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## Aspen Plus

Getting Started Modeling Processes with Solids

#### Version Number: V8.4 November 2013

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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:

chapter	
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.

### Follow the steps in this To learn how to

## **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-todate 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.

Blank and Recent Solids	Preview
My Templates Installed Templates Air Separation Chemical Processes Electrolytes Gas Processing Metallurgy Pharmaceutical Polymers Refinery Solids	Solids Simulation with English Units : F, psi, Ib/hr, Ibmol/hr, Btu/hr, cuft/hr. Property Method: None Flow basis for input: Mass

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:

Component ID	Туре	Component name	Alias
H20	Conventional	WATER	H20
N2	Conventional	NITROGEN	N2
02	Conventional	OXYGEN	02
COAL	Nonconventional		

**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**.

Property methods & o	ptions —	Me	thod name:		
Method filter:	COMMON	× 11	EAL V	Methods as	sistant
Base method:	IDEAL				
Henry components:			Modify		
- Petroleum calculatio	n ontions	V	apor EOS:	ESIG	~
Free-water method:	STEAM-TA		ata set:	1	* ¥
Water solubility:	3	V	iquid gamma:	GMIDL	2
		E	ata set:	1	
Electrolyte calculatio	n options		iquid molar enthalpy:	HLMX82	2
Chemistry ID:		<b>×</b>   L	iquid molar volume:	VLMX01	X
Use true compon	ents		Heat of mixing		
			Povoting correction		

2 Click No 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 <sup>▶</sup> 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 Manual and select DCOALIGT.

#### The **Property Methods** sheet is complete:

om	ponent:	<b>⊘</b> COAL		~				
Pro	perty mode	els for nonc	onver	ntional	comp	onents		
		Model nan	ne		Opt	ion cod	es	T
	Enthalpy	HCOALGE	N	•	1	1	1	1
•	Density	DCOALIG	Г	~				

#### **3** Click № to continue.

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

Required Properties Input Complete	
Next step:	
Run Property Analysis / Setup	
Modify required property specifications	
Enter property parameters	
Enter experimental data	
O Go to Simulation environment	
	_
OK Cancel	

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**.

Simulation Properties Basis	Pressure:	%.0f	Custom1	Ţ	%.2f		-	
Files Flowsheet	Vapor fraction:	%.2f	Custom2	Ţ	%.2f		•	
Plots	Mole flow rate:	%.0f	Custom3	Ţ	%.2f		-	
Upward Compatibility Advanced	Mass flow rate:	%.0f	Custom4		%.2f		-	
Startup	Volume flow rate:	%.0f	Custom5		%.2f		-	
	Heat/Work:	%.0f	Custom6	-	%.2f			
	Status display on Process	Flowsheet window						
	Show error	Show warning	Show inactive					-
	Stream and unit operatio	n labels						
	Automatically assign block name with prefix:							
	📝 Display block name							
	Automatically assign	stream name with prefix:	S					
	📝 Display stream name							
	Label Font	8 pt. Arial						
	Placement options							
4	Automatically place b	locks when importing						

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
- o MIXCISLD for the global Stream class
- **3** In the **Stream class** field, click **MIXNCPSD**.

🎯 Global	Oescription	Accounting [	Diagnostics	Information	
Title:	Getting Started	with Solids – Simula	ation 1		
		Global settings	;		
Global unit set:	set: ENG	Input mode:	Steady-	Steady-State MIXNCPSD Mass	
		Stream class: Flow basis: Ambient pressure:	MIXNC		
			Mass		
			ure: 14.6959	psi	•
		Ambient temp	50	F	2
		Valid phases:			~
		Free water:	No		~
		Operational ye	ar: 8766	hr	

#### **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.

General	Flowsheet	Block	Stream 🤡	@ Pro	perty	ADA	
Generate	a standard strea included in stre	m report am report –	<b>V</b> Include	stream de	escriptions	•	
Flow ba	sis e s iq.volume onents with zero	Fraction bas Mole Mass Std.liq.vo	olume	ream forn F: SOL Standard Wide (13 Sort stre	nat <mark>IDS</mark> I (80 colur 2 column ams alpha	nn) ) enumerica	Ily
Include S	Streams	xclude Strea	ms Proj	erty Sets	Cor	mponent /	Attributes
Stream N	ames	Batch Opera	tion	upplemer	ntary Strea	m	

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.
- o 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:

Compo	nent	Value					
N2		0.999					
02		0.001			_		
🕜 Mixed	CI Solid	🕜 NC Solid	Flash Option	ns EO	Options	Costing	Information
Specifica	itions						
Flash Type:		Temperature	Pressure	×	Compos	ition ———	
- State varia	bles				Mole-Fr	rac 💌	) [ [
Temperatu	ure:	270	F			Component	Value
Pressure:		14.7	psia	•	H2C	)	
Vapor frac	tion:				N2		0.999
7.0					02		0.001
	basis:	Mass	~				
Total flow							
Total flow Total flow	rate:	50000	lb/hr	~			

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

Mixed	CI Solid	🖉 NC Solid	Flash Options	EO Opti	ons C	osting Info	ormation		
🕗 🥝 Compo	nent Attribu Size Distribu	te							
PSD mesh ID:	PSD	► Edit	PSD Mesh		Interval	Lower limit	Upper limit	Weight fraction	Cumulative weight fractic
- Populate PS	D using				1	0	20	0	0
Oser-spe	cified values				2	20	40	0	0
O A distribu	ution functio	n			3	40	60	0	0
- Distribution	function				4	60	80	0	0
Type of dist	ribution func	tion: Normal			5	80	100	0	0
Type of dise	noutorrane	Horn Hornat			6	100	120	0	0
			Calculat	e	7	120	140	0.1	0.1
					8	140	160	0.2	0.3
					9	160	180	0.3	0.6
					10	190	200	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

Co	mponent ID:	@COAL	~
Att	ribute ID:	PROXANAL	×
	Elemer	nt Val	ue
	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 **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.
- o ULTANAL value for ash equals the PROXANAL value for ash.
- ULTANAL values sum to 100.
- o PROXANAL values for FC, VM, and ASH sum to 100.
- **14** Click No 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 M 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 Mark 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.

