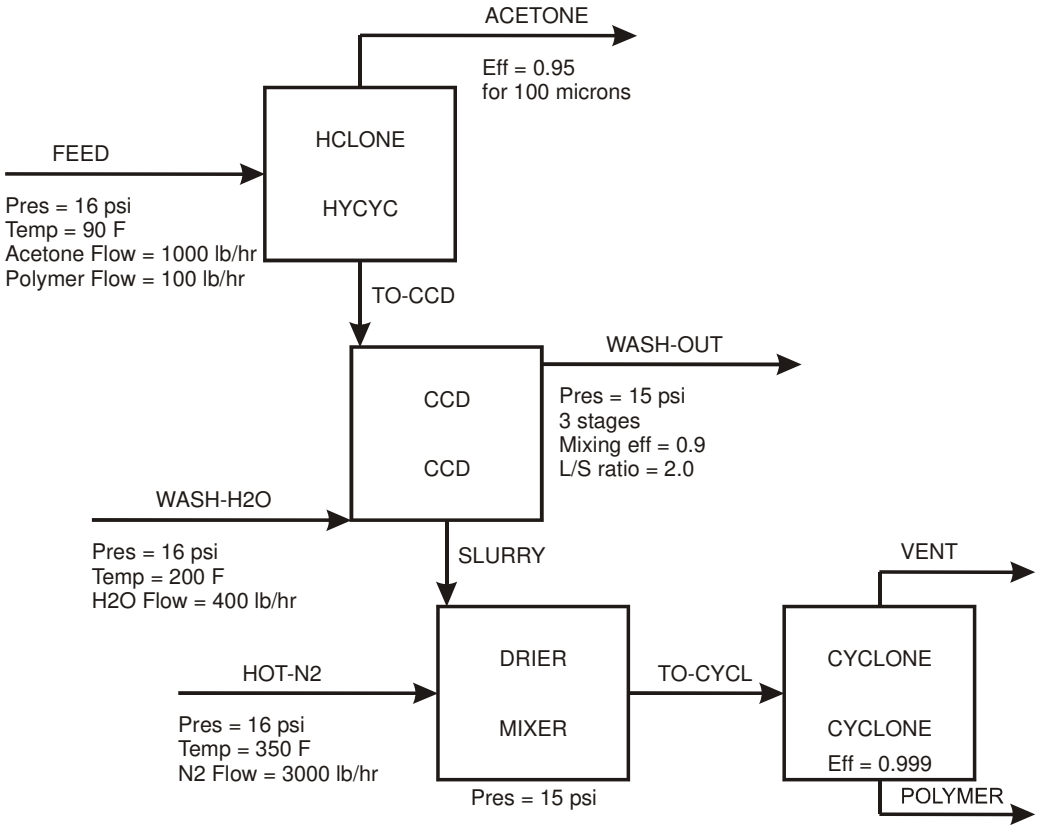
- Component attribute GENANAL to characterize a nonconventional (NC) component.
- The hydrocyclone model (HyCyc).
- The counter-current decanter model (CCD).
- The cyclone model (Cyclone).

Allow about 30 minutes to do this simulation.

Polymer Recovery Flowsheet

The process flow diagram and operating conditions for this simulation are shown in the following figure.

The feed stream FEED, a dilute slurry of polymer in acetone, is concentrated in a hydrocyclone. The concentrated slurry of polymer in acetone is then washed with water in a countercurrent decanter. The resulting slurry of polymer in water is dried with nitrogen. The gases from drying are separated from the solid polymer in a cyclone.



Starting Aspen Plus

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

2 Select **AspenTech | Process Modeling <version> | Aspen Plus | Aspen Plus <version>**.

The **Start Using Aspen Plus** window appears in the main window. In this simulation, use an Aspen Plus template.

3 Click **New**.

The **New** dialog box appears.

Use the **New** dialog box to specify the template for the new run. Aspen Plus uses the template you choose to automatically set various defaults appropriate to your application.

To Specify the Template for the New Run

4 Select the **Solids with English Units** template in the **Recently Selected Templates** field.

5 Click **Create** to apply these options.

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

Specifying Components

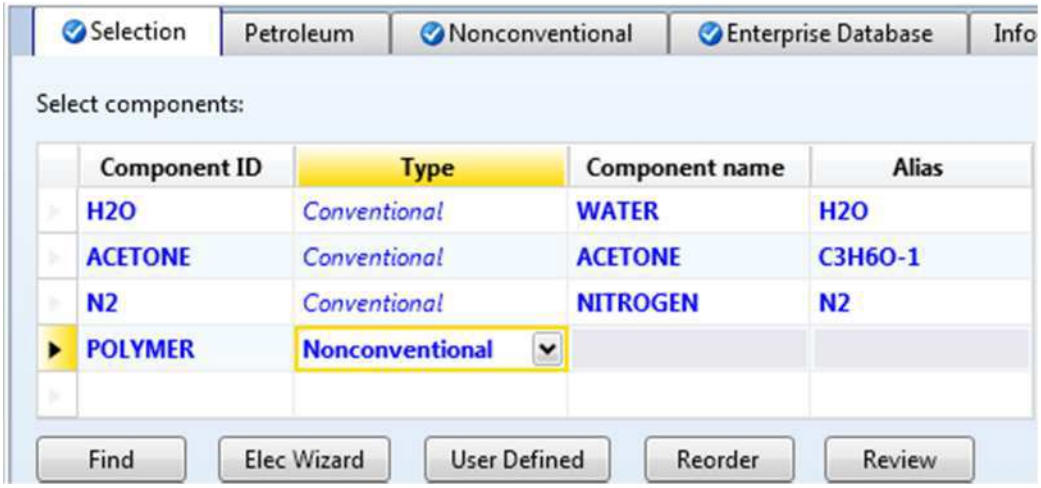
Use the **Components - Specifications | Selection** sheet to enter the components present in the simulation.

The components for this simulation are water, acetone, nitrogen, and polymer.

1 On the first four **Component ID** fields, enter **H2O**, **ACETONE**, **N2**, and **POLYMER**.

Aspen Plus is able to find WATER, ACETONE and NITROGEN in the databanks. POLYMER is not found, so the **Component name** field for polymer is empty.

By default, Aspen Plus assumes all components have a **Type** of **Conventional**, indicating that they participate in phase equilibrium calculations. Change the Type for POLYMER to indicate that it is a solid. Because POLYMER does not have a precise molecular weight, assign POLYMER the Type **Nonconventional**.



2 In the **Type** field for POLYMER, click and select **Nonconventional**.

3 Click to continue.

The **Methods - Specifications | Global** sheet appears.

