2 Modeling Coal Combustion

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

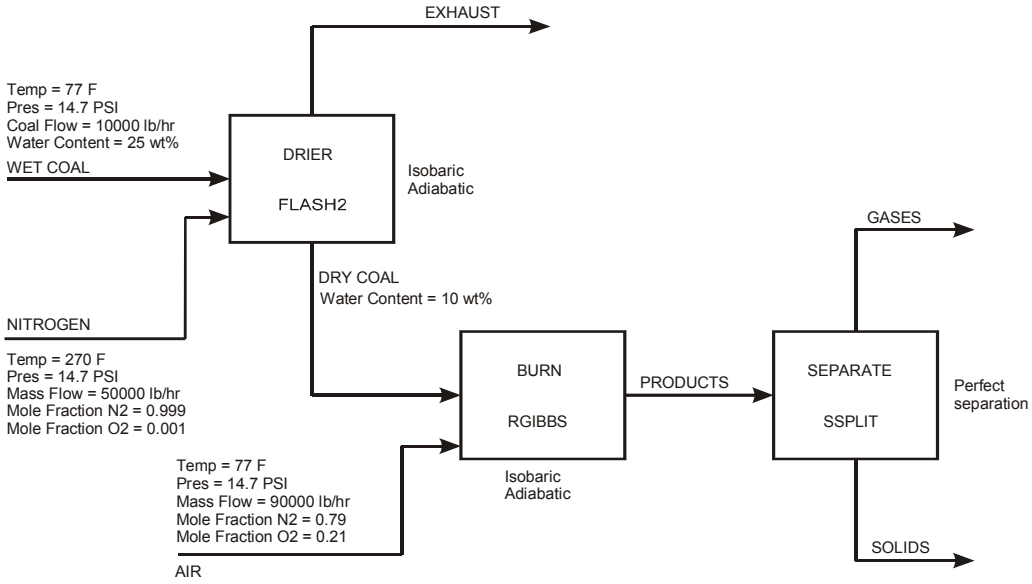
You will:

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

Allow about 45 minutes to complete this simulation.

Coal Combustion Flowsheet

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



Starting Aspen Plus

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

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

Opening an Existing Run

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

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

If Your Saved File Solid1.apw is Not Displayed

1 Click **Open**.

The **Open** dialog box appears.

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

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

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

To Access the Examples Folder

1 Click **Open File**.
The **Open** dialog box appears.
2 At the left, under **Favorites**, click **Aspen Plus** <*version*> **Examples**.
By default, this folder contains folders that are provided with Aspen Plus.
3 Double-click the **Examples** folder, then the **GSG_Solids** folder.
4 Select **Solid1.bkp** and click **Open**.

Saving a Run Under a New Name

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

1 From the ribbon, select **File | Save As | Aspen Plus Document**.
2 In the **Save As** dialog box, choose the directory where you want to save the simulation.
3 In the **File name** field, enter **Solid2**.
4 Click **Save** to save the simulation and continue.
Aspen Plus creates a new simulation model, Solid2, which is a copy of the base case simulation, Solid1.

