

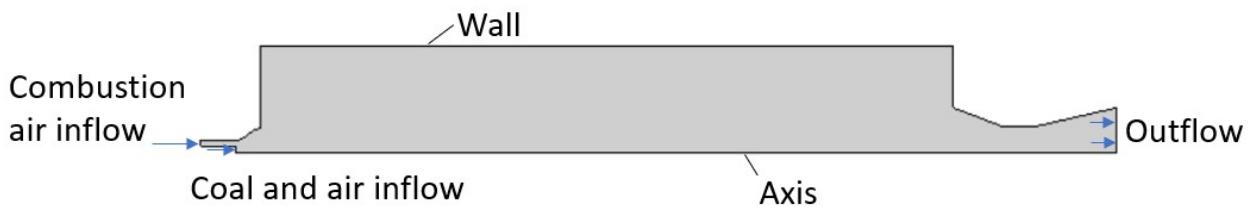
Eddy Break-Up: Coal Combustion

The combustion of pulverized coal is still one of the main primary energy conversion mechanisms worldwide.

In this tutorial, you simulate the flow and combustion of coal particles in an axisymmetric coal combustor. Coal furnaces are often used to provide heat for a specific purpose. Therefore, it is useful to simulate the temperature and monitor any products of incomplete combustion at the outlet—such as carbon particles or carbon monoxide gas. Since coal often contains sulfur impurities, it is also prudent to monitor sulfur dioxide emissions (a pollutant which contributes significantly to acid rain).

The coal particles enter the computational domain together with transport air at a velocity of 23m/s and a temperature of $70\text{ }^{\circ}\text{C}$. At a different boundary, combustion air inflow is specified as a velocity profile $V_Z(r)$ with swirl $V_\theta(r)$.

The following diagram shows the geometry of the coal combustor:



Initially, the combustion chamber is filled with hot air at a temperature of $527\text{ }^{\circ}\text{C}$. Upon injection of the coal particles into the combustor, the coal particles devolatilize to form the combustible gaseous fuel. The high initial temperature around the coal particles ensures that devolatilization begins and also ignites the gas-phase combustion.

The Lagrangian Multiphase model is used to simulate the dispersed phase of solid coal particles, and the Radiation model is used to simulate radiative heat transfer within the system.

To set up a coal combustion simulation in Simcenter STAR-CCM+, you require the following information:

- Proximate and ultimate analysis of the coal sample
- Calorific value of the coal sample (LCV)
- Specific heat of coal
- Particle density of coal

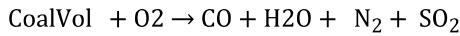
In the particle phase, the multi-component coal particle consists of four components: raw coal, char, ash and moisture (water). The exact composition of these components depends on the proximate analysis of the coal. The coal particles undergo several processes once they are injected and flow through the domain.

Simcenter STAR-CCM+ provides the following models to describe each of the processes:

- Evaporation of the moisture content in the coal is modeled by the Coal Moisture Evaporation model
- Coal volatile formation is modeled by the Coal Devolatilization model
- Oxidation of the remaining char is modeled by the Char Oxidation model

The Coal Moisture Evaporation Model is based on a quasi-steady evaporation process where the driving force for evaporation is the departure from the vapor-liquid equilibrium using the Ranz-Marshall correlation.

The coal volatile that is released into the gas phase as a result of the coal Devolatilization model mixes with the surrounding gases to undergo an oxidation process. The gas-phase combustion reactions consist of two steps:



To properly define the gas-phase reactions, you require the coal volatile composition, which is computed based on the proximate and the ultimate analysis as well as the coal volatile specific heat.

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Prerequisites

The instructions in this tutorial assume that you are already familiar with certain techniques in Simcenter STAR-CCM+.

Technique	Tutorial
The Simcenter STAR-CCM+ workflow	Introduction to STAR-CCM+
Using visualization tools, scenes, and plots	Introduction to STAR-CCM+

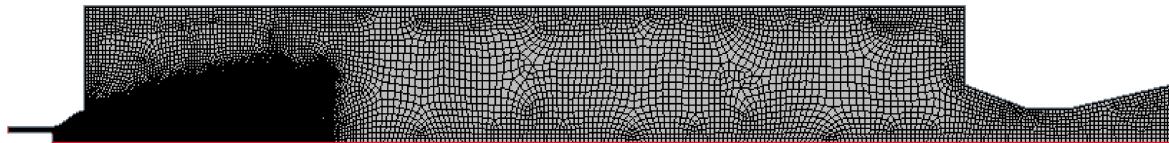
If you have not already done so, download the tutorial files bundle. See [Downloading the Tutorial Files from the Support Center Portal](#).

Loading the Starting Simulation File

For this tutorial, you are provided with a starting simulation file that contains the mesh operations necessary for generating a 2D axisymmetric mesh of the coal combustor.

To import the starting simulation file:

1. Launch Simcenter STAR-CCM+.
2. Select **File > Load**.
3. In the *Load a File* dialog, navigate to the `reactingFlow` folder of the downloaded tutorial files, select `coalCombustion_start.sim`, then click **OK**.
4. To generate the 2D axisymmetric combustor mesh, right-click the **Geometry > Operations** node and select **Execute All**.
The mesh generation process takes a few minutes to complete. You can monitor the progress in the output window.
5. When mesh generation has finished, create a mesh scene to view the mesh.



The quadrilateral cell mesh is refined using wake refinement at an angle of twelve degrees from the inlet surfaces for a distance of two metres.

6. Save the simulation as `EBU_Coal.sim`.

Selecting Physics Models

The standard EBU version of the Eddy Break-Up model is used to represent the combustion reactions that occur within the coal combustor, since the reaction rates are limited by the rate at which turbulence mixes the reactants and heat into the flame zone.