Defining Properties

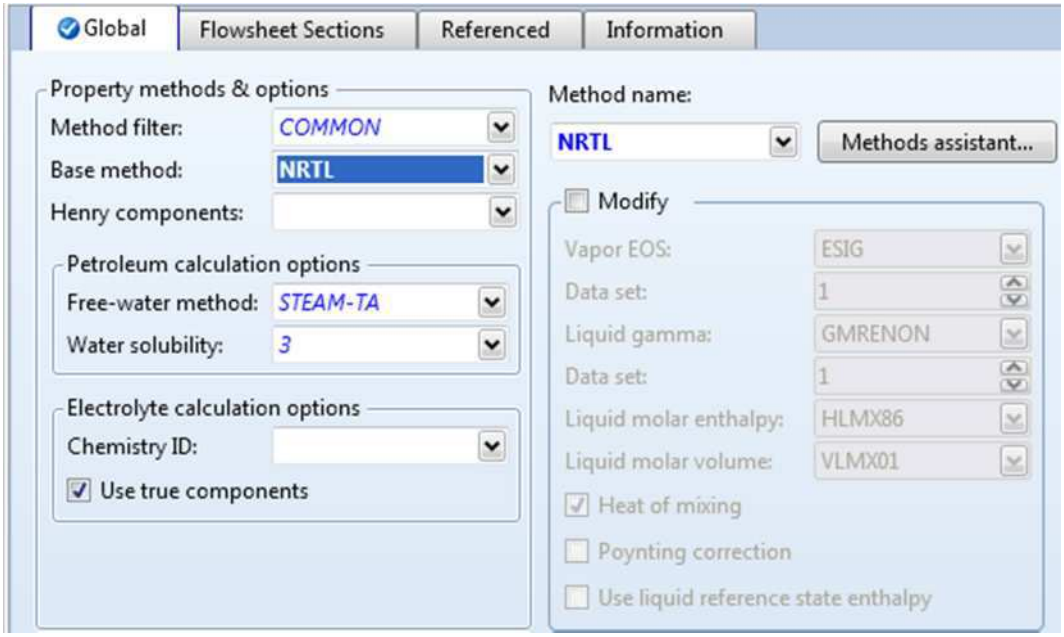
Use the **Methods - Specifications | Global** sheet to select the thermodynamic methods used to calculate properties such as K-values, enthalpy, and density. Property methods in Aspen Plus are arranged according to process types.

Select a Property Method

All property methods use the same physical property models for solid components. Therefore, the selection of the appropriate property method

depends on the components that participate in phase equilibrium. Since acetone and water form a non-ideal solution, use an activity-coefficient-based option set. For this simulation, use the NRTL property method.

1 In the **Base method** field, click and select **NRTL**.



2 Click to continue.

The **Binary Interaction - NRTL-1 (T-DEPENDENT) | Input** sheet appears.

On this sheet, Aspen Plus displays binary interaction parameters for the NRTL activity coefficient model. Binary parameters are retrieved for all binary combinations present in the database. If you had data for binary pairs that are not present in the database, or you wanted to override the parameters in the database, you could enter your parameters on this sheet.

Aspen Plus requires you to use this sheet to see what parameters are available. No further action is required to accept the database values for the binary interaction parameters. Aspen Plus marks this sheet as complete as soon as it is displayed.

In this example, parameters are retrieved for the acetone-water pair from the Aspen Plus VLE-IG databank. Aspen Plus displays the value of the parameters, and temperature range in which they were regressed. Use the vertical scrollbar at the bottom right to see all the parameter values.

3 Click to continue.

Specify Nonconventional Component Property Methods

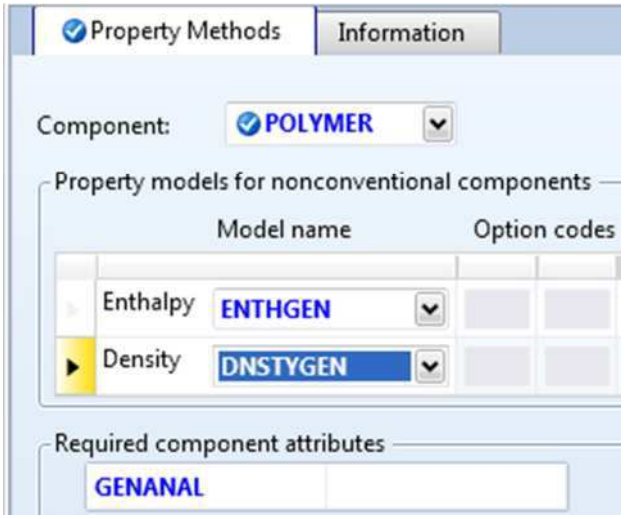
The **Methods - NC Props | Property Methods** sheet appears.

Specify the methods for Aspen Plus to calculate the enthalpy and density of the nonconventional component POLYMER. Use the general enthalpy model (ENTHGEN) and the general density model (DNSTYGEN) in this simulation.

1 In the **Model name** field for **Enthalpy**, click and select **ENTHGEN**.

As soon as you select ENTHGEN, Aspen Plus assigns the attribute **GENANAL** to the component POLYMER.

2 In the **Model name** field for **Density**, click and select **DNSTYGEN**.



You use GENANAL to characterize a nonconventional solid in terms of the weight percent of its constituents. Each nonconventional component may be characterized by up to 20 constituents.

For example, if you were to characterize paper as a nonconventional component, you might use the first seven constituents of GENANAL to represent: cellulose, hemicellulose, lignin, extractives, moisture, and inerts. Note that there is no way to tell Aspen Plus that the third constituent of paper represents lignin. You must develop and maintain a consistent nomenclature outside of Aspen Plus.

In this simulation, use only the first constituent to characterize the component POLYMER. Thus, POLYMER will be composed of 100% constituent 1.

Specify Parameters Used to Calculate POLYMER Properties

Now provide Aspen Plus with the required parameters to calculate enthalpy and density for the nonconventional component POLYMER.

1 In the Navigation Pane, select **Methods | Parameters | Pure Components**.

The **Pure Components** object manager appears.

2 Click **New**.

The **New Pure Component Parameters** dialog box appears. The enthalpy and density parameters for the POLYMER are of a Nonconventional type.

3 Select the **Nonconventional** option.

4 Click **OK** to accept the default ID, **NC-1**.

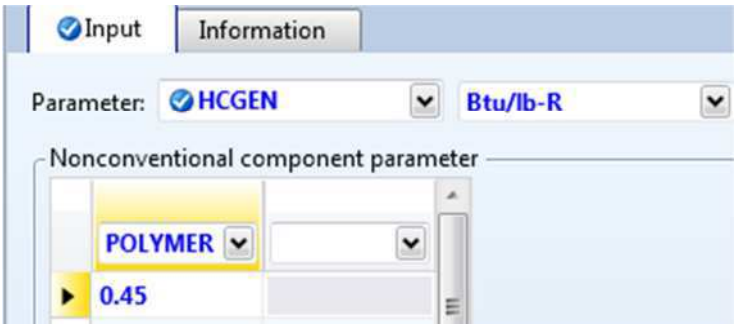
The **Pure Components - NC-1 | Input** sheet appears.

The ENTHGEN model calculates enthalpy from the parameters DHFGEN and HCGEN. In this simulation DHFGEN (heat of formation) is not required since POLYMER does not participate in any chemical reactions. You must provide HCGEN (heat capacity). For this simulation, POLYMER is assumed to have a constant heat capacity of 0.45 Btu/lb-R.

5 In the **Parameter** field, click and select **HCGEN**.

6 In the first field in the **Nonconventional component parameter** frame, click and select **POLYMER**.

7 In the first parameter value field directly below, enter **0.45**.



The first four elements of HCGEN are used to calculate the heat capacity of the first constituent of GENANAL, using the following equation:

$$C_p = HCGEN(1) + HCGEN(2) \times T + HCGEN(3) \times T^2 + HCGEN(4) \times T^3$$

HCGEN(2), HCGEN(3) and HCGEN(4) default to zero. Since only the first constituent of GENANAL will be used to characterize POLYMER, POLYMER will have a constant heat capacity of 0.45 Btu/lb-R.