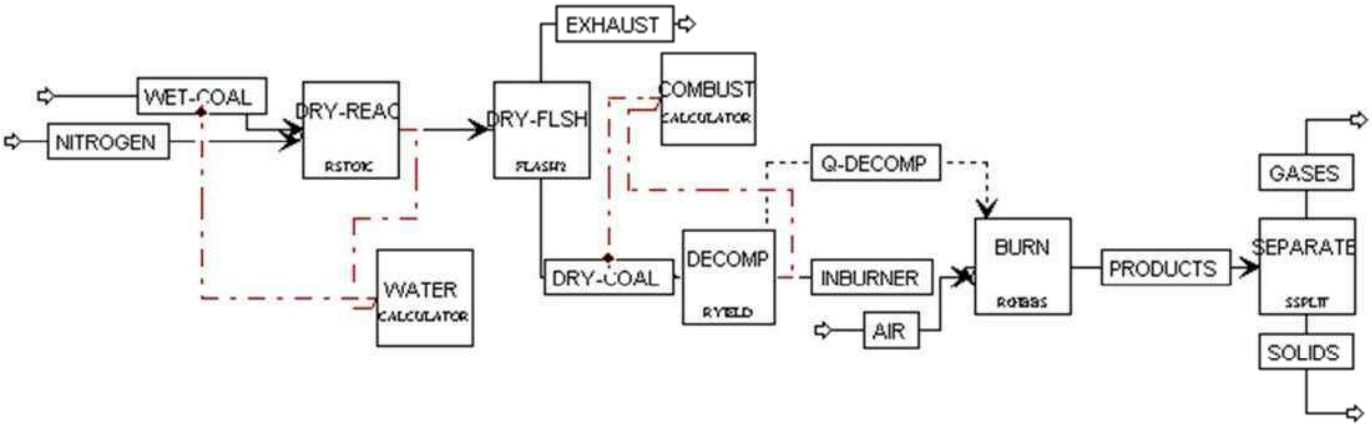
Modifying the Flowsheet

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

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

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

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



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

Changing the Stream Class

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

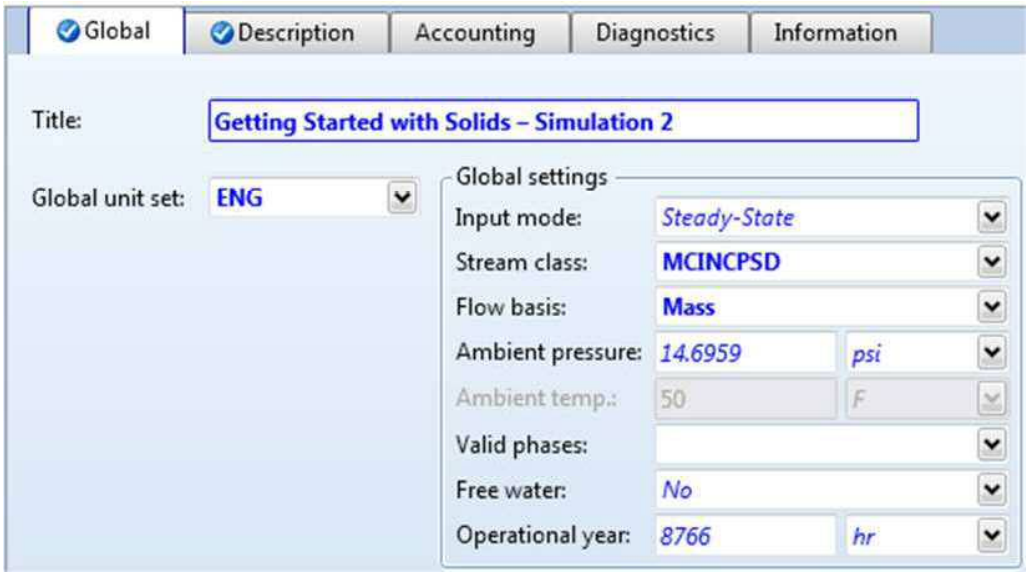
- MIXED
- CIPSD
- NCPSD

To Change the Global Stream Class

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

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

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



Adding Components to the Model

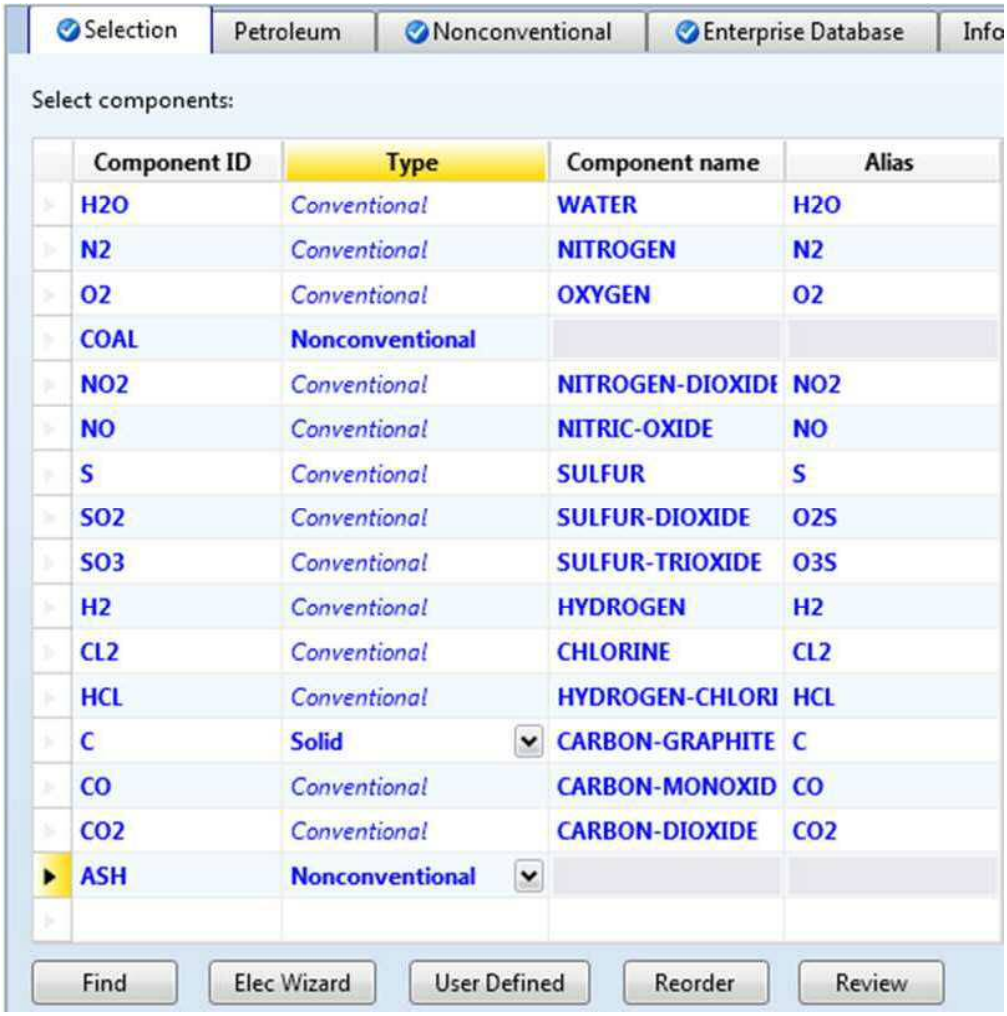
Simulation 1 had four components: H2O, N2, O2, and COAL. Add the components that are formed by decomposing and combusting coal.