To select the physics models:

1. Rename the **Continua > Physics 1** node to **Coal Combustion**.
2. For models in the **Coal Combustion** continuum:
 - a) In the *Enabled Models* group box, deselect **Two Dimensional**.
 - b) Select the following models in order:

Group Box	Model
Space	Axisymmetric
Time	Steady
Material	Multi-Component Gas
Reaction Regime	Reacting
Reacting Flow Models	Reacting Species Transport
Reacting Species Models	Eddy Break-Up

Group Box	Model
Flow	Segregated Flow (selected automatically)
	Gradients (selected automatically)
	Segregated Species (selected automatically)
	Segregated Fluid Enthalpy (selected automatically)
Equation of State	Ideal Gas
Viscous Regime	Turbulent
	Reynolds-Averaged Navier-Stokes (selected automatically)
Reynolds-Averaged Turbulence	K-Epsilon Turbulence
	Realizable K-Epsilon Two-Layer (selected automatically)
	Wall Distance (selected automatically)
	Two-Layer All y+ Wall Treatment (selected automatically)
Optional Models	Axisymmetric Swirl
	Lagrangian Multiphase
	Radiation Surface Materials (selected automatically)
Radiation	Participating Media Radiation (DOM)
Radiation Spectrum (Participating)	Gray Thermal Radiation

3. Click **Close**.
4. Select the **Models > Eddy Break-Up** node and set the following properties:

Property	Setting
<i>Reaction Control</i>	Standard EBU
<i>Source Term Limiting</i>	Activate

5. Right-click the **Models > Multi-Component Gas > Gas Components** node and select **Select Mixture Components**.
6. In the *Select Mixture Components* dialog, select the following:
 - CO (Carbon Monoxide)
 - CO₂ (Carbon Dioxide)
 - CoalVolatile (Coal Volatile)
 - H₂ (Hydrogen)
 - H₂O (Water)
 - N₂ (Nitrogen)
 - O₂ (Oxygen)
 - SO₂ (Sulphur Dioxide)

7. Click **Apply**, then click **Close**.
8. Save the simulation.

Setting Material Properties

Since the composition of different types of coal varies, it is important to define the correct composition of the type of coal that is used in the combustor.

The raw coal devolatilizes into char in the particle phase and **CoalVolatile** in the gas phase. The composition of the coal volatile species is not fixed, but depends on the properties of the coal type being simulated. The proximate and ultimate analysis of the coal sample determines the coal volatile composition. In addition to the proximate and ultimate analysis, the calorific value of the coal type is needed to estimate the heat of formation of the coal volatile.

The proximate analysis is given by:

Component	Mass Fraction (-)
Volatile Matter	0.5502
Fixed Carbon	0.3668
Ash	0.083
H ₂ O	0.0

The ultimate analysis (dry ash free) is given by:

Component	Mass Fraction(%)
C	80.36
H	5.08
N	1.45
S	0.94
O	12.17

The proximate analysis gives us a yield of 0.6, the low calorific value of coal is 7.1 *kcal/g* and the specific heat of coal is 1100 *J/kg K*.

To set the material properties:

1. For the **Coal Combustion** continuum, select the **Models > Multi-Component Gas > Material Properties > Thermal Conductivity** node and set *Method* to **Mass Weighted Mixture**.
2. Expand the **Multi-Component Gas > Gas Components** node.
3. Multi-select all of the **[Gas Component] > Material Properties > Molecular Weight** nodes and set *Method* to **Elemental Composition**.
4. Define the composition of the **CoalVolatile**.
 - a) Expand the **Gas Components > CoalVolatile > Material Properties > Elemental Composition** node.

- b) Right-click the **Elemental Composition > Elemental Composition Method > Atoms** node and select **New Atom**.
- c) In the *Add atom to elemental composition* dialog, set *Choose atom* to **S** and click **OK**.
- d) Expand the **Atoms** node and set the following properties:

Node	Property	Setting
C	Value	2.8029
H	Value	4.2329
N	Value	0.0860
O	Value	0.6340
S	Value	0.0240

5. Expand the **Gas Components > CoalVolatile > Material Properties** node and set properties:

Node	Property	Value
Specific Heat	<i>Method</i>	Constant
└ Constant		1100.0 J/kg-K
Heat of Formation		
└ Constant		-4725729.0 J/kg

6. Expand the **Multi-Component Gas > Material Properties** node and set the following properties:

Node	Property	Setting
Absorption Coefficient	<i>Method</i>	Weighted Sum of Gray Gases
└ Weighted Sum of Gray Gases	<i>Optical Path Length</i>	1.8 m

7. Define the surface materials and specify radiation properties:

- a) Select the **Coal Combustion > Models > Surface Materials > Surface Materials > Default** node and rename it to **Cooling Loops**.
- b) Select the **Cooling Loops > Material Properties > Emissivity > Constant** node and set *Value* to **0.4**.
- c) Right-click the **Surface Materials > Surface Materials** node and select **Select Surface Materials**.
- d) In the *Select Surface Materials* dialog, select **Cast Iron (Cast Iron)**.
- e) Click **Apply** twice, then click **Close**.
- f) Rename the **Cast Iron** node to **Furnace** and the **Cast Iron 1** node to **Inlet Ducts**.
- g) Set the following properties:

Node	Property	Setting
Furnace > Material Properties > Emissivity > Constant	Value	0.5
Inlet Ducts > Material Properties > Emissivity > Constant		0.6

- Save the simulation.

Defining Reactions

Due to the heating of the coal particles, the coal volatile matter is released to the gas phase. The coal volatile mixes with the surrounding gases to undergo an oxidation process. In this tutorial, you specify the gas phase reactions in two steps.