Reactants		Products	
Component Coe	efficient	Component	Coefficient
COAL -1		H2O	0.0555084
Products generation			
Products generation O Molar extent:		bmol/hr	

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  $\frown$  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 **Sector** 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.)

Specificatio	ns ØReactions	Comb	oustion	h Heat of	Reaction	Selectivity	PSD	Component Attr
ubstream ID:	3 NCPSD	•						
Component att	ributes		_					
Component ID:	@COAL	•		Element	Value			
Attribute ID:	<b>OPROXANAL</b>	~	•	MOISTURE	1			
				FC				
				VM				
				ASH				

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:

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

/ariable name:	<b>OH2OIN</b>	×	Reference —		2.2	
Category		122201	Type: Stream:	Compattr-Var	*	
		12		WET-COAL		
Blocks     Streams			Substream: Component:	NCPSD		
				COAL	~	
O Model Utili	tv		Attribute:	PROXANAL		
Physical Property Parameters			Element:	1		
O Reactions						
Information fl	ow ariable OD	(port variab	le 🔿 Tearva	riable	2	
EO input						
	1					
Open variable						

#### **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 **H20DRY** variables as shown:

/aviable waves	(CONV		<ul> <li>Reference –</li> </ul>					
ranapie name:	CONV		Туре:	Block-Var	V			
Category —		r.	Block:	DRY-REAC	~			
O All			Variable:	CONV	▼ (#)			
Blocks			Sentence	CONV				
Streams     Model Utility			ID1.	1				
O Model Utili	ty _	3L	101.					
O Physical Pr	operty Parameters	5						
Reactions								
<ul> <li>Edit selecte</li> </ul>	d variable							
<ul> <li>Edit selecte</li> <li>/ariable name:</li> </ul>	d variable	•	Reference – Type:	Block-Var				
Edit selecte     Ariable name:     Category	d variable		- Reference - Type: Block:	Block-Var DRY-REAC	×			
Edit selecte     dariable name:     Category     All     Blocks	d variable		Reference – Type: Block: Variable:	Block-Var DRY-REAC COMPATT	× ×			
<ul> <li>Edit selecte</li> <li>'ariable name:</li> <li>Category —</li> <li>All</li> <li>Blocks</li> <li>Streams</li> </ul>	d variable		Reference – Type: Block: Variable: Sentence:	Block-Var DRY-REAC COMPATT COMP-ATTR	× ×			
<ul> <li>Edit selecte</li> <li>Category —</li> <li>All</li> <li>Blocks</li> <li>Streams</li> <li>Model Utili</li> </ul>	ty		Reference – Type: Block: Variable: Sentence: ID1:	Block-Var DRY-REAC COMPATT COMP-ATTR NCPSD	× × ×			
<ul> <li>Edit selecte</li> <li>Category</li> <li>All</li> <li>Blocks</li> <li>Streams</li> <li>Model Utili</li> <li>Physical Pr</li> </ul>	ty		Reference – Type: Block: Variable: Sentence: ID1: ID2:	Block-Var DRY-REAC COMPATT COMP-ATTR NCPSD COAL	× × *			
<ul> <li>Edit selecte</li> <li>Category</li> <li>All</li> <li>Blocks</li> <li>Streams</li> <li>Model Utili</li> <li>Physical Pr</li> <li>Reactions</li> </ul>	ty operty Parameters		Reference – Type: Block: Variable: Sentence: ID1: ID2: ID3:	Block-Var DRY-REAC COMPATT COMP-ATTR NCPSD COAL PROXANAL	× × × ×			

2 Click No 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 No 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 **Select Before**.
- 2 In the **Block type** field, click **and** select **Unit operation**.
- **3** In the **Block name** field, click **M** and select **DRY-REAC**.

	Sequence	Tears	Stream Flash	Information	
ecution sequ	Jence	Block type:		Block name:	
	×	Unit operati	on 💌	DRY-REAC	8
ort or expo	t				
	ecution sequ	ecution sequence	Block type: Unit operation of export	Block type:  Unit operation  Fort or export	Block type: Block name: Unit operation  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.

Mate	rial Heat	Load	Work	Vol.% Cur	ves	Wt. % Curve	5	Petro, Curve	s	Poly, Curves			
Displi	ay: All streams	6	Form	at: SOLIDS			•	Stream Table					
14				DRY-COAL	¥	EXHAUST		IN-DRIER	¥	NITROGEN	¥	WET-COAL	¥
Þ	Temperature F			116.6		116.6		116.6		270		77	
×.	Pressure psia			14.7		14.7		14.7		14.7		14.7	
$\mathcal{F}_{i}$	Mass VFrac			0		1		0.861		1		0	
P.	Mass SFrac			1		0		0.139		0		1	
Þ.	*** ALL PHASES **	18											
$\left  \mathbf{F} \right $	Mass Flow Ib/hr			8333.33		51666.7		60000		50000		10000	
Þ.	Volume Flow cuft/	/hr		96.255		789719		789816		950620		115.506	
$ \mathbf{F} $	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	
E.	Mass Flow Ib/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 **Solution** 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.