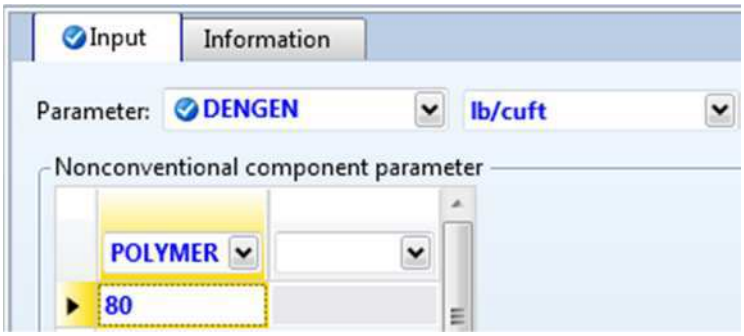
If POLYMER were characterized with other constituents, use elements 5 through 8 of HCGEN to calculate the heat capacity of the second constituent, and so on.

Enter the parameters required for the DNSTYGEN model on this sheet. DNSTYGEN calculates density for a nonconventional solid from the DENGEN parameter. For this simulation, POLYMER is assumed to have a constant density of 80 lb/cuft.

8 In the **Parameter** field, click and select **DENGEN**.

9 In the first field in the **Nonconventional component parameter** frame, click and select **POLYMER**.

10 In the first parameter value field, enter **80**.



11 Click to continue.

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

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

12 Select **Go to Simulation environment** and click **OK** to move to the next required input in the **Simulation** environment.

Drawing the Flowsheet

In this simulation, begin building the process flowsheet. Since you will enter your own block and stream IDs, turn off the automatic naming of blocks and streams, which provide these IDs automatically.

1 From the ribbon, select **File | Options**.

The **Aspen Plus Options** dialog box appears.

2 Click **Flowsheet** on the panel on the left side of the dialog box.

3 Clear the **Automatically Assign Block Name with Prefix** and **Automatically Assign Stream Name with Prefix** check boxes.

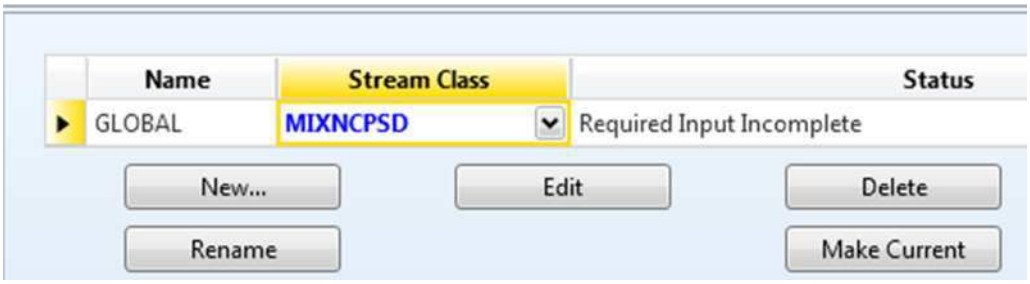
4 Click **Apply** and then **OK** to apply the changes and close the dialog box.

To Change the Stream Class for the Simulation

1 From the Navigation Pane, click **Flowsheet | Section**.

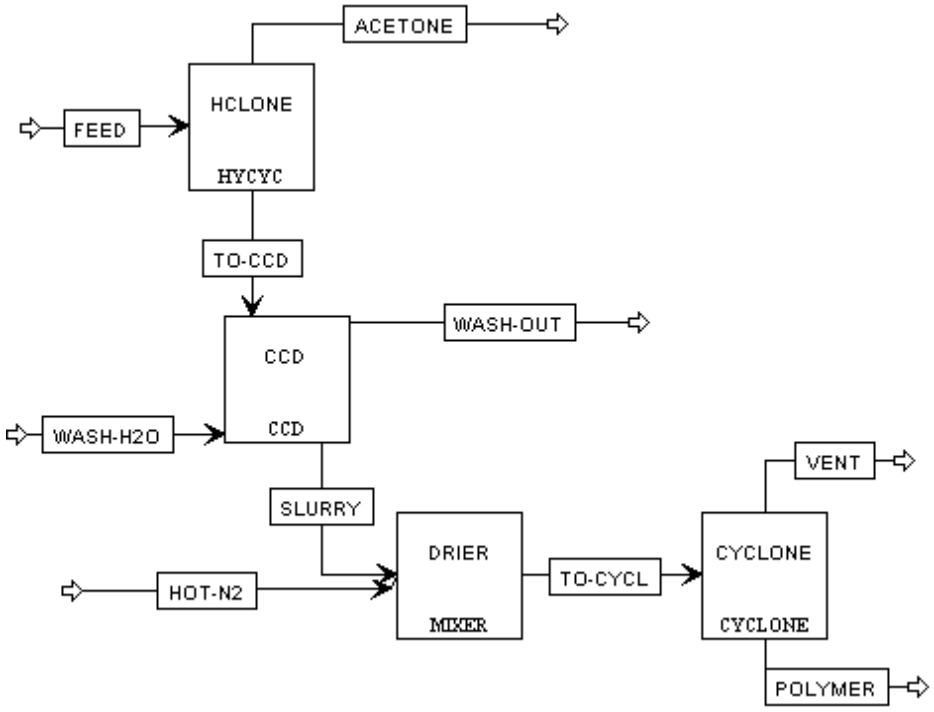
The **Section** object Manager appears.

2 In the **Stream class** field, click and select **MIXNCPSD**.



3 Go to the **Main Flowsheet** window.

4 Place the flowsheet blocks and streams to create the graphical simulation flowsheet shown below. (See *Getting Started Building and Running a Process Model*, Chapter 2, if you need to review how to create a graphical simulation flowsheet.)



Specifying Title, Stream Properties, and Global Options

1 From the Navigation Pane, go to **Setup | Specifications**.

The **Setup - Specifications | Global** sheet displays defaults Aspen Plus uses for other forms. 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 Solids with English Units template.

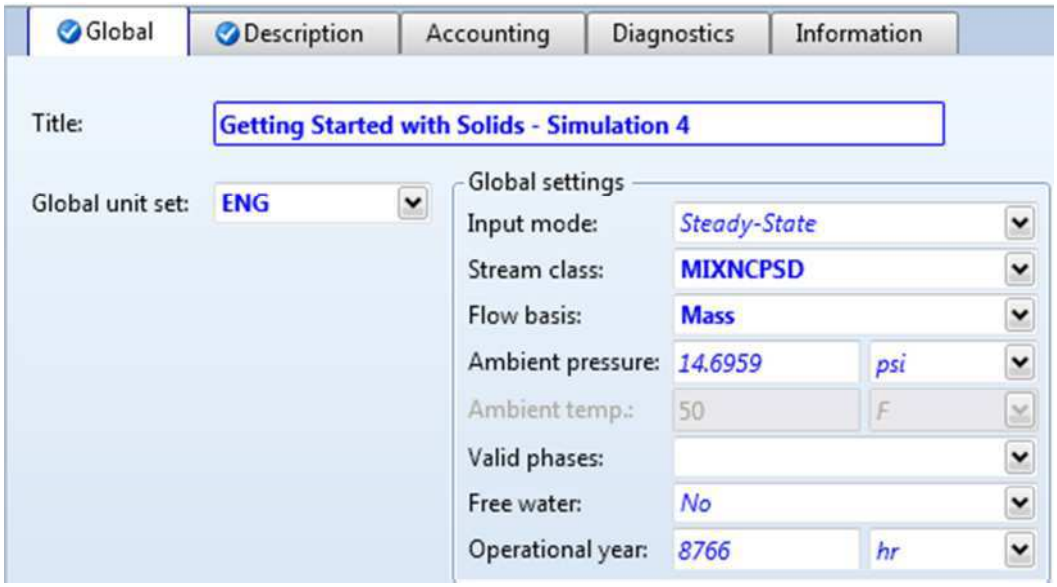
It is always good practice to describe your simulation by entering a title for the simulation.