To define reactions:

- For the **Coal Combustion** continuum, right-click the **Models > Reacting > Reactions** node and select **New Reaction**.
- Rename the **Reactions > Reaction 1** node to **CoalVol + O₂ → CO+H₂O+N₂+SO₂**.
- Set up the sub-nodes of the **CoalVol + O₂ → CO+H₂O+N₂+SO₂** node as follows:

Node	Action
Reactants	Right-click and select: a. Add Reactant > Gas Mixture > Coal Volatile. b. Add Reactant > Gas Mixture > O ₂
└ O ₂	Set Stoich. Coeff to 2.16675.
Products	Right-click and select: a. Add Product > Gas Mixture > N ₂ b. Add Product > Gas Mixture > CO c. Add Product > Gas Mixture > H ₂ O d. Add Product > Gas Mixture > SO ₂
└ N ₂	Set Stoich. Coeff to 0.043.
└ CO	Set Stoich. Coeff to 2.803.
└ H ₂ O	Set Stoich. Coeff to 2.1165.
└ SO ₂	Set Stoich. Coeff to 0.024.

- Create one more **[Reaction]** node and rename it as **CO + 0.5O₂ → CO₂**:
- Set up the sub-nodes of the **CO + 0.5O₂ → CO₂** node as follows:

Node	Action
Reactants	Right-click and select: a. Add Reactant > Gas Mixture > CO. b. Add Reactant > Gas Mixture > O2.
L_{O_2}	Set Stoich Coeff to 0.5.
Products	Right-click and select Add Product > Gas Mixture > CO2.

- Save the simulation.

Defining the Coal Particles

The Lagrangian Multiphase model is used to define the interaction between a discrete phase of solid coal particles and the continuous background phase of the fluid domain within the coal combustor.

Coal is defined as a multi-component coal particle consisting of the four components raw coal, char, ash, and water. The injected coal particles undergo several processes flowing through the combustor:

- Evaporation of moisture content
- Coal volatile formation
- Oxidation of the remaining char

The evaporation of the moisture content of the coal particle is modeled by the coal moisture evaporation model. This model is based on a quasi-steady evaporation process where the driving force for evaporation is the departure from the vapor-liquid equilibrium using the Ranz-Marshall correlation. The Coal Devolatilization model determines the rate at which the coal volatile escapes from the coal particle and is released to the gas phase. In this tutorial, you use the half-order char oxidation model to calculate the char oxidation. With this model, char is oxidized through O_2 , H_2O and CO_2 .

To define the coal particles:

- Within the **Coal Combustion** continuum, right-click the **Models > Lagrangian Multiphase > Lagrangian Phases** node and select **New > Free-stream Phase**.
- Rename the **Lagrangian Phases > Phase 1** node to **Coal**.
- For the **Coal** phase, select the following models in order:

Group Box	Model
Particle Type	Material Particles
	Residence Time (selected automatically)
	Pressure Gradient Force (selected automatically)
	Spherical Particles (selected automatically)
Material	Multi-Component Coal
	Species (selected automatically)
Equation of State	Constant Density

Group Box	Model
<i>Mass Transfer</i>	Coal Combustion
	Two-Way Coupling (selected automatically)
	Energy (selected automatically)
	Coal Moisture Evaporation (selected automatically)
<i>Char Oxidation</i>	Half-Order Char Oxidation
<i>Raw Coal Devolatilization</i>	User-Defined Devolatilization
<i>Track Sampling</i>	Boundary Sampling
	Track File
<i>Optional Particle Forces</i>	Drag Force
<i>Optional Models</i>	Turbulent Dispersion
	Particle Radiation
	Parcel Depletion

4. Click **Close**.
5. To allow you to track particles at the outlet boundary, select the **Coal > Models > Boundary Sampling** node and set the following properties:

Property	Setting
<i>Scalars</i>	Click  (Custom Editor) and select: <ul style="list-style-type: none"> ◦ Particle > Mole Fraction > Particle Mole Fraction of Ash ◦ Particle > Mole Fraction > Particle Mole Fraction of Char ◦ Particle > Mole Fraction > Particle Mole Fraction of H2O ◦ Particle > Mole Fraction > Particle Mole Fraction of RawCoal
<i>Boundaries</i>	OUTLET

6. Expand the **Half-Order Char Oxidation** node, multi-select all **[reaction]** nodes and set the *Temperature Exponent, Beta* to **0.5**.
7. To prevent the tracking of very small ash particles and to reduce the calculation time, set the maximum mass fraction of ash that is tracked. Select the **Coal > Models > Parcel Depletion** node and set the following properties:

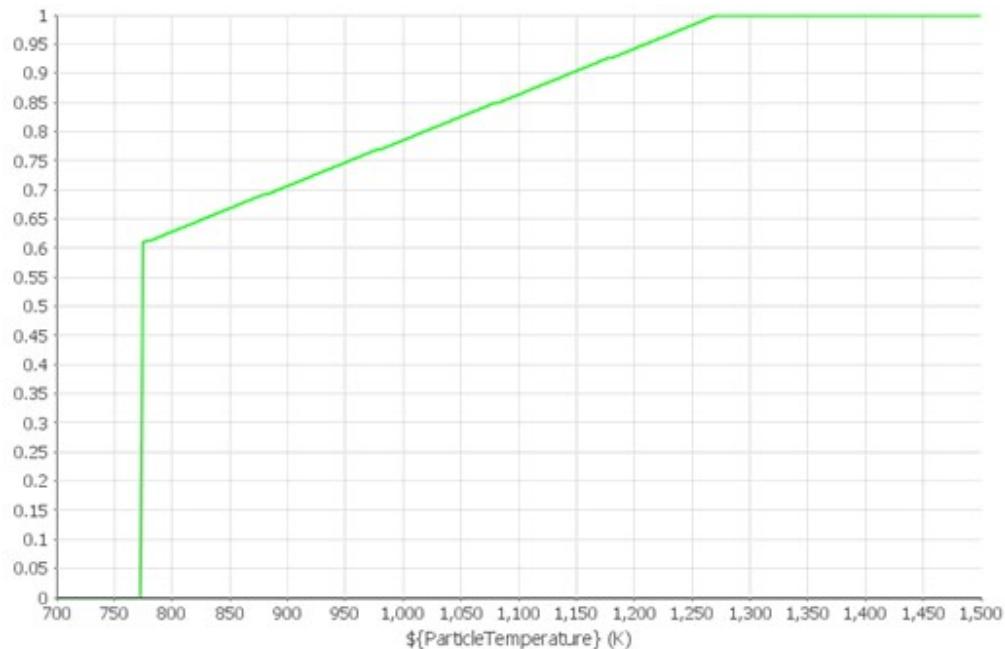
Property	Setting
<i>Depletion Criterion</i>	\$ParticleMassFractionAsh>0.999