Summary	Balance	Phase Equilibriu	m Utility	Usage	Status
Block results	summary —				
Outlet temperature:		116.622009	F	•	
Outlet pressure:		14.7	psia	•	
Vapor fractio	n:	1			
Heat duty:		0	Btu/hr	•	
Net duty:		0	Btu/hr	•	
1st liquid / T	otal liquid:				

#### **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.

Summary	Balance	Phase Equ	uilibrium	Reactions	
RStoic results	;				
Outlet tempe	erature:	116.62201	F	<b>×</b>	
Outlet pressu	ire:	14.7	psia		
Heat duty:		0	Btu/hr	~	
Net heat duty:		0	Btu/hr	~	
Vapor fraction:		1			
1st liquid / To	otal liquid:				

**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**

- 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.

Global	Oescription	Accounting Dia	agnostics	Information	
Title:	Getting Started	with Solids – Simulat	on 2		
Clabel with each	THE	Global settings -			
Global unit set:	ENG	Input mode:	Steady-S	State	~
		Stream class:	MCINCP	SD	~
		Flow basis:	Mass		~
		Ambient pressu	e: 14.6959	psi	~
		Ambient temp.:	50	F	×
		Valid phases:			~
		Free water:	No		~
		Operational year	8766	hr	~

## 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	Туре	Component Name
NO2	Conventional	NITROGEN DIOXIDE
NO	Conventional	NITRIC OXIDE
S	Conventional	SULFUR
S02	Conventional	SULFUR-DIOXIDE
S03	Conventional	SULFUR-TRIOXIDE
H2	Conventional	HYDROGEN
CL2	Conventional	CHLORINE
HCL	Conventional	HYDROGEN-CHLORIDE
С	Solid	CARBON-GRAPHITE
CO	Conventional	CARBON-MONOXIDE
CO2	Conventional	CARBON-DIOXIDE
ASH	Nonconventional	

Component ID	Туре	Component name	Alias
H20	Conventional	WATER	H20
N2	Conventional	NITROGEN	N2
02	Conventional	OXYGEN	02
COAL	Nonconventional		
NO2	Conventional	NITROGEN-DIOXIDE	NO2
NO	Conventional	NITRIC-OXIDE	NO
S	Conventional	SULFUR	S
SO2	Conventional	SULFUR-DIOXIDE	025
SO3	Conventional	SULFUR-TRIOXIDE	035
H2	Conventional	HYDROGEN	H2
CL2	Conventional	CHLORINE	CL2
HCL	Conventional	HYDROGEN-CHLORI	HCL
С	Solid	CARBON-GRAPHITE	С
со	Conventional	CARBON-MONOXID	со
CO2	Conventional	CARBON-DIOXIDE	CO2
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 № 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**.

m	ponent:	<b>⊘COAL</b>	~				
oro	perty mode	els for nonconv	entional	comp	onents		
		Model name		Opt	ion cod	es	
	Enthalpy	HCOALGEN	×	6	1	1	1
•	Density	DCOALIGT	~				

#### **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 **Second Second Second**

om	ponent:	<b>Ø</b> ASH	~				
Pro	perty mode	els for nonconv Model name	entional	comp Onti	onents	ec	
		modermanne		ope	lon cou		
	Enthalpy	HCOALGEN		1	1	1	1
	Density	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:

HCOMB = Heat of Combustion (wet) \*  $\frac{100}{100 - \%}$  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
02	0.21

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

Ø Mixed	🕜 CI Solid	I 🛛 🥑 NC S	olid Flas	h Options	EO Options	Costing	Information
Specificat	tions						
Flash Type:		Temperature	Y Press	ure 💌	Compositi	on ———	
- State variah	ales				Mole-Fra	. 🖌	
Temperatu	re:	77	F	•	Ca	mponent	Value
Pressure:		14.7	psia	×	H2O		
Vapor fract	ion:			1	N2		0.79
1					02		0.21
Total flow I	basis:	Mass	•		- NO2		
Total flow i	rate:	90000	lb/hr	~	NO		
6 I.S. 6					S		
Solvent				1. Ale	SO2		

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.

Component	Phase	Component	Phase
H2O	Mixed	SO3	Mixed
N2	Mixed	H2	Mixed
02	Mixed	CL2	Mixed
NO2	Mixed	HCL	Mixed
NO	Mixed	С	PureSolid
S	Mixed	СО	Mixed
S02	Mixed	CO2	Mixed

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

Ø	Specifications	Products	Assign Streams	Inerts
) R(	Gibbs considers all	components as	products	
Id	entify possible pro	ducts		
D	efine phases in whi	ich products app	ear	
		0		
нус	drate-check:	Rigorous		
Pro	ducts			
	Compone	ent	Valid phases	
2	H20	Mix	ed	
	N2	Mix	ed	
	02	Mix	ed	
	NO2	Mix	ed	
	NO	Mix	ed	
	S	Mix	ed	
	SO2	Mix	ed	
	SO3	Mix	ed	
	H2	Mix	ed	
	CL2	Mix	ed	
	HCL	Mix	ed	
۲	С	Pur	eSolid	~
	со	Mix	ed	
je.	CO2	Mix	ed	