2 In the **Title** field, enter **Getting Started with Solids - Simulation 4**.

The Solids with English Units template sets the following global defaults for solids applications:

- **ENG** units (English Engineering Units).
- **Mass** Flow basis for all flow inputs.

There are no other changes required on the **Setup - Specifications | Global** sheet.

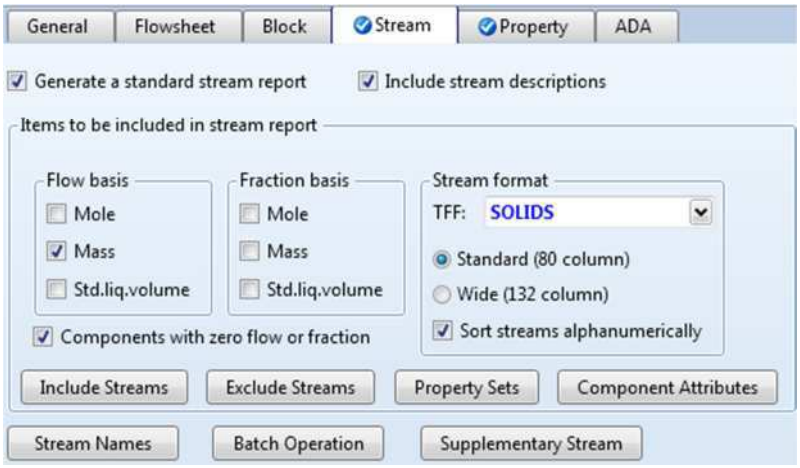


Since you chose the Solids with English Units template when you started this simulation, Aspen Plus has set the following defaults for calculating and reporting stream properties:

- The component mass flow rates will be included in the stream report.
- The stream results will be displayed using the **SOLIDS** Stream Format.
- Property set **ALL-SUBS** (properties for the entire stream, all substreams combined) will be reported for each stream.

To Review the Report Options Specified in the Selected Template

1. From the Navigation Pane, select the **Setup | Report Options** form.
2. Click the **Stream** tab to view the **Setup - Report Options | Stream** sheet.



3 Click **Property Sets** to view the selected property sets.

4 Click **Close** to return to the **Setup - Report Options | Stream** sheet.

5 Click to continue.

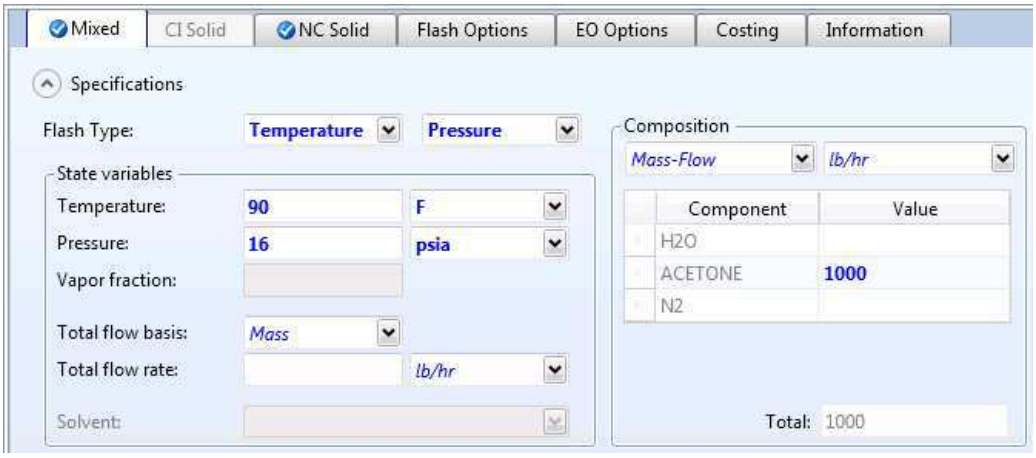
Defining Stream Conditions

The **FEED (MATERIAL) - Input | Mixed** sheet appears.

For the MIXED substream, Aspen Plus requires two thermodynamic specifications, and enough information to calculate the flow rate of each component.

1 Enter the following specifications:

Parameter	Value
Temperature	90 F
Pressure	16 psia
Composition	Mass-Flow
ACETONE value	1000 lb/hr

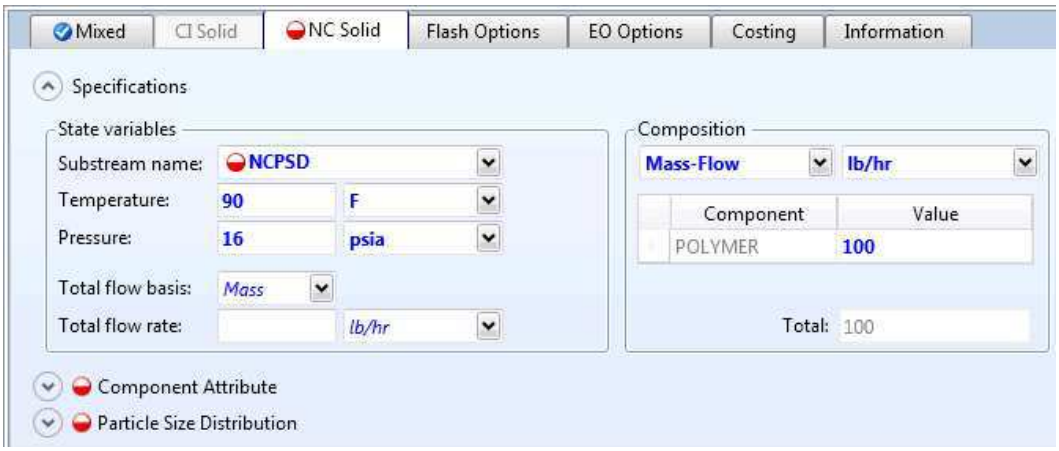


2 Click the **NC Solid** tab to display the **FEED (MATERIAL) - Input | NC Solid** sheet.

3 In the **Substream name** field, click and select **NCPSD**.

4 Enter the following specifications for the mixed substream:

Parameter	Value
Temperature	90 F
Pressure	16 psia
Composition	Mass-Flow
POLYMER value	100 lb/hr

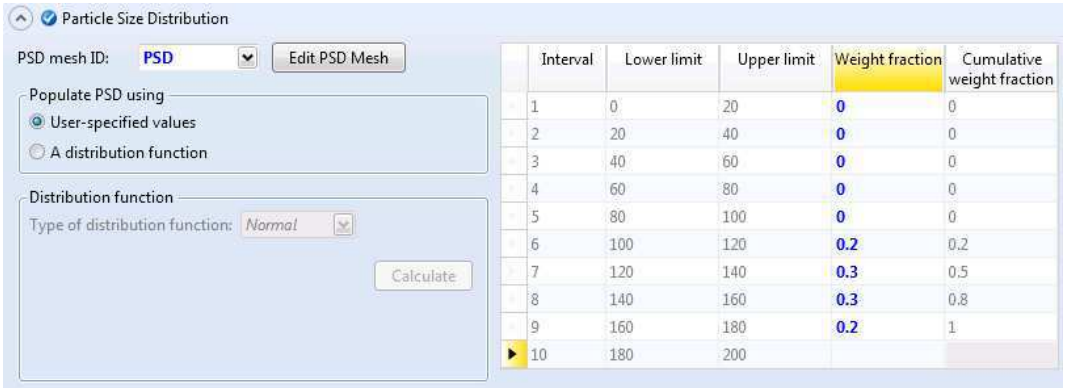


5 Click the arrow in front of **Particle Size Distribution**.

Use this sheet to define the particle size distribution for the POLYMER that you placed in the NCPSD substream. By default, Aspen Plus uses a particle size distribution of 10 size ranges covering 20 microns each. The default size ranges are appropriate for this simulation. On this sheet, enter the weight fraction of coal in each size range.