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

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

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

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



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

3 Click to continue.

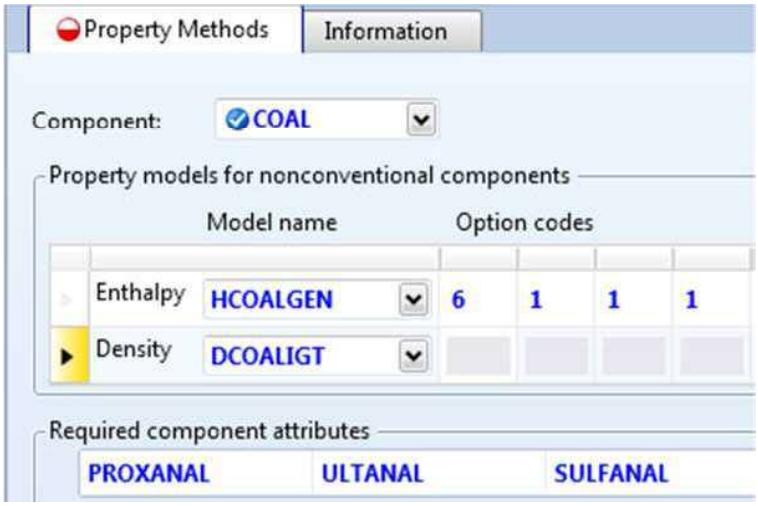
The **Methods - NC Props | Property Methods** sheet appears.

Defining Properties

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

Change the Heat of Combustion Method for Coal

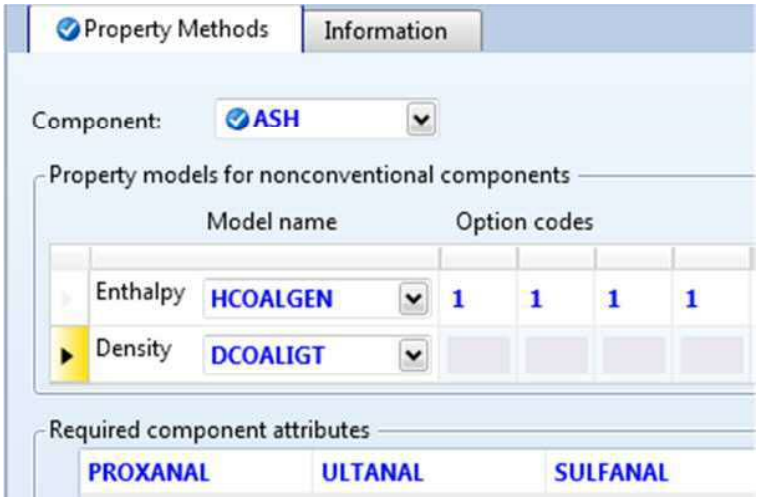
1 In the **Component** field, click and select **COAL**.
2 Change the first HCOALGEN **Option codes** field from **1** to **6**.