#### **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

✓ Spec	ifications	⊘Yield Flash	Options 🛛 🥑	PSD 🛛 🥝 C	omp. Attr.	Comp.
Operatir Flash Ty	ng conditions pe:	Temperature	Pre:	ssure	•	
Temper	<b>ature:</b> ature change:	77	F	*		
Pressure	2	14.7	psia	~		
Duty: Vapor fr	action:		Btu/hr	*		
-Valid ph	ases —					
Vapor-	Liquid	~				

2 Click No 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
<u>C (CIPSD)</u>	Mass	0.1
H2	Mass	0.1
N2	Mass	0.1
CL2	Mass	0.1
S	Mass	0.1
02	Mass	0.1

eld	options: Co	omponent yields			•
Con	nponent yields				
	Com	ponent	Basi	s	Basi Yiel
	H20		Mass	×	0.2
	ASH		Mass	~	0.2
	C (CIPSD)		Mass	*	0.1
	H2		Mass	*	0.1
	N2		Mass	~	0.1
	CL2		<ul> <li>Mass</li> </ul>	*	0.1
	S	6	<ul> <li>Mass</li> </ul>	~	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.

0	Specifications	<b>⊘</b> Yield	Flash Options	ØPSD
Sub	ostream ID:	<b>⊘ CIPSD</b>	•	
Par	ticle size distrib	ution ———		
PSE	D mesh ID:	PSD	Units:	mu
	Interval	Lower limit	Upper limit	Weight fraction
	1	0	20	0
	2	20	40	0
	3	40	60	0
	4	60	80	0
	5	80	100	0
	6	100	120	0
	7	120	140	0.1
	8	140	160	0.2
	9	160	180	0.3
	10	180	200	0.4

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

- **4** In the **Substream ID** field, click **Markov** 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

Specification	os 🕜 Yield	Flash Options	⊘PSD	🕝 Comp. Attr.
ubstream ID: 🤇	NCPSD			
Component attri	ibutes —			
Component ID:	<b>ØASH</b>		Element	Value
Attribute ID:	PROXANAL		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 Խ 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

0	Specifications Flash		n Options	Key Components		Information	
Spe	ecification for e	ach subst	ream				
Stre	eam names:	GASES			•		
	Substream	Name	Specif	fication	Basis		Value
	MIXED		Split fract	tion		1	
	CIPSD		Split fract	tion		0	
	NCPSD		Split fract	tion		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.

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

- **4** Create and define the following two variables using category **Streams**:
- **5** Also define the following eight mass yield variables using category **Blocks**.

Variable Name		ID1	ID2
H2O	Type <b>Block-Var</b> Block <b>DECOMP</b> Variable <b>MASS-YIELD</b> for all eight variables.	H2O	MIXED
ASH		ASH	NCPSD
CARB		С	CIPSD
H2		H2	MIXED
N2		N2	MIXED
CL2		CL2	MIXED
SULF		S	MIXED
02		02	MIXED

Calculate 
 Gequence Tears Stream Flash Information

Variable name	Info. flow	Definition					
ULT		Compattr-Vec Stream=DRY-COAL Substream=NCPSD Component=COAL Attribute=ULTANAL					
WATER		Compattr-Var Stream=DRY-COAL Substream=NCPSD Component=COAL Attribute=PROXANAL Element=					
H2O		Block-Var Block=DECOMP Variable=MASS-YIELD Sentence=MASS-YIELD ID1=H2O ID2=MIXED					
ASH		lock-Var Block=DECOMP Variable=MASS-YIELD Sentence=MASS-YIELD ID1=ASH ID2=NCPSD					
CARB		Block-Var Block=DECOMP Variable=MASS-YIELD Sentence=MASS-YIELD ID1=C ID2=CIPSD					
H2		llock-Var Block=DECOMP Variable=MASS-YIELD Sentence=MASS-YIELD ID1=H2 ID2=MIXED					
N2		Block-Var Block=DECOMP Variable=MASS-YIELD Sentence=MASS-YIELD ID1=N2 ID2=MIXED					
CL2		Block-Var Block=DECOMP Variable=MASS-YIELD Sentence=MASS-YIELD ID1=CL2 ID2=MIXED					
SULF		Block-Var Block=DECOMP Variable=MASS-YIELD Sentence=MASS-YIELD ID1=S ID2=MIXED					
02		Block-Var Block=DECOMP Variable=MASS-YIELD Sentence=MASS-YIELD ID1=O2 ID2=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) / 100H2O = 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 **Second** and select **Before**.

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

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

<b>O</b> Define	⊘Calculate	Sequence	Tears	Stream Fla	ash	Information	
Calculator b	olock execution seq	uence	Block type:		Blo	ck name:	
Before		×	Unit opera	tion	• D	ECOMP	<b>×</b>
List variable	s as import or expo	rt —					
Import varia	ables:						
Export varia	bles:						

12 Click Խ 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**

- 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 M and select **INBURNER**, **AIR**, **PRODUCTS**, **GASES**, and **SOLIDS**.