8. To set the absorption and scattering efficiencies of the coal particles, edit the **Coal > Models > Multi-Component Coal > Material Properties** node and set the following properties:

Node	Property	Setting
Particle Absorption Efficiency > Constant	<i>Value</i>	1.1
Particle Scattering Efficiency > Constant	<i>Value</i>	1.2

9. Select the **Coal > Models > Track File** node and using  (Custom Editor), select the following Scalars:
- **Particle > Particle Diameter**
 - **Particle > Mass Fraction > Particle Mass Fraction of Ash**
 - **Particle > Mass Fraction > Particle Mass Fraction of Char**
 - **Particle > Mass Fraction > Particle Mass Fraction of H₂O**
 - **Particle > Mass Fraction > Particle Mass Fraction of RawCoal**
 - **Particle > Mole Fraction > Particle Mole Fraction of Ash**
 - **Particle > Mole Fraction > Particle Mole Fraction of Char**
 - **Particle > Mole Fraction > Particle Mole Fraction of H₂O**
 - **Particle > Mole Fraction > Particle Mole Fraction of RawCoal**
 - **Particle > Particle Temperature**

It is possible to estimate the kinetics of devolatilization by heating coal particles at a constant rate and monitoring the loss in mass. In this tutorial, the devolatilization rate is defined by a user-defined field function **UserDevolatilizationRate** that is a function of the particle temperature according to [\[1014\]](#):



10. Select the **Coal > Models > User-Defined Devolatilization** node and set the following properties:

Node	Property	Setting
User-Defined Devolatilization	<i>Volatile Yield</i>	0.6
	<i>Volatile Vapor Component</i>	CoalVolatile
L User Devolatilization Rate	<i>Method</i>	Field Function
	<i>Scalar Function</i>	UserDevolatilizationRate

- Save the simulation.

Setting the Initial Conditions

Before the combustion occurs, hot air is present in the coal combustor. High initial temperature assists with coal devolatilization and ignition so it is not necessary to define an ignitor.

To set the initial conditions:

- Select the **Continua > Coal Combustion > Initial Conditions > Species Mass Fraction** node and next to the *Value* property, click  (Custom Editor).
- In the *Species Mass Fraction - Value* dialog, set *N2* to 0.767 and *O2* to 0.233, then click **OK**.
- Select the **Initial Conditions > Static Temperature** node and set *Value* to 800 K.
- Save the simulation.

Setting the Boundary Conditions

The coal particles transport air enters the computational domain through a velocity inlet boundary at a constant velocity of 23 m/s. The combustion air flows in as a radial velocity profile with a swirl around the axis. You specify this velocity profile as a radial table with respect to a local cylindrical coordinate system.

At the individual walls of the combustor, you specify constant temperatures together with radiation properties.

To set the boundary conditions:

- Edit the **Regions > coalCombustor > Boundaries > COALANDTRANSPORTAIRINLET** node and set the following properties:

Node	Property	Setting
Physics Conditions		
L Turbulence Specification	<i>Method</i>	Intensity + Length Scale
Physics Values		
L Radiation Temperature	<i>Value</i>	343.15 K
L Species Mass Fraction	<i>Value</i>	<ul style="list-style-type: none"> ◦ N2: 0.767 ◦ O2: 0.233

Node	Property	Setting
└ Static Temperature	<i>Value</i>	343.15 K
└ Surface Material	<i>Surface Material</i>	Inlet Ducts
└ Turbulence Intensity	<i>Value</i>	0.1
└ Turbulent Length Scale	<i>Value</i>	6.5 mm
└ Velocity Magnitude	<i>Value</i>	23.0 m/s

2. Edit the **COMBUSTIONAIRINLET** node and set the following properties:

Node	Property	Setting
Physics Conditions		
└ Turbulence Specification	<i>Method</i>	Intensity + Length Scale
└ Velocity Specification	<i>Method</i>	Components
Physics Values		
└ Radiation Temperature	<i>Value</i>	573.15 K
└ Species Mass Fraction	<i>Value</i>	<ul style="list-style-type: none"> ◦ N2: 0.767 ◦ O2: 0.233
└ Surface Material	<i>Surface Material</i>	Inlet Ducts
└ Turbulence Intensity	<i>Value</i>	0.2
└ Turbulent Length Scale	<i>Value</i>	2.35 cm
└ Velocity	<i>Method</i>	Table (r)
	<i>Coordinate System</i>	Laboratory -> Cylindrical 1
└ Table (r)	<i>Table</i>	AirInletProfile
	<i>Table: X-Data</i>	V-radial
	<i>Table: Y-Data</i>	V-theta
	<i>Table: Z-Data</i>	V-z

3. Select the **OUTLET** node and set the following properties:

Node	Property	Setting
Physics Values		
└ Radiation Temperature	<i>Value</i>	300 K
└ Surface Material	<i>Surface Material</i>	Furnace