Specify Methods for Calculating Ash Properties

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

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



Specify the Heat of Combustion for Coal

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

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

The **Pure Components** object manager appears.

2 Click **New**.

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

3 Select the **Nonconventional** option.

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

5 Click **OK**.

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

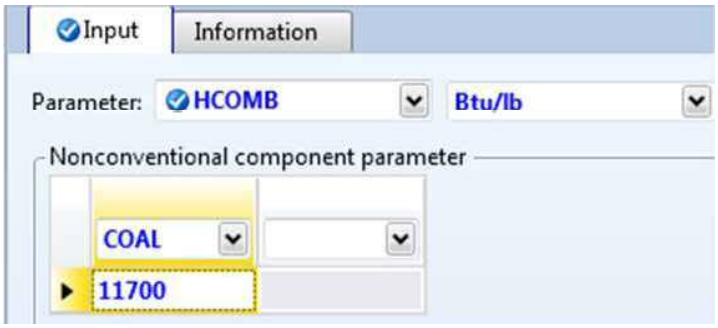
6 In the **Parameter** field, click and select **HCOMB**.

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

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

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

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



9 Click to continue.

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

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

Specifying the Air Stream

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

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

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

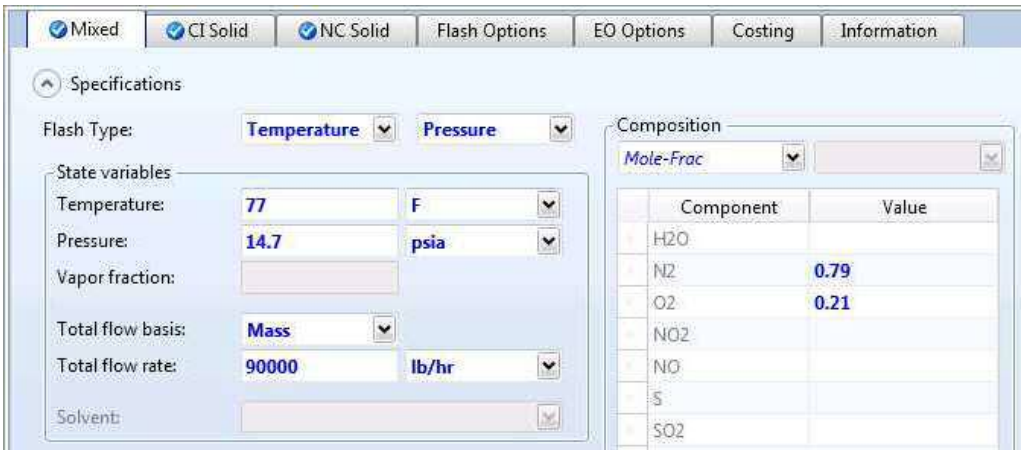
Parameter	Value
Temperature	77 F
Pressure	14.7 psia