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

Disp	lay: Streams 💌 For	mat: FULL	-	Stream Table		
		INBURNER 💌	AIR 💌	PRODUCTS 💌	GASES 💌	SOLIDS 💌
Þ.	Mass Flow Ib/hr					
÷.	H2O	833.333	0	4046.16	4046.16	0
1	N2	82.5	69037.5	68976.2	68976.2	0
þ.	02	1230	20962.5	5687.51	5687.51	0
÷.	NO2	0	0	0.451699	0.451699	0
÷.	NO	0	0	307.764	307.764	0
3×	s	97.5	0	2.58099e-06	2.58099e-06	0
Þ.	SO2	0	0	194.469	194.469	0
p.	SO3	0	0	0.408278	0.408278	0
÷.	H2	360	0	0.277068	0.277068	0
þ.	CL2	7.5	0	3.64932e-05	3.64932e-05	0
3.,	нсі	0	0	7 71 310	7 71 319	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:

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

Material		Heat	Load	Work
Dis	play:	All stream	s	¥
۲			Q-DEC	OMP
	QCAL	C Btu/hr	-55061	56.19
	TBEGI	IN F	116.62	201
	TEND	F	77.	

#### **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.

Summary Ba	lance	Phase Equi	Weight Dist	
RYield results			n*-	
Outlet temperature	e:	77	F	•
Outlet pressure:		14.7	psia	~
Heat duty:		5.50616e+06	Btu/hr	~
Net heat duty:		5.50616e+06	Btu/hr	~
Vapor fraction:		0.841371		
1st liquid / Total li	quid:	1		

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.

Summary	Balance	nce Phase Composition		ds
-RGibbs result	·s			
Outlet tempe	erature:	2980.99001	F	~
Outlet pressu	ire:	14.7	psia	Y
Heat duty:		-5.50616e+06	Btu/hr	~
Net heat dut	y:	0	Btu/hr	¥
Vapor fractio	n:	1		
Number of fl	uid phases:	1		
Maximum nu	umber of pure s	olids: 1		

- 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

- 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

⊘ Mesh Info	rmation					
PSD mesh ID:	PSD		Pa	nticle size dist	ribution mesh —	
- DSD Mech				Int.	Lower	Upper
PSD mesh tune	Upper	1		1	0	1
PSD mesh type.	OSE/			2	1	2
No. of intervals:	6		•	3	2	4
Lower limit:	Upper limit:	Size units:		4	4	8
		mu		5	8	16
		Create PSD Mesh	ר ר	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

0	Specifications	🕜 Yield	Fla	sh Options	🥑 PSD	
Substream ID:			•			
Par	ticle size distrib	ution —				
PSE	) mesh ID:	PSD		Units:	mu	
	Interval	Lower limit	U	lpper limit	Weight fractio	on
	1	0	1		0.1	
	2	1	2		0.1	
	3	2	4		0.2	
	4	4	8		0.2	
	5	8	16		0.2	
	6	16	32		0.2	

**9** In the **Substream** field, click **Second Second Second** 

- **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 **I** to continue.

## Specifying the Solids-Handling Blocks

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

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.

Specifications	Coefficient Model	Efficiency	Outlet flash	Information				
Calculation options								
Model:		Fabric filter						
Mode:		Design				¥		
Filtration area calcu	lation:	Calculate from e	estimated velocity	and baghouse ch	aracteristics	¥		
Pressure drop/Filtrat	tion time							
Pressure drop calcul	lation method:	Filtration velo	city function					
		O Calculate from specific resistance						
		🔘 Constant						
Average pressure dr	op:		psi		20			
Filtration time:			hr	2				
Maximum pressu	ure drop:	0.5	psi	psi				
Filter media resis	tance Kr:	3.048e+08	1/ft		*			
O Pressure drop of	filter media:	0.0362594	psi		2			
Oust resistance c	oefficient:	60000						
🚫 Filter cake resista	ince Ks:		ft/lb		X			
Porosity of filter	cake:	0.75						
Outlet solids stream	pressure:	Use ambient pr	essure		×			
Specify outlet solids	stream pressure:		psia		X			
Filter operation con	ditions							
Filtration velocity:		0.015	m/sec		~			
Maximum velocity:		0.0833333	ft/sec		~			

- 9 Click No continue.
   The Efficiency sheet appears.
- **10** In the **Separation Efficiency** field, click **and select Piecewise**.
- **11** Click **I** 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 **I** 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 <u>Sheet Help</u>.

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

- **3** In the **See Also** list at the end of the topic, click the <u>Specifying Cyclone</u> 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 Mark 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 **Stairmand-HE**.
- **10** In the **Separation efficiency** field, enter a separation efficiency of **0.8**. No further specifications are required for CYCLONE.

Specifications Dimensions	Ratios Efficie	ncy Solids Loading	Outlet Flash	Information
Calculation options				
Model:	Cyclone		-	
Mode:	Design		-	
Calculation method:	Leith-Licht		-	
Type:	Stair m and-HE		-	
Efficiency correlation parameter	rs			
Vane constant:	16			
Wall friction coefficient:	0.0075			
Constant D:	3			
Constant Kg:	0.025			
Consider secondary flow				
- Design parameters				
Separation efficiency:	0.8			
Maximum pressure drop:	0.217557	psi 🔹		
Maximum no. of cyclones:	100			
Design convergence options —				
Maximum iterations:	30			
Error tolerance:	0.0001			

#### **11** Click **I** to continue.

The **ESP (ESP) - Input | Specifications** sheet appears.