4. Set the thermal specifications at the coal combustor walls.

- Expand the **Regions > coalCombustor > Boundaries** node and multi-edit the following boundary nodes:
 - **BURNERQUARLWALL**
 - **CHIMNEYWALL**
 - **COALGUNFRONTWALL01**
 - **COALGUNFRONTWALL02**
 - **COOLINGLOOPS**
 - **FURNACEBACKWALL**
 - **FURNACECYLINDERWALL**
 - **FURNACEFRONTWALL**
 - **INLETDUCTWALL-INNER**
 - **INLETDUCTWALLS-OUTER**
- In the *Multiple Objects* dialog, select the **Physics Conditions > Thermal Specification** node and set *Condition* to **Temperature**, then click **Close**.
- Select the **BURNERQUARLWALL** node and set the following properties:

Node	Property	Setting
Physics Values		
└ Static Temperature	<i>Value</i>	1273.0 K
└ Surface Material	<i>Surface Material</i>	Inlet Ducts

- Select the **CHIMNEYWALL** node and set the following properties:

Node	Property	Setting
Physics Values		
└ Static Temperature	<i>Value</i>	1300.0 K
└ Surface Material	<i>Surface Material</i>	Furnace

- Multi-select the **COALGUNFRONTWALL01** and the **COALGUNFRONTWALL02** nodes, and set the following properties:

Node	Property	Setting
Physics Values		
└ Static Temperature	<i>Value</i>	800.0 K
└ Surface Material	<i>Surface Material</i>	Inlet Ducts

- Select the **COOLINGLOOPS** node and set the following properties:

Node	Property	Setting
Physics Values		
└ Static Temperature	<i>Value</i>	1000.0 K
└ Surface Material	<i>Surface Material</i>	Cooling Loops

- g) Select the **FURNACEBACKWALL** node and set the following properties:

Node	Property	Setting
Physics Values		
└ Static Temperature	<i>Value</i>	1300.0 K
└ Surface Material	<i>Surface Material</i>	Furnace

- h) Select the **FURNACECYLINDERWALL** and the **FURNACEFRONTWALL** nodes and set the following properties:

Node	Property	Setting
Physics Values		
└ Static Temperature	<i>Value</i>	1400.0 K
└ Surface Material	<i>Surface Material</i>	Furnace

- i) Select the **INLETDUCTWALL-INNER** node and set the following properties:

Node	Property	Setting
Physics Values		
└ Surface Material	<i>Surface Material</i>	Inlet Ducts

- j) Select the **INLETDUCTWALLS-OUTER** node and set the following properties:

Node	Property	Setting
Physics Values		
└ Static Temperature	<i>Value</i>	573.0 K
└ Surface Material	<i>Surface Material</i>	Inlet Ducts

5. Save the simulation.

Defining the Coal Particle Injector

The injector introduces coal particles into the reactive domain in a given direction, at a specified rate. The diameter of the coal particles is defined using the Rosin-Rammler method.

You specify the species mass fraction at the injector based on the proximate analysis. The proximate analysis gives the mass fractions of volatile matter, fixed carbon, ash, and moisture content (see [Setting Material Properties](#)). The mass fraction of raw coal is equal to the sum of volatile matter and fixed carbon. You are advised to set the value of char to 0.

To define the coal particle injector:

1. Right-click the **Injectors** node and select **New**.
2. Rename the **Injector 1** node to **Fuel** and set the following properties:

Node	Property	Setting
Fuel	<i>Lagrangian Phase</i>	Coal
	<i>Type</i>	Part Injector
	<i>Inputs</i>	Regions > coalCombustor > COALANDTRANSPORTAIRINLET

3. Select the **Fuel > Conditions > Velocity Specification** node and set *Method* to **Magnitude + Direction**.
4. Expand the **Fuel > Values** node and set the following properties:

Node	Property	Setting
Parcel Streams	<i>Value</i>	5.0
Point Inclusion Probability	<i>Value</i>	1
Injection Direction	<i>Value</i>	[1.0, 0.0]
Mass Flow Rate	<i>Value</i>	0.01162 kg/s As the tutorial simulation is 2D axisymmetric, you obtain this mass flow rate value that you specify by dividing the mass flow rate of the 360° combustor geometry by 2π .
Particle Diameter	<i>Method</i>	Rosin-Rammler
	<i>Minimum</i>	1.0E-5 m
	<i>Maximum</i>	5.0E-4 m
	<i>Reference</i>	2.0E-4 m
	<i>Exponent</i>	1.36
Particle Temperature	<i>Value</i>	800 K

Node	Property	Setting
Species Mass Fraction	Value	Click  (Custom Editor) and set: o RawCoal: 0.917 o Ash: 0.083
Velocity Magnitude	Value	23.0 m/s

- Save the simulation.

Specifying Solver Parameters

To let the flow solution stabilize initially, the flow and energy solvers run without the Lagrangian solver for 500 iterations in the beginning of the simulation. The DO Radiation and the Lagrangian solver update only every 20th iteration, which speeds up the runtime of this tutorial.

To set up the solvers:

- Edit the **Solvers** node and set the following properties:

Node	Property	Setting
Lagrangian Multiphase	<i>Maximum Courant Number</i>	0.5
	<i>Minimum Courant Number</i>	0.2
 Steady	<i>Maximum Residence Time</i>	40.0 s
 Iteration Update Frequency	<i>First Iteration</i>	500
	<i>Update Frequency</i>	20
 Two-Way Coupling	<i>Under-Relaxation Factor</i>	0.8
Segregated Flow		
 Velocity	<i>Under-Relaxation Factor</i>	0.5
DO Radiation		
 Update Frequency		
 Steady	<i>Iteration Update Frequency</i>	20

- Save the simulation.

Monitoring and Plotting Carbon

You compare the mass of carbon entering the computational domain with the mass of carbon leaving it. When the two mass flow rates reach the same value, you can assume that the solution has converged.