6 In the **Weight fraction** fields, enter the following values:

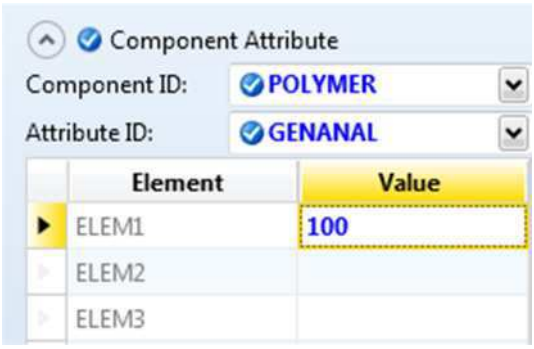
Interval	Weight Fraction
6	0.2
7	0.3
8	0.3
9	0.2



7 Click the arrow in front of **Component Attribute**.

On this sheet, define the component POLYMER in terms of the constituents in its GENANAL. Aspen Plus does not require you to use all 20 constituents. Since you are using only the first constituent to characterize POLYMER, the first element of GENANAL is 100%.

8 In the **ELEM1** field, enter a value of **100**.



9 Click to continue.

The **HOT-N2 (MATERIAL) | Mixed** sheet appears. Stream HOT-N2 is the feed stream used to dry the polymer.

10 Enter the following specifications:

Parameter	Value
Temperature	350 F
Pressure	16 psia
Composition	Mass-Flow
N2 value	3000 lb/hr

11 Click to continue.

The **WASH-H2O (MATERIAL) | Mixed** sheet appears. Stream WASH-H2O is the feed stream used to wash the polymer in the CCD.

12 Enter the following specifications:

Parameter	Value
Temperature	200 F
Pressure	16 psia
Composition	Mass-Flow
H2O value	400 lb/hr

13 Click to continue.

Entering Block Specifications

The **CCD (CCD) | Specifications** sheet appears.

Enter Specifications for the CCD Model

Make the following specifications for a countercurrent decanter:

- Number of stages.

- Operating pressure.
- Mixing efficiency.
- Liquid/solid ratio.

If you do not provide mixing efficiency or liquid/solid ratio for all stages, Aspen Plus determines the values for missing stages by linear interpolation. If you provide only a single value for mixing efficiency or liquid/solid ratio, Aspen Plus uses that value for all stages.

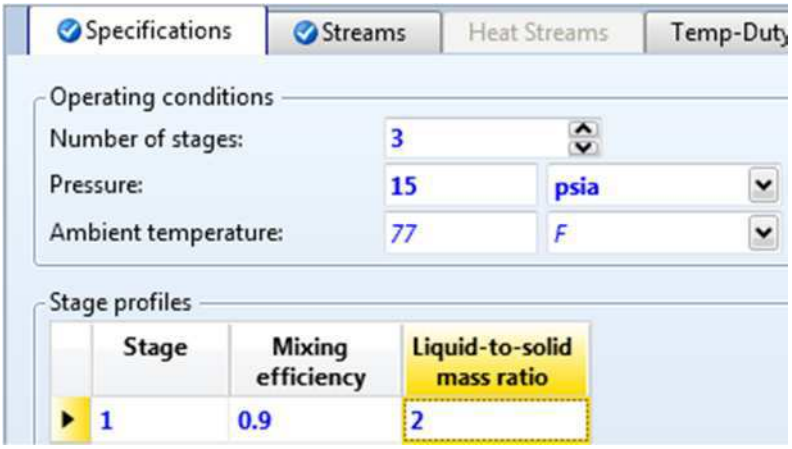
By default, Aspen Plus assumes each stage of a countercurrent decanter to be adiabatic. Alternatively, you could specify a temperature, a heat duty, or a heat transfer coefficient for each stage.

1 Enter the following operating conditions:

Field	Value
Number of stages	3
Pressure	15 psia

2 For the stage profiles, enter:

Field	Value
Stage	1
Mixing efficiency	0.9
Liquid-to-solid mass ratio	2



3 Click the **Streams** tab.

The **CCD (CCD) | Streams** sheet describes the connections of the streams to the stages of the CCD. It is already complete.

4 Click  to continue.

The **CYCLONE (Cyclone) | Specifications** sheet appears.

To Learn More about the Cyclone Model Using Help

1 Click anywhere on the **CYCLONE (Cyclone) | Specifications** sheet.

2 Press **F1**. If a help window without a blue heading bar appears, click the link for Sheet Help.

The help for the **Cyclone Input Specifications Sheet** appears.

3 In the list of **See Also** links, click the Specifying Cyclone hypertext link.

4 Use the links, scrollbars, and arrow keys to move through the topics.

5 After reviewing the help, close the help window.

You can use the Cyclone model in simulation mode or design mode. In this simulation, use Cyclone in design mode. Aspen Plus will determine the dimensions and the number of cyclones required to achieve a specified efficiency for solids removal.

Enter Specifications for the Cyclone Model

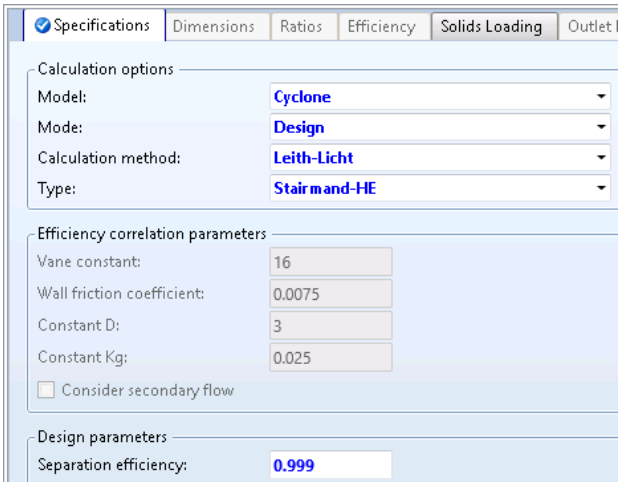
1 In the **Model** field, click and select **Cyclone**.

2 In the **Mode** field, click and select **Design**.

3 In the **Calculation method** field, click and select **Leith-Licht**.

4 In the **Type** field, click and select **Stairmand-HE**.

5 In the **Separation efficiency** field, enter a separation efficiency of **0.999**.



6 From the Navigation Pane, click **Blocks | DRIER**.

The **DRIER (Mixer) | Flash Options** sheet appears. The sheet is marked complete, since there are no specifications required for a Mixer block. However, Aspen Plus does allow the pressure of the Mixer as an optional specification.