**12** In the **Model** field, click **Second Second Second Plate**.

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

14 In the Calculation Method field, click and select Crawford.
15 In the Separation efficiency field, enter 0.995.

Specifications 🤤	Dielectric Constant	Operation Options	Out
Calculation options —			
Model:	Plate	•	
Mode:	Design	-	
Calculation method:	Crawford	-	
Exponent K:	1		
Exponent alpha:	0.53		
Design parameters —			
Separation efficiency:	0.995		
Gas velocity:	6.56168	ft/sec	•
Maximum height:	27.5591	ft	•
Maximum width:	27.5591	ft	•
Minimum length:	0.328084	ft	•
Maximum length:	20.6693	ft	•

#### 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.

0	Specifications	🖉 Die	electric Constant
Die	lectric constant f	or each s	ubstream ——
	Substream	ID	Dielectric constant
•	MIXED		
	CIPSD		5
5	NCPSD		5

**18** Click No 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 **Streams**.
- 6 At the top of each column, click M and select COOLPROD, CYC-SOL, FILT-SOL, ESP-SOL, and ESP-GAS.

Mat	erial Heat Load W	ork Vol.% Curves	Wt. % Curves	Petro, Curves	Poly, Curves	
Disp	ilay: Streams	Format: SOLIDS		Stream Table		
		COOLPROD 💌	CYC-SOL	FILT-SOL	ESP-SOL	ESP-GAS
1	s	trace				trace
×.	SO2	194.469				194.469
Ŀ.	SO3	0.408				0.408
Þ	H2	0.277				0.277
$\left  \mathbf{F} \right $	CL2	< 0.001				< 0.001
Ж	HCL	7.713				7.713
$\mathbf{F}$	с					
þ.	со	30.284				30.284
F	CO2	18392.1				18392.1
$\left  \mathbf{F} \right $	COAL					
Þ.	ASH	690	551.998	125.565	12.302	0.134
dir	*** SURSTREAM 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.

Summary Balance Effici	ency 🕺 🥝 Stati	us
Type of cyclone:	High Efficienc	-y
Number of cyclones:	24	
Efficiency:	0.799998	
Pressure drop:	0.215033	psi 🔹
Diameter of cylinder:	1.71713	ft 🔹
Length of vortex:	4.25436	ft 🔹
Length of cylinder:	2.5757	ft 🔹
Length of cone section:	4.29283	ft 🔹
Diameter of overflow:	0.858565	ft 🔹
Length of vortex finder:	0.858565	ft 🔹
Width of gas inlet:	0.343426	ft 🔹
Height of gas inlet:	0.858565	ft 🔹
Diameter of underflow:	0.643924	ft 🔹
Number of gas turns:	7	
Inlet / saltation velocity ratio:	0.869544	

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.

Summary Balance Separation Effici	ency 🛛 🥑 Status	
Minimum pressure drop:	0.0362594	psi 🔹
Average pressure drop:	0.26813	psi 🔹
Maximum pressure drop:	0.5	psi 🔹
Filtration time:	222.53	hr 🔻
Overall collection efficiency:	0.909882	
D50 of inlet:	5.81805e-06	ft 🔹
D50 of solid outlet:	6.45669e-06	ft 🔹
D50 of vapor outlet:	1.73071e-06	ft 🔹
Solid concentration at inlet:	6.57148e-05	lb/cuft ▼
Solid concentration at outlet:	5.7177e-06	lb/cuft 🝷
Filtration velocity:	0.0260807	ft/sec 🔻
Total filter area:	22366.5	sqft 🔻
Required floor space:	1399.68	sqft 👻
Number of cells:	19	
Number of cells being cleaned:	1	
Number of bags per cell:	78	

**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.

Summary	Balance	Sep	paration Efficiend	.y	Status	
ESP results –						
Gas velocity:			1.64042	ft/	sec	•
Number of pl	lates:		26			
Plate height:			19.6951	ft		•
Plate length:			20.6693	ft		•
Overall collec	tion efficiency	y:	0.995109			
Corona volta	ge:		13468.4			
Power require	ement:		5.57344	hp	)	•
Total width o	f precipitator:		18.7008	ft		~
Pressure drop	0:		0.00118637	ps	ia	•

## **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**.

Component ID	Туре	Component name	Alias
H2O	Conventional	WATER	H2O
ACETONE	Conventional	ACETONE	C3H6O-1
N2	Conventional	NITROGEN	N2
POLYMER	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 **Mathematical State** and select **NRTL**.

	Flowsheet Sections	Referenced	Information		
Property metho	ds & options	Me	thod name:		
Method filter:	COMMON	× N	RTI	✓ Methods ass	sistant
Base method:	NRTL				ngeorien
Henry compone	ents:		Modify —		
- Petroleum cal	culation ontions	V	apor EOS:	ESIG	×
Free-water me	thod: STEAM-TA		ata set:	1	Â
Water solubilit	tv: 3	V L	iquid gamma:	GMRENON	×
	,		ata set:	1	A V
Electrolyte cal	culation options	L	iquid molar enthalpy	HLMX86	×
Chemistry ID:		<b>X</b>	iquid molar volume:	VLMX01	×
Use true co	omponents		7 Heat of mixing		
			Povnting correctio	n	
			Use liquid referenc	e state enthalny	
				e store entrialpy	

### 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 <sup>▶</sup> 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 Manual and select DNSTYGEN.