The mass flow rate of carbon at the inlet boundaries is calculated as a product of mass flow rate of coal at the injector, the mass fraction of carbon in the ultimate analysis, and the mass fraction of raw coal at the injector.

$$\dot{m}_{\text{in}, C} = 0.01162 \frac{\text{kg}}{\text{s}} * 0.8036 * 0.917 = 0.0085628 \frac{\text{kg}}{\text{s}}$$

By considering all species in the reaction mechanism that contain carbon, the mass outflow rate of carbon can be defined as:

$$\dot{m}_{\text{out}, C} = \dot{m}_{\text{tot}} \left(\frac{A_r(C)}{M_W(CO_2)} Y_{CO_2} + \frac{A_r(C)}{M_W(CO)} Y_{CO} + \frac{2.803 A_r(C)}{M_W(\text{CoalVolatile})} Y_{\text{CoalVolatile}} \right)$$

where \dot{m}_{tot} is the total mass flow rate, $M_W(i)$ is the molecular weight, $A_r(i)$ is the atomic weight, and Y_i is the mass fraction of species i .

The mass flow rate of carbon can then be written as:

$$\dot{m}_{\text{out}}(C) = \dot{m}_{\text{tot}}(0.27Y_{CO_2} + 0.43Y_{CO} + 0.673Y_{\text{CoalVolatile}}) \quad (5360)$$

From the ingoing and outgoing carbon mass flow rates, you create a monitor for a normalized carbon balance $(\dot{m}_{\text{in}} - \dot{m}_{\text{out}})/\dot{m}_{\text{in}}$ that you use later on to define a monitor-based stopping criterion.

To monitor and plot carbon:

1. Create a report for the mass flow rate of incoming carbon.
 - a) Right-click the **Reports** node and select **New > User > Expression**.
 - b) Rename the **Expression 1** node as **Carbon In**.
 - c) Select the **Carbon In** node and set the following properties:

Property	Setting
<i>Definition</i>	0.0085628
<i>Dimensions</i>	Click  (Custom Editor). In the <i>Carbon In - Dimensions</i> window, set Mass to 1, set Time to -1.

2. Create a report for the mass flow rate of carbon leaving the computational domain.
 - a) Right-click the **Reports** node and select **New > User > Sum**.
 - b) Rename the **Sum 1** node as **Carbon Out**.
 - c) Select the **Carbon Out** node and set the following properties:

Property	Setting
<i>Field Function</i>	Carbon This user-defined field function has been pre-defined on the starting simulation file of the tutorial. Its definition corresponds to Eqn. (5360) .
<i>Parts</i>	Regions > coalCombustor > Boundaries > OUTLET

3. Create a plot to display the ingoing and outgoing mass flow rate of carbon:
 - a) Multi-select the **Carbon In** and the **Carbon Out** report nodes, right-click one of the selected nodes and select **Create Monitor and Plot from Report**.
 - b) In the *Create Plot From Reports* dialog, click **Single Plot**.
 - c) Rename the **Plots > Reports Plot** node Carbon Balance.
4. Create a report and monitor to calculate the normalized carbon balance.
 - a) Right-click the **Reports node** and select **New > User > Expression**.
 - b) Rename the **Expression 1** node as Normalized Carbon Balance.
 - c) Select the **Normalized Carbon Balance** node and *Definition* to $(\{\text{Carbon In}\} - \{\text{Carbon Out}\}) / \{\text{Carbon In}\}$.
 - d) Right-click the **Normalized Carbon Balance** node and select **Create Monitor from Report**.
5. Create one more report to analyze the char burnout of the coal particles.
 - a) Right-click the **Reports node** and select **New > Combustion > Char Burn Out**.
 - b) Rename the **Char Burn Out 1** node as Char Burnout.
 - c) Select the **Char Burnout** node and set *Parts* to **Coal**.
6. Within the **Monitors** node, multi-select the following nodes and set *Normalization Option* to **Off**.
 - CO
 - CO2
 - CoalVolatile
 - Continuity
 - Energy
 - H2
 - H2O
 - N2
 - O2
 - Tdr
 - Tke
 - SO2
 - X-momentum
 - Y-momentum
 - Z-momentum
7. Save the simulation.

Visualizing Coal Combustion Products, Temperature, and Velocity

You visualize the distribution of the mass fraction of CO, CO₂, and SO₂ as well as the temperature in the form of contour plots. The velocity field is displayed as a line integral convolution plot.

To visualize the results:

1. Create a transform that reflects the coal combustor geometry along the symmetry axis.
 - a) Right-click the **Tools > Transforms** node and select **New Graphics Transform > Graphics Symmetry Transform**.
 - b) Select the **Graphics Symmetry Transform 1** node and set *Plane* to [0.0, 1.0, 0.0, 0.0].

2. Create a scalar scene that is reflected along the symmetry axis.
 - a) Right-click the **Scenes** node and select **New > Scalar**.
 - b) Change to the **Scene/Plot** tab, select the **Outline 1** node and set *Transform* to **Graphics Symmetry Transform 1**.
 - c) Select the **Outline 1 > Parts** node and set *Parts* to all region boundaries except **AXIS**.
 - d) Select the **Scalar 1** node and set *Transform* to **Graphics Symmetry Transform 1**.
 - e) Change to the **Simulation** tab, right-click the **Scenes > Scalar Scene 1** node, then copy and paste it onto the **Scenes** node. Repeat this step four times to obtain a total of five scalar scenes.