To Specify That the Mixer Block DRIER Operates at 15 psia

1 In the **Pressure** field, enter **15** psia.

2 Click to continue.

The **HCLONE (HyCyc) | Specifications** sheet appears.

Enter Specifications for the HyCyc Model

1 Click anywhere on the **Specifications** sheet.

2 Press **F1**.

3 Use the links, scrollbars, and arrow keys to move through the topics.

4 After reviewing the help, close the help window.

You can use HyCyc in simulation mode or design mode. In this example, use HyCyc in design mode. In design mode, make the following specifications:

- Particle size for design efficiency.
- Design separation efficiency.
- Maximum diameter of the hydrocyclone.
- Maximum pressure drop.

5 In the **Model** field, click and select **Hydrocyclone**.

6 In the **Mode** field, click and select **Design**.

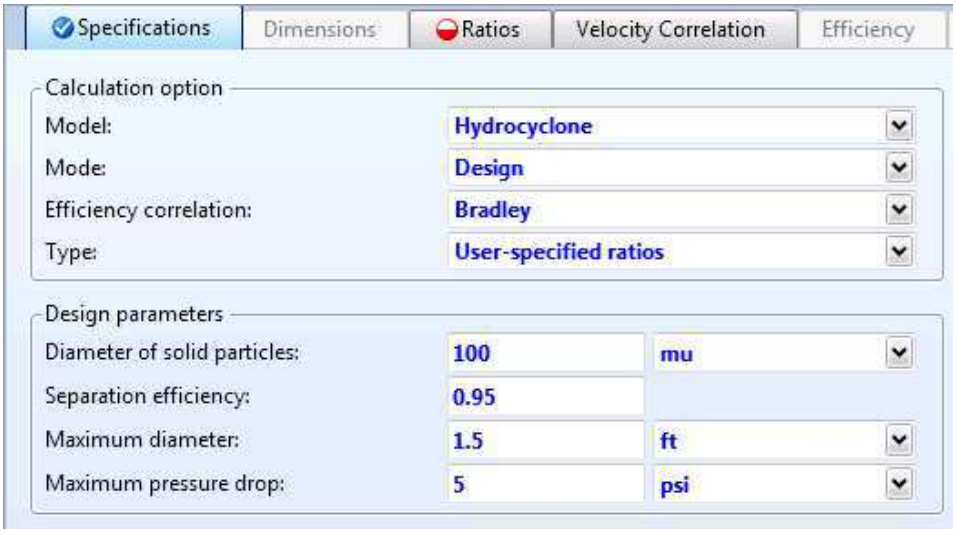
7 In the **Efficiency Correlation** field, click and select **Bradley**.

8 In the **Type** field, click and select **User-specified ratios**.

9 Enter the following specifications:

Field	Value
Diameter of solid particles	100 mu (microns)
Separation efficiency	0.95
Maximum diameter	1.5 ft
Maximum pressure drop	5 psi

Be sure to specify the units of measure for the particle diameter.

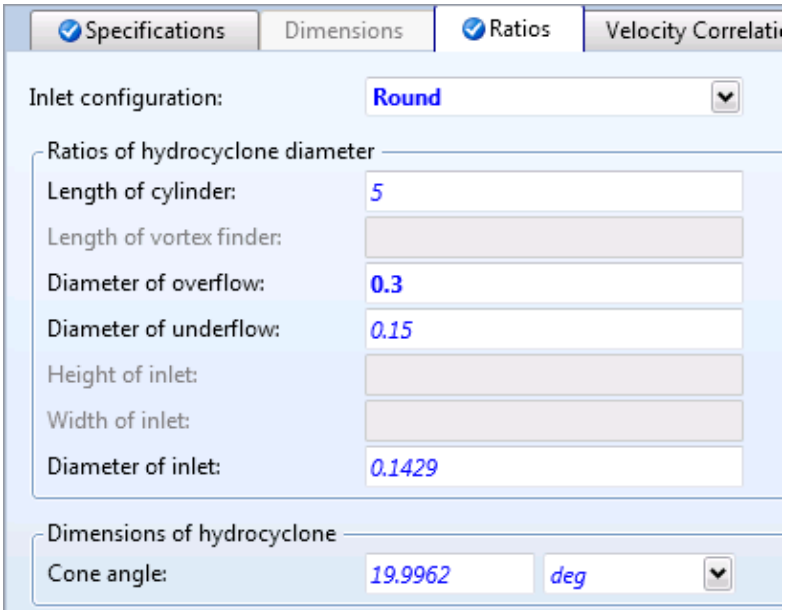


To help concentrate the solid slurry, change the default geometry of the hydroclone. Increasing the size of the overflow diameter increases the amount of liquid product in stream ACETONE. Specify that the ratio of the overflow diameter to the hydroclone diameter be equal to 0.3.

10 Click the **Ratios** tab.

11 In the **Inlet Configuration** field, click and select **Round**.

12 In the **Diameter of overflow** field, enter **0.3**.



13 Click to continue.

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

Running the Simulation

You have now entered the data and specifications for this simulation.

1 Click **OK** to run the simulation.

The **Control Panel** allows you to monitor and interact with the Aspen Plus simulations calculations. As Aspen Plus performs the simulation, status messages display in the **Control Panel**.

GENANAL is defined as having 20 constituents. If you only use a portion of the constituents available in GENANAL, Aspen Plus generates a warning. Since you need only one element in GENANAL for this simulation, ignore this warning. The remainder of the simulation completes without warnings or errors.

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 see the messages.

3 Examine the results of your run.

Examining Results

To View the Stream Results

1 In the Control Panel, click **Check Status**.

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

2 On the **Home** tab of the ribbon, in **Summary**, click the arrow beside **Stream Summary**, and then click **Stream Summary**.

The **Results Summary - Streams | Material** sheet appears.

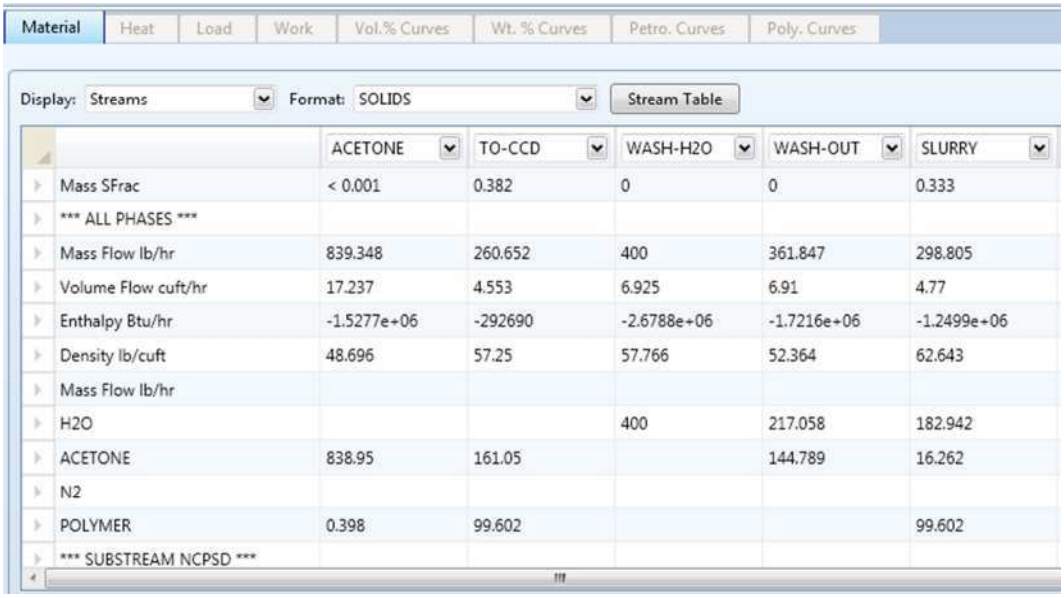
3 Review the results on this sheet.