Com	ponent:	OPOL	YMER	•	
- Pro	perty mode	els for non Model na	iconvent ame	ional	components – Option codes
	Enthalpy	ENTHGE	N	~	
				Parameter (	

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/Ib-R.

- **5** In the **Parameter** field, click **M** 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**.

0	Input	Information			
Parar	neter:	<b>OHCGEN</b>	•	Btu/lb-R	
No	nconve	entional compon	ent parame	ter	
			-		
	POL	YMER 💌			
1.0	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**.

01	Input	Information			
Paran	neter:	<b>Ø DENGEN</b>	•	lb/cuft	(
Nor	nconve	entional compone	nt param	eter	
	POL		•	1	
•	80			E	

#### **11** Click **I** 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.

	Name	Stream Clas	ss		Statu
Þ	GLOBAL	MIXNCPSD	•	Required Inpu	t Incomplete
	New		Edi	t	Delete

- **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.

Global	Oescription	Accounting [	agnostics	Information	
Title:	Getting Started	with Solids - Simula	tion 4		
Clabel and ast	THE	Global settings	;		
Global unit set:	ENG	Input mode:	Steady-	State	
	Stream cla	Stream class:	MIXNCPSD	PSD	•
		Flow basis: Ambient pressure:	Mass	Mass	
			ure: 14.6959	psi	•
		Ambient temp	.: 50	F	2
		Valid phases:			•
	Free water:	No		~	
		Operational ye	ar: 8766	hr	~

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.

General	Flowsheet	Block	Stream 🎯	O Proper	rty ADA	
Generate Items to be	a standard stre included in sti	am report ream report —	<b>V</b> Include s	tream descr	iptions	
Flow ba	sis e s iq.volume onents with ze	Fraction bas Mole Mass Std.liq.vc	is Stre TFF olume	eam format SOLIDS Standard (8) Wide (132 c Sort stream	5 0 column) olumn) is alphanume	rically
Include	Streams	Exclude Strear	ns Prope	erty Sets	Compone	ent Attributes
Stream N	ames	Batch Operat	tion Su	pplementa	ry Stream	

- 3 Click **Property Sets** to view the selected property sets.
- 4 Click Close to return to the Setup Report Options | Stream sheet.
- **5** Click No 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

🕜 Mixed	CI Solid	ONC Solid	Flash Options	EO	Options	Costing	Information
Specifica	tions	T	D		Compos	ition	
- State varial	bles —	remperature 💽	rressure		Mass-Fl	low 🖌	lb/hr
Temperatu	ire:	90	F	~		Component	Value
Pressure:		16	psia	~	H2C	)	
Vapor fract	tion:				ACE	TONE	1000
194 194					N2		
Total flow	basis:	Mass 👻			10000		
Total flow	rate:		lb/hr	~			
Solventi				*		Total:	1000

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	

State variables —				Com	position ———		
Substream name:	<b>⊖</b> NCPSD		Y	Mas	s-Flow	lb/hr	
Temperature:	90	F	~	157	Component	Value	
Pressure:	16	psia	~	• 1	OLYMER	100	
Total flow basis:	Mass	•					
Total flow rate:		lb/hr	~		Total:	100	

#### 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

📀 🥝 Particle Size Distribution

2SD mesh ID: PSD 💌 Edit PSD Mesh	Interval	Lower limit	Upper limit	Weight fraction	Cumulative weight fraction
Populate PSD using	1	0	20	0	0
Oser-specified values	2	20	40	0	0
O A distribution function	- 3	40	60	0	0
Distribution function	4	60	80	0	0
Type of distribution function: Normal	5	80	100	0	0
	6	100	120	0.2	0.2
Calculate	> 7	120	140	0.3	0.5
	8	140	160	0.3	0.8
	9	160	180	0.2	1
	▶ 10	180	200		

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**.

Component ID: Attribute ID:		ØF	<b>OPOLYMER</b>	
		@ GENANAL		
	Elemen	ıt	Value	
۲	ELEM1		100	
	ELEM2			
	ELEM3			

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

**13** Click No 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

0	Specification	s 🕜 Stream	ns	Heat Streams	Temp-Dut
Оре	erating condit	tions —	2	~	
NUI	mber of stage	is:	3	Y	
Pre	ssure:		15	psia	~
Am	bient temper	ature:	77	F	•
Stag	ge profiles —				
	Stage	Mixing efficiency	Liqui	id-to-solid ass ratio	
۲	1	0.9	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 <u>Sheet Help</u>.

The help for the Cyclone Input Specifications Sheet appears.

- **3** In the list of **See Also** links, click the <u>Specifying Cyclone</u> 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**.

Specifications	Dimensions	Ratios	Efficiency	Solids Loading	Outlet I			
Calculation options								
Model:	Model:		Cyclone -					
Mode:	Mode:				-			
Calculation metho	Calculation method:		ht		-			
Type:		Stair mar	nd-HE		-			
_ Efficiency correlati	ion parameters							
Vane constant:		16						
Wall friction coeffi	Wall friction coefficient:							
Constant D:		3						
Constant Kg:		0.025						
Consider secor	Consider secondary flow							
- Design parameters	;							
Separation efficier	icy:	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.
- 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 Sand select Bradley.
- 8 In the **Type** field, click **Sector** 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.