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

3 Enter the following mole fractions:

Component	Value
N2	0.79
O2	0.21

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



5 Click to continue.

Specifying Unit Operation Models

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

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

Specify the RGibbs Reactor Model

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

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

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

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

3 Click the **Products** tab.

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

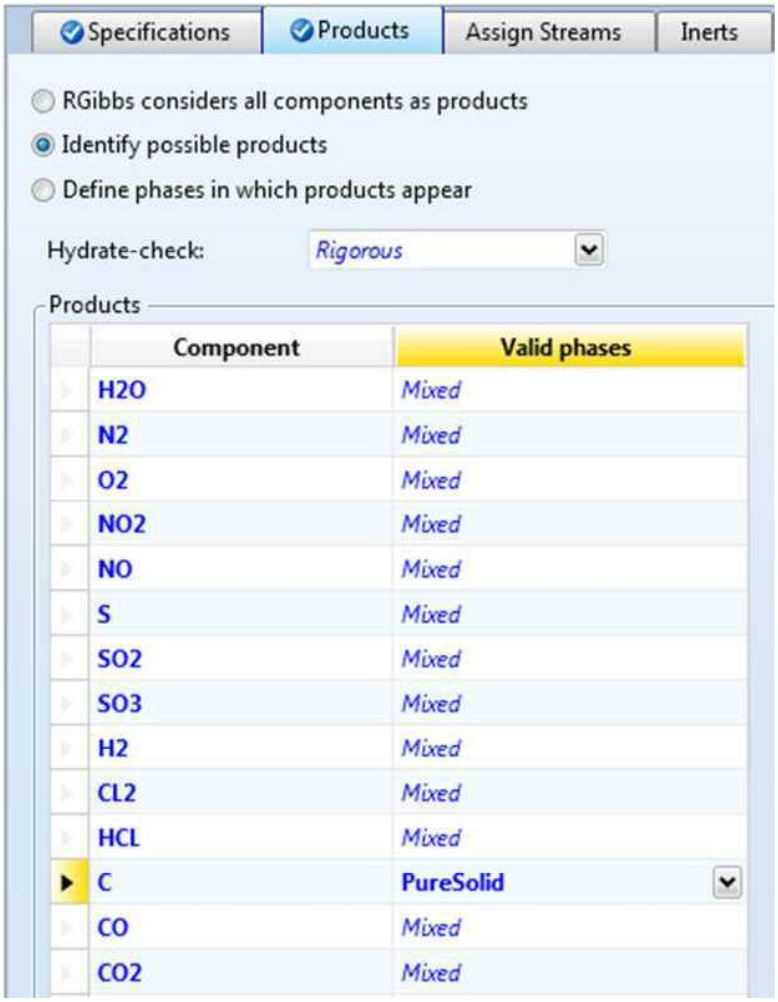
By default, RGibbs assumes that all of the components that are listed on the **Components - Specifications | Selection** sheet are potential products in the vapor phase or the liquid phase. This default is not appropriate for this simulation, since any carbon that remains after combustion would be solid.

4 Select **Identify possible products**.

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

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

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



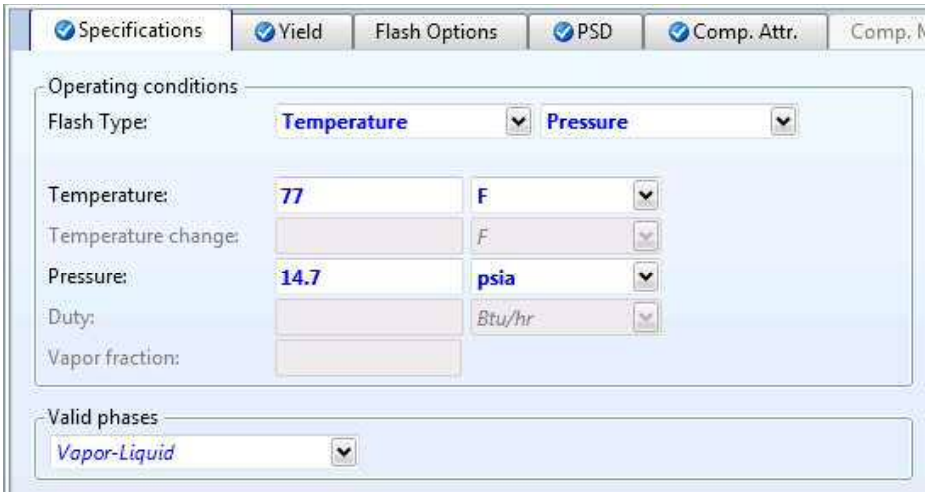
6 Click to continue.

Specify the RYield Reactor Model

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

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

Parameter	Value
Pressure	14.7 psia
Temperature	77 F



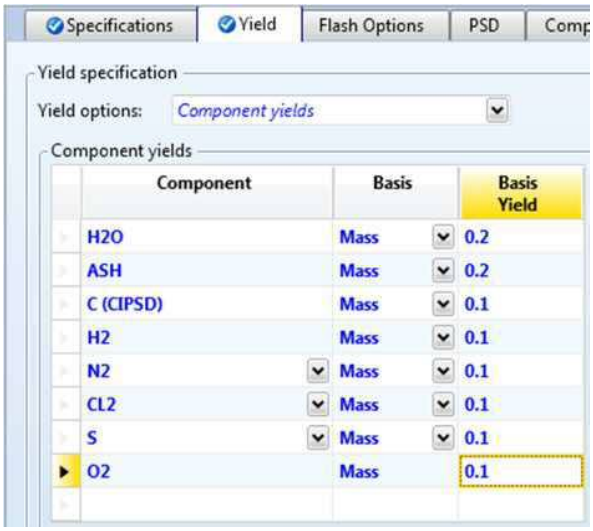
2 Click to continue.

The **Yield** sheet appears.