Note: Since this is a scrolling sheet, use the scrollbars to review results that are off the screen.

4 In the **Display** field, select **Streams**.

5 At the top of the blank column of results, click  and select **ACETONE**. In subsequent columns, select **TO-CCD**, **WASH-H2O**, **WASH-OUT**, and **SLURRY**.

6 Evaluate the performance of the hydrocyclone by comparing its outlet streams: ACETONE and TO-CCD.



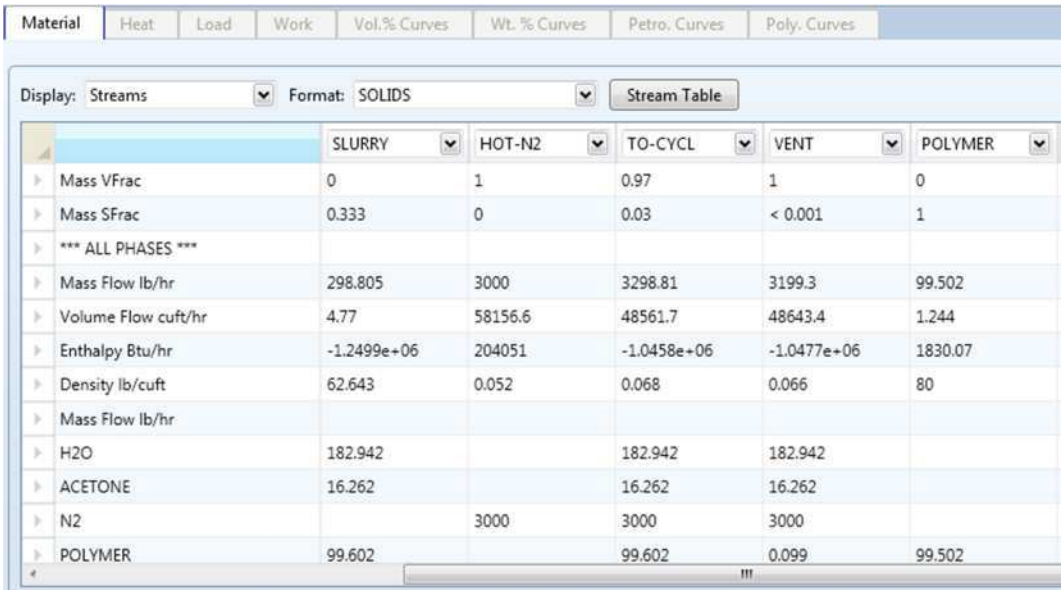
	ACETONE	TO-CCD	WASH-H2O	WASH-OUT	SLURRY
Mass SFrac	< 0.001	0.382	0	0	0.333
*** ALL PHASES ***					
Mass Flow lb/hr	839.348	260.652	400	361.847	298.805
Volume Flow cuft/hr	17.237	4.553	6.925	6.91	4.77
Enthalpy Btu/hr	-1.5277e+06	-292690	-2.6788e+06	-1.7216e+06	-1.2499e+06
Density lb/cuft	48.696	57.25	57.766	52.364	62.643
Mass Flow lb/hr					
H2O			400	217.058	182.942
ACETONE	838.95	161.05		144.789	16.262
N2					
POLYMER	0.398	99.602			99.602
*** SUBSTREAM NCPSD ***					

Most of the acetone and very little of the polymer are in stream ACETONE. The hydrocyclone has substantially concentrated the dilute slurry of polymer in acetone to feed to the CCD.

7 Evaluate the performance of the countercurrent decanter by comparing streams TO-CCD, WASH-OUT, and SLURRY.

Most of the acetone in TO-CCD is removed by the wash water. Stream SLURRY contains polymer in a water rich environment. Note that stream WASH-OUT contains no polymer.

8 After the SLURRY column, click and select the following streams **HOT-N2**, **TO-CYCL**, **VENT**, and **POLYMER**.



	SLURRY	HOT-N2	TO-CYCL	VENT	POLYMER
Mass VFrac	0	1	0.97	1	0
Mass SFrac	0.333	0	0.03	< 0.001	1
*** ALL PHASES ***					
Mass Flow lb/hr	298.805	3000	3298.81	3199.3	99.502
Volume Flow cuft/hr	4.77	58156.6	48561.7	48643.4	1.244
Enthalpy Btu/hr	-1.2499e+06	204051	-1.0458e+06	-1.0477e+06	1830.07
Density lb/cuft	62.643	0.052	0.068	0.066	80
Mass Flow lb/hr					
H2O	182.942		182.942	182.942	
ACETONE	16.262		16.262	16.262	
N2		3000	3000	3000	
POLYMER	99.602		99.602	0.099	99.502

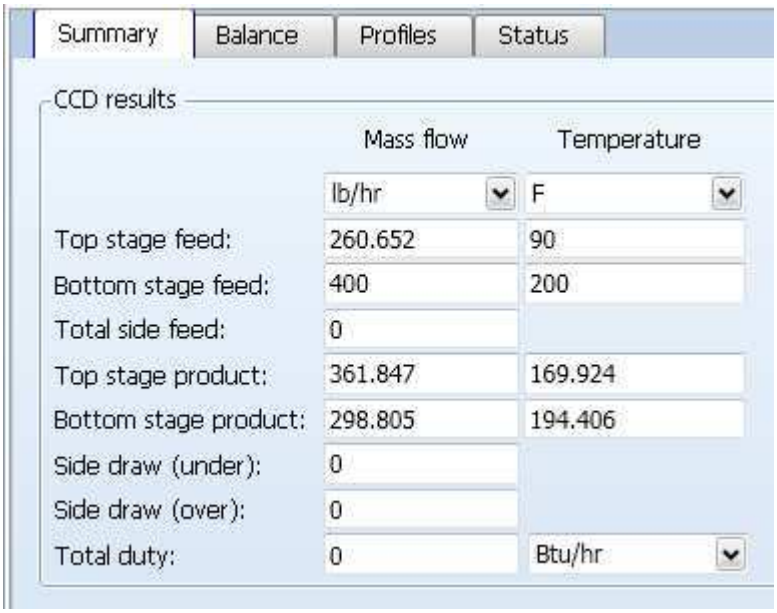
The DRIER block operates by mixing streams SLURRY and HOT-N2. There is enough hot nitrogen to adiabatically evaporate all of the liquid in stream SLURRY (VFrac + SFrac =1 in stream TO-CYCL).

The CYCLONE block separates the solid polymer from the gas. Because the Cyclone model neglects the interstitial flow of gas in the separated solids, stream POLYMER has no flow of H2O, ACETONE, or N2.

To View the Block Results

1 In the Flowsheet, right-click the **CCD** block. From the shortcut menu, select **Results**.

The **CCD (CCD) - Results | Summary** sheet appears. This sheet displays summary flow and temperature information for the first and last stages.