3. Visualize the mass fraction of CO:
 - a) Select the **Scenes > Scalar Scene 1** node and rename it as **CO**.
 - b) Select the **CO > Scalar 1** node and set the following properties:

Node	Property	Setting
Scalar 1	<i>Contour Style</i>	Smooth Filled
L Scalar Field	<i>Function</i>	Mass Fraction of CO

4. Visualize the mass fraction of CO2:
 - a) Select the first copy and rename it as **CO2**.
 - b) Select the **CO2 > Scalar 1** node and set the following properties:

Node	Property	Setting
Scalar 1	<i>Contour Style</i>	Smooth Filled
L Scalar Field	<i>Function</i>	Mass Fraction of CO2

5. Visualize the mass fraction of SO2:
 - a) Select the second copy and rename it as **SO2**.
 - b) Select the **SO2 > Scalar 1** node and set the following properties:

Node	Property	Setting
Scalar 1	<i>Contour Style</i>	Smooth Filled
L Scalar Field	<i>Function</i>	Mass Fraction of SO2

6. Visualize the temperature:
 - a) Select the third copy and rename it as **Temperature**.
 - b) Select the **Temperature > Scalar 1** node and set the following properties:

Node	Property	Setting
Scalar 1	<i>Contour Style</i>	Smooth Filled
L Scalar Field	<i>Function</i>	Temperature

7. Visualize the tracks of the coal particles:

- Select the fourth copy and rename it as **Particles: Mass Fraction of Char**.
- Delete the **Particles: Mass Fraction of Char > Scalar 1** node.
- Right-click the **Particles: Mass Fraction of Char** node and select **New Displayer > Streamline**.
- Edit the **Streamlines 1** node and set the following properties:

Node	Property	Setting
Streamlines 1	<i>Mode</i>	Tubes
	<i>Transform</i>	Graphics Symmetry Transform 1
L Color Bar	<i>Color Map</i>	white-red

8. Visualize the velocity field:

- Create a vector scene and rename it as **Velocity**.
- Select the **Outline 1** node and set *Transform* to **Graphics Symmetry Transform 1**.
- Select the **Outline 1 > Parts** node and set *Parts* to all region boundaries except **AXIS**.
- Select the **Vector 1** node and set the following properties:

Node	Property	Setting
Vector 1	<i>Display Mode</i>	Line Integral Convolution
	<i>Transform</i>	Graphics Symmetry Transform 1
L Vector Field	<i>Function</i>	Velocity > Lab Reference Frame (default)

9. Save the simulation.

Running the Simulation

You set the stopping criteria before running the simulation.

To run the simulation:

- Select the **Stopping Criteria > Maximum Steps** node and set *Maximum Steps* to 7000.
- Click  (**Run**).
- When the simulation is complete, click **Save**.

Visualizing the Results

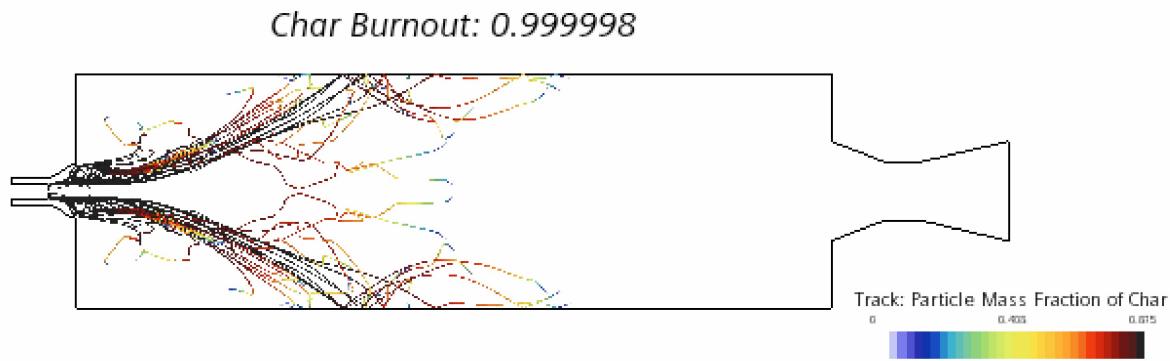
You load the track file that contains the coal particles tracks after the simulation has finished.

To visualize the results:

1. Load the particle track file.
 - a) Right-click the **Tools > Track Files** node and select **Track File**.
 - b) In the **Open** dialog, select the `EBU_Coal.trk` file and click **Open**.
2. Finalize the particle tracks scene.
 - a) Expand the **Scenes > Particles: Mass Fraction of Char > Streamlines 1** node and set the following properties:

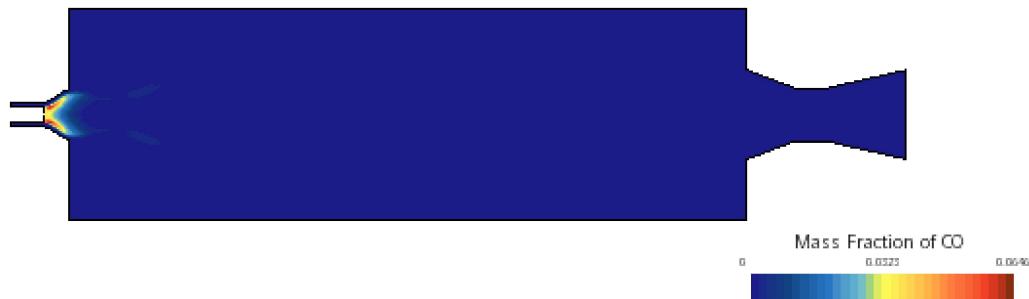
Node	Method	Setting
Parts	<i>Parts</i>	Coal tracks
Scalar Field	<i>Function</i>	Track > Track: Particle Mass Fraction of Char

- b) Right-click the **Reports > Char Burnout** node and select **Create Text Annotation from Report**.
 - c) Select the **Tools > Annotations > Char Burnout** node, then drag and drop it onto the graphics window with the particle tracks scene.