Specifications	Dimensions	<b>Q</b> Ratios	Velocity Correlation	Efficiency
- Calculation option -	2			
Model:		Hydrocyc	×	
Mode:		Design		
Efficiency correlation:		Bradley	~	
Туре:		User-spe	×	
Design parameters -		1		
Diameter of solid pa	rticles:	100	mu	~
Separation efficienc	y:	0.95		
Maximum diameter		1.5	ft	×
Maximum pressure	drop:	5	psi	×

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.

Specifications	Dimensions	Ratios	Velocity Correlation
Inlet configuration:	Roun	d	
Ratios of hydrocyclor	ne diameter —		
Length of cylinder:	5		
Length of vortex find	er:		
Diameter of overflow	: <b>0.3</b>		
Diameter of underflo	w: 0.15		
Height of inlet:			
Width of inlet:			
Diameter of inlet:	0.142	9	
Dimensions of hydro	cyclone		
Cone angle:	19.99	62 de	g 💌

### **13** Click **I** 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.

- 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 <sup>▶</sup> 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.

lisp	lay: Streams 💽 Fe	ormat: SOLIDS	~	Stream Table		
		ACETONE	TO-CCD	WASH-H20	WASH-OUT	SLURRY ¥
ř.	Mass SFrac	< 0.001	0.382	0	0	0.333
Þ.	*** ALL PHASES ***					
Þ.	Mass Flow Ib/hr	839.348	260.652	400	361.847	298.805
þ.	Volume Flow cuft/hr	17.237	4.553	6.925	6.91	4.77
Þ.	Enthalpy Btu/hr	-1.5277e+06	-292690	-2.6788e+06	-1.7216e+06	-1.2499e+06
F.	Density lb/cuft	48.696	57.25	57.766	52.364	62.643
E	Mass Flow Ib/hr					
Þ	H2O			400	217.058	182.942
Þ.	ACETONE	838.95	161.05		144.789	16.262
P.	N2					
F	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 in and select the following streams HOT-N2, TO-CYCL, VENT, and POLYMER.

Mat	erial Heat Load	Work	c Vol.% Cu	rves	Wt. % Cur	ves	Petro, Curve	s	Poly. Curves			
Disp	lay: Streams	💌 Fo	rmat: SOLIDS				Stream Table					
			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 Ib/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	
Þ.	Density lb/cuft		62.643		0.052		0.068		0.066		80	
÷	Mass Flow lb/hr											
${\mathbb P}_i$	H2O		182.942				182.942		182.942			
5	ACETONE		16.262				16.262		16.262			
Þ.	N2				3000		3000		3000			
×.	POLYMER		99.602				99.602		0.099		99.502	
4			141					III				

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.

Summary	Balance	Profiles	St	atus		
CCD results	-			177.45 X		
		Mass flov	٧	Tempera	ature	
		lb/hr	•	F	Y	
Top stage fe	ed:	260.652		90		
Bottom stag	e feed:	400		200		
Total side fe	otal side feed: op stage product:			169.924		
Top stage p						
Bottom stag	e product:	298.805		194.406		
Side draw (under):		0				
Side draw (d	over):	0				
Total duty:		0		Btu/hr		

- 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.

Su	mmary	Baland	e	Profiles	St	atus									
	Stage	Tempera	ature	Duty	/	Underf	low	Overfl	ow	Fee	ł	Under Pi	roduct	Over	Product
		F	•	Btu/hr		lb/hr	•	lb/hr	•	lb/hr	¥	lb/hr	~	lb/hr	~
۲	1	169.924		0		99.6017		561.05		260.652		0		361.84	7
	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.

Summary Balance Efficiency 🖉 Status							
Type of cyclone:	High Efficiency						
Number of cyclones:	1						
Efficiency:	0.999003						
Pressure drop:	0.0255742	psi 🔹					
Diameter of cylinder:	2.38592	ft 🔹					
Length of vortex:	5.91134	ft 🔹					
Length of cylinder:	3.57888	ft 🔹					
Length of cone section:	5.96479	ft 🔹					
Diameter of overflow:	1.19296	ft 🔹					
Length of vortex finder:	1.19296	ft 🔹					
Width of gas inlet:	0.477183	ft 🔹					
Height of gas inlet:	1.19296	ft 🔹					
Diameter of underflow:	0.894719	ft 🔹					
Number of gas turns:	7						
Inlet / saltation velocity ratio:	1.08617						

- 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.

Summary	Balance	Status		
Mixer results				
Outlet tempe	Outlet temperature:		F	×
Outlet pressu	Outlet pressure:		psia	~
Vapor fraction:		1		
1st liquid/Tot	tal liquid:	1		

- 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.

Summary Bal	ance Separ	ation Efficiency	Status 🎯			
Pressure drop:		0.04733	17 psi	•		
Overall separation	n efficiency:	0.99601	7			
Overflow volume	flow:	17.2365	cuft	/hr 🔻		
Underflow volum	e flow:	4.5529	cuft	cuft/hr 🔻		
Liquid from split	to underflow:	0.16105	j			
Liquid volumetric	flow per cyc	lone: 20.5394	cuft	/hr 🔻		
Cylinder length:		2.09245	ft	-		
Overflow diamete	er:	0.12554	7 ft	-		
Underflow diame	ter:	0.06277	'34 ft	-		
Number of cyclo	nes:	1				
Diameter of inlet:		0.05980	21 ft	•		
Diameter of cylin	der:	0.41848	9 ft	-		
Inlet liquid veloci	ty:	2.03124	ft/s	ec 🔹		

# **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.