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

3 Enter the component yields as follows:

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



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

Specify the Particle Size Distributions

1 Click the **PSD** tab.

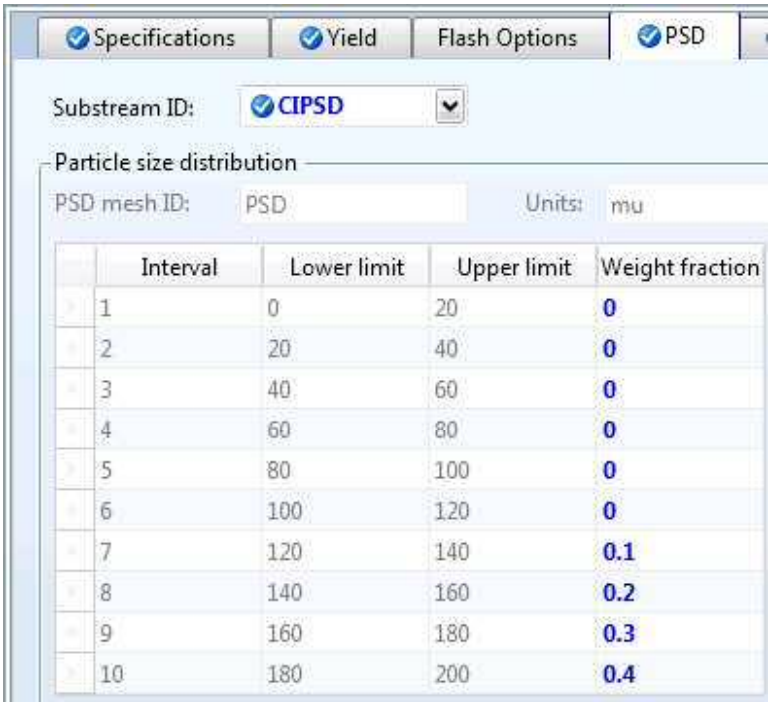
The **DECOMP (RYield) - Setup | PSD** sheet appears.

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

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

Interval	Weight Fraction
7	0.1
8	0.2
9	0.3
10	0.4

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



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

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

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

Specify the Component Attributes for Ash

1 Click the **Comp. Attr.** tab.
The attributes PROXANAL, ULTANAL, and SULFANAL are required for RYield to calculate the enthalpy and density of ash.

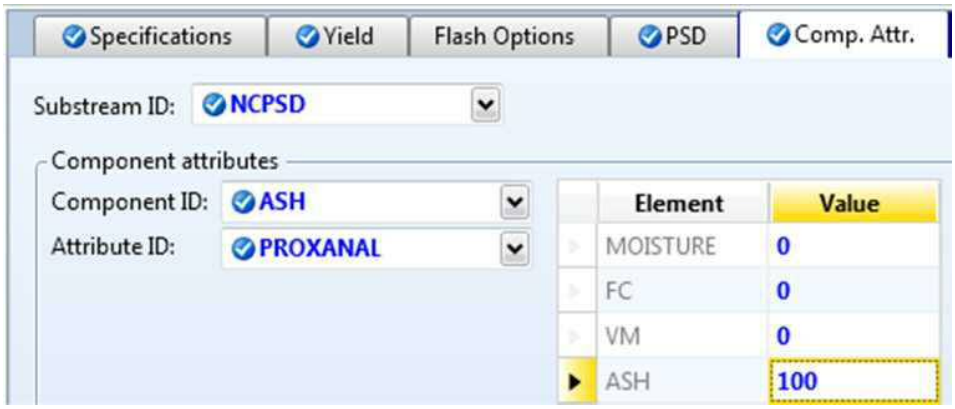
2 In the **Substream ID** field, click and select **NCPSD**.