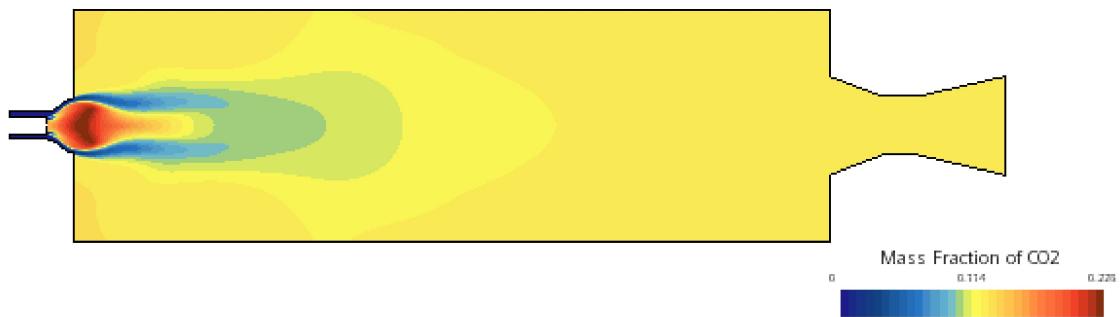


3. Open the following scenes: *CO, CO₂, SO₂, Temperature and Velocity*.

Mass Fraction of CO



Mass Fraction of CO₂

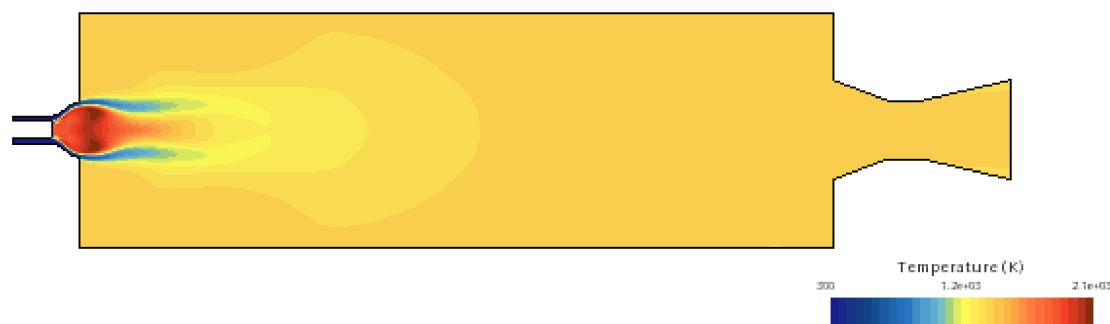


Mass Fraction of SO₂

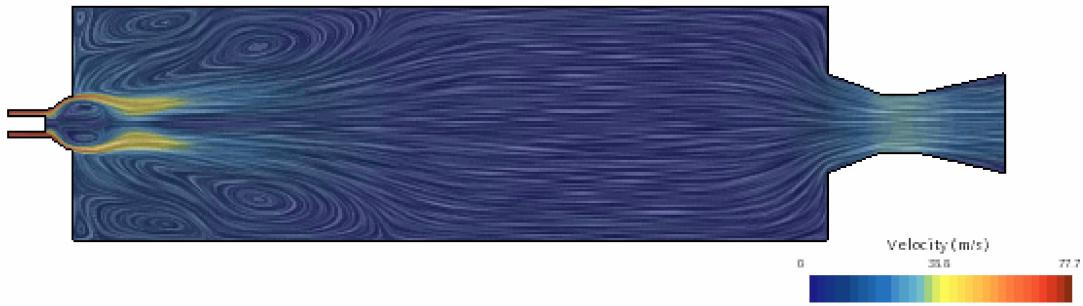


Sulfur dioxide gas is generated by the combustion of sulfur impurities in the coal.

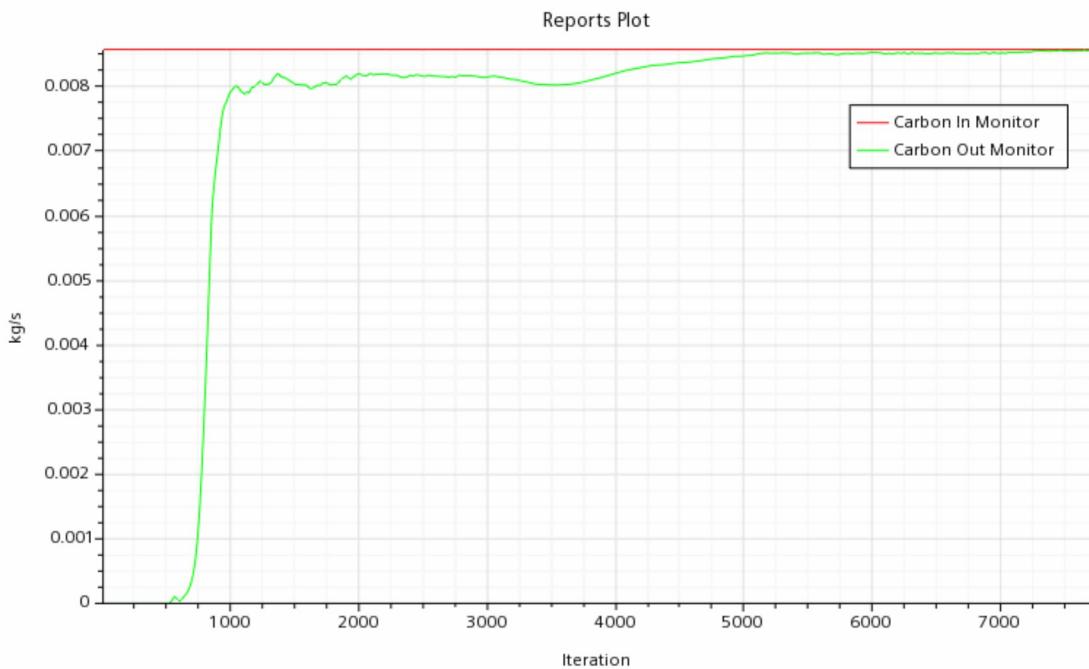
Temperature



Velocity



4. Open the **Carbon Balance** plot:



Bibliography

[1014] Ranade,V.V. and Gupta, D.F. 2015. "Computational Modeling of Pulverized Coal Fired Boilers". CRC Press.