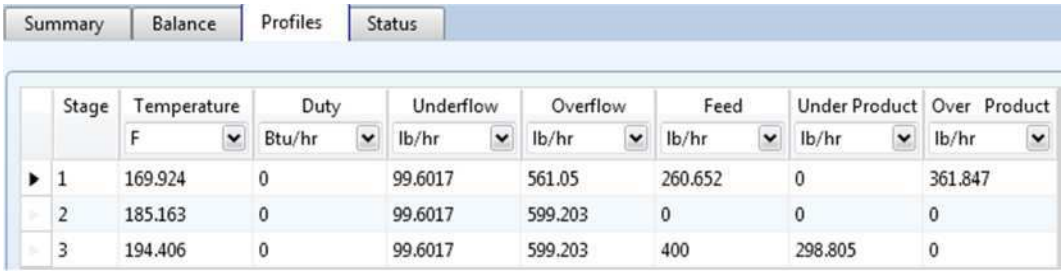


2 Click the **Balance** tab to the next sheet with results.

The **CCD (CCD) - Results | Balance** sheet appears. This sheet displays the overall mass and energy balance for the block.

3 Click the **Profiles** tab.

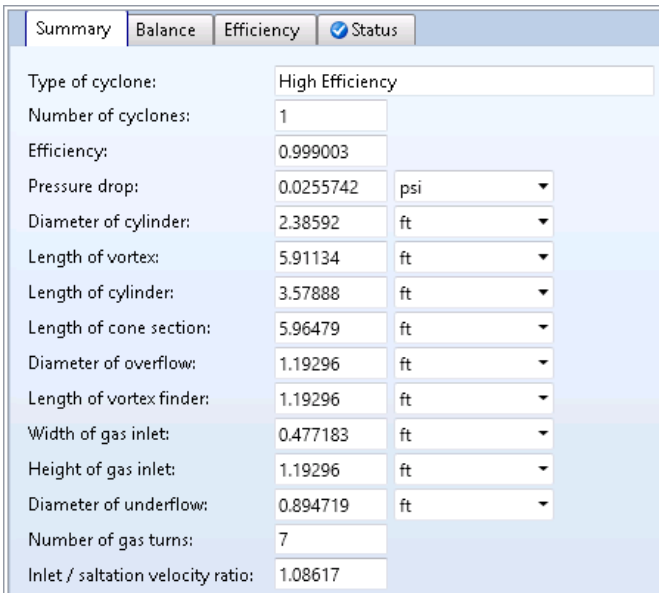
The **CCD (CCD) - Results | Profiles** sheet appears. This sheet displays the temperature, duty, underflow, and overflow for each stage of the CCD.



	Stage	Temperature	Duty	Underflow	Overflow	Feed	Under Product	Over Product
		F	Btu/hr	lb/hr	lb/hr	lb/hr	lb/hr	lb/hr
▶	1	169.924	0	99.6017	561.05	260.652	0	361.847
	2	185.163	0	99.6017	599.203	0	0	0
	3	194.406	0	99.6017	599.203	400	298.805	0

4 In the Flowsheet, right-click the **CYCLONE** block. From the shortcut menu, select **Results**.

The **CYCLONE (Cyclone) - Results | Summary** sheet appears. This sheet displays the calculated geometry for the cyclone.

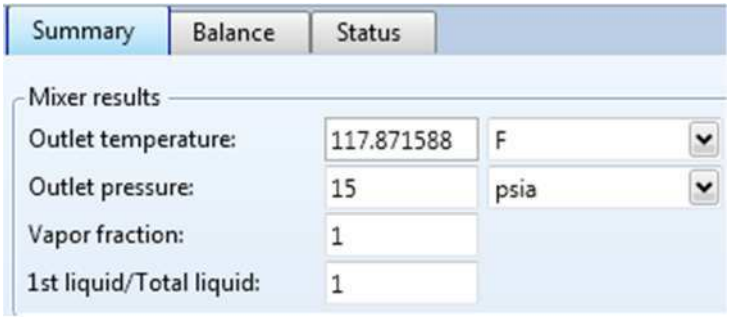


5 Click the **Balance** tab to move to the next sheet with results.

The **CYCLONE (Cyclone) - Results | Balance** sheet appears. This sheet displays the overall mass and energy balance for the block.

6 In the Flowsheet, right-click the **DRIER** block. From the shortcut menu, select **Results**.

The **DRIER (Mixer) - Results | Summary** sheet appears. This sheet displays the outlet thermodynamic conditions for the block.

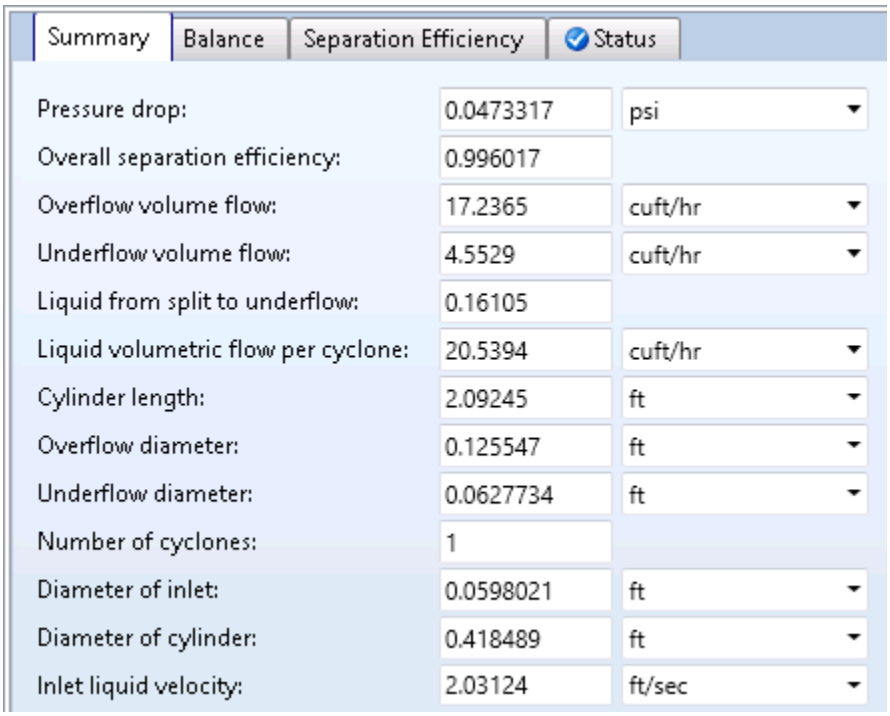


7 Click the **Balance** tab to move to the next sheet with results.

The **DRIER (Mixer) - Results | Balance** sheet appears. This sheet displays the overall mass and energy balance for the block.

8 In the Flowsheet, right-click the **HCLONE** block. From the shortcut menu, select **Results**.

The **HCLONE (HyCyc) - Results | Summary** sheet appears. This sheet displays the calculated geometry for the block.



Exiting Aspen Plus

When you are finished working with this model, you can exit Aspen Plus as follows:

1. From the ribbon, select **File | Exit**.

   The **Aspen Plus** dialog box appears.
2. Click **Yes** to save the simulation.
3. In the **Save As** dialog box, enter **Solid4** in the **File name** box.

   Aspen Plus saves the simulation as the Aspen Plus Document file, Solid4.apw, in your default working directory (displayed in the **Save in** box).

   This simulation is delivered as backup file **solid4** in the online Aspen Plus Examples Library. You can use this backup file to check your results.