3 In the **Component ID** field, click and select **ASH**.
ASH has the attributes PROXANAL, ULTANAL, and SULFANAL.

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

5 For the attribute PROXANAL, enter these values:

Element	Value
Moisture	0
FC	0
VM	0
Ash	100



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

7 For the attribute ULTANAL, enter these values:

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

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

9 For the attribute SULFANAL, enter these values:

Element	Value
Pyritic	0

Element	Value
Sulfate	0
Organic	0

10 Click  to continue.

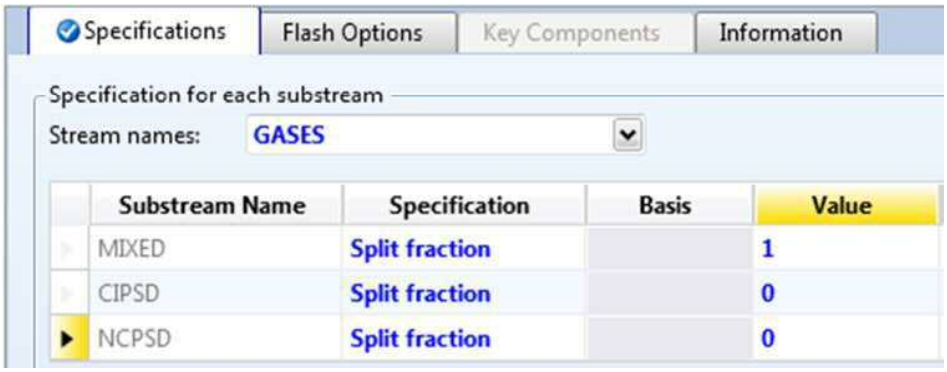
Specify the Splits for the SSplit Block

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

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

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

Substream Name	Value
MIXED	1
CIPSD	0
NCPSD	0



Defining a Calculator Block

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

Create the Calculator Block

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

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

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

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

Define the Calculator Variables

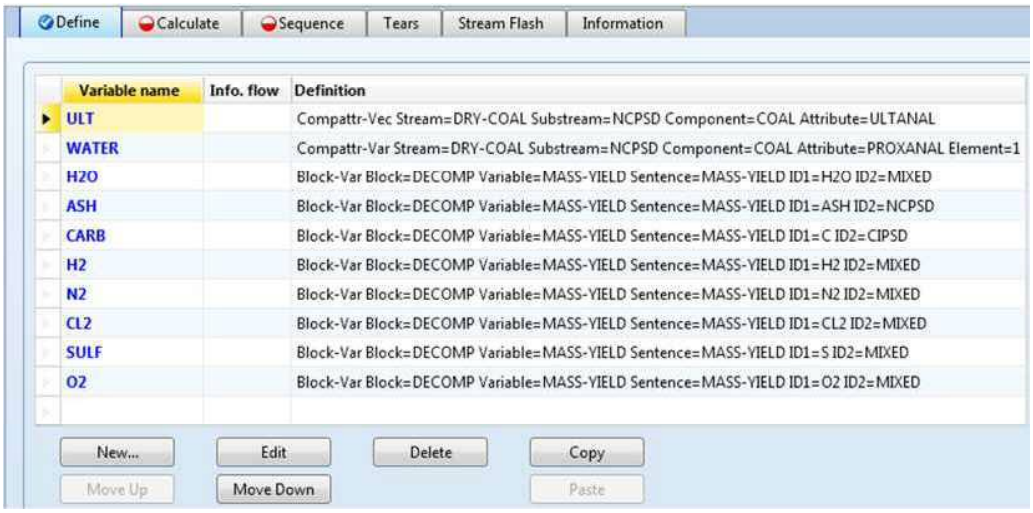
The **COMBUST | Define** sheet appears. Use this sheet to access the flowsheet variables you want to use in the Fortran block. In the simulation in chapter 1, you accessed individual elements of component attributes. You can also access component attributes as a vector. In this simulation, access the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

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

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

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

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



6 Click the **Calculate** tab.

Specify the Calculations to be Performed

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

7 Enter the following Fortran statements:

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

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

8 Click the **Sequence** tab.

Specify When the Calculator Block Should be Run

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

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

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

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

12 Click to continue.

Running the Simulation

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

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

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

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

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

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

2 Examine the results of your simulation.

Examining Results

View the Stream Results

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

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

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

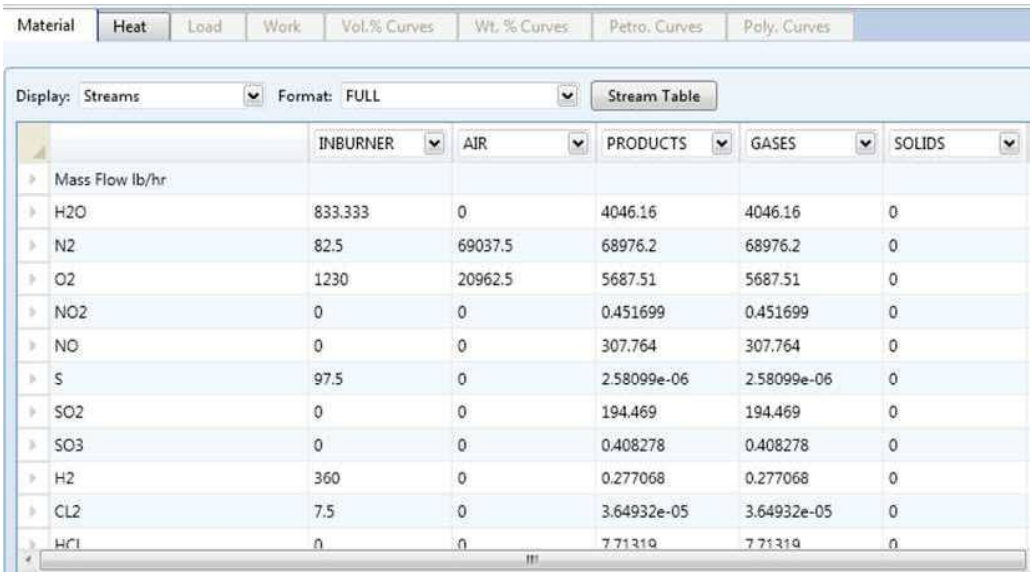
The **Results Summary - Streams | Material** sheet appears.

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

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

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

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



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

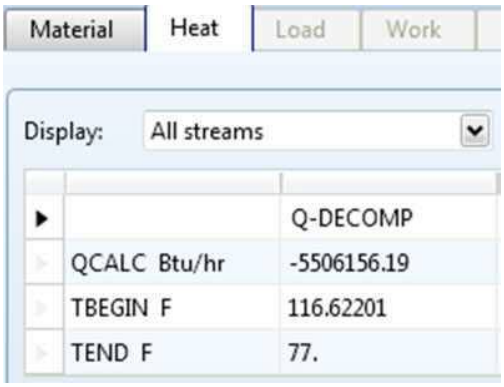
6 Review the results on this sheet. Use the scrollbars to review results that are off the screen.

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

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

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

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



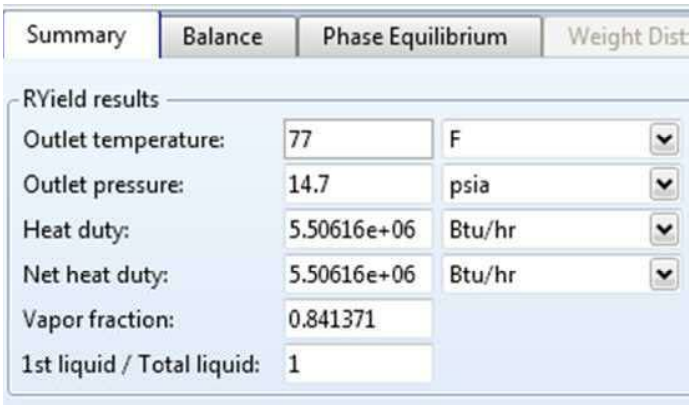
View the Block Results

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

1 In the Flowsheet, select the DECOMP block.

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

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



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

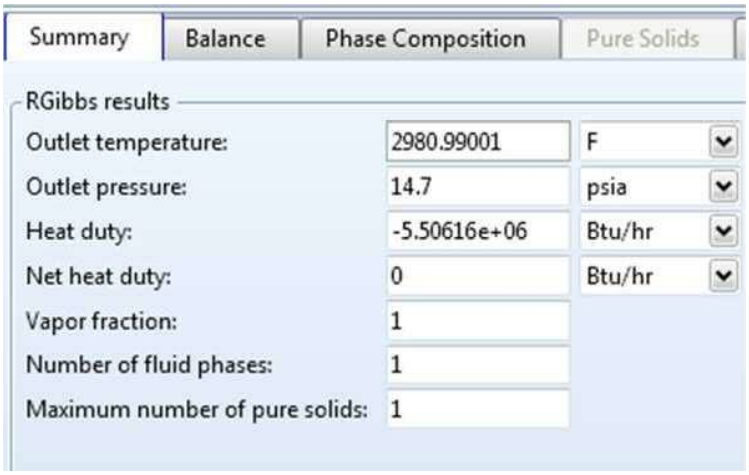
The **DECOMP (RYield) - Results | Balance** sheet appears. Use this sheet to report the mass and energy balance for the block. Because RYield has a net reaction from nonconventional components to conventional components, the mass balance for both conventional components and nonconventional components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

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

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

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

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



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

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

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

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

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

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

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

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

Exiting Aspen Plus

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

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

The **Aspen Plus** dialog box appears.

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

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

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