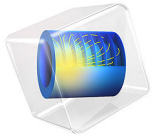

Chemical Reactions and Soot Build-Up in a Diesel Filter

Introduction

This example deals with a model of a filter system for a diesel engine. A porous filter separates soot particles from exhaust gases passing through it, leading to the formation of a soot layer. Both catalytic and non-catalytic reactions suppress the layer's build-up; carbon is oxidized to carbon monoxide and carbon dioxide, which both pass through the membrane.

Diesel filters are used to remove particulate matter in diesel-engine exhaust gases. A filter system's efficiency and durability are closely related to the manner in which it removes soot deposits from the porous filter walls. For instance, one method is to remove the soot layer by means of non-catalytic reactions with oxygen. However, this scheme requires that the exhaust temperature is increased above normal operating conditions. Another approach involves introducing cerium additives to the fuel. Cerium oxide species are subsequently present in the soot layer, acting as a catalyst in carbon-oxidation reactions. Under these conditions, it is possible to remove carbon deposits in the filter without increasing the exhaust temperature. The following model illustrates both of these working conditions.

Diesel filters are typically of a monolithic type with narrow channels running through a cylindrical structure. The silicon carbide filter under study is 15 cm long with a total of 2000 channels. Filter channels are open only at one end and are arranged in an alternating

fashion in the monolith. The channels are separated by porous walls, as illustrated in Figure 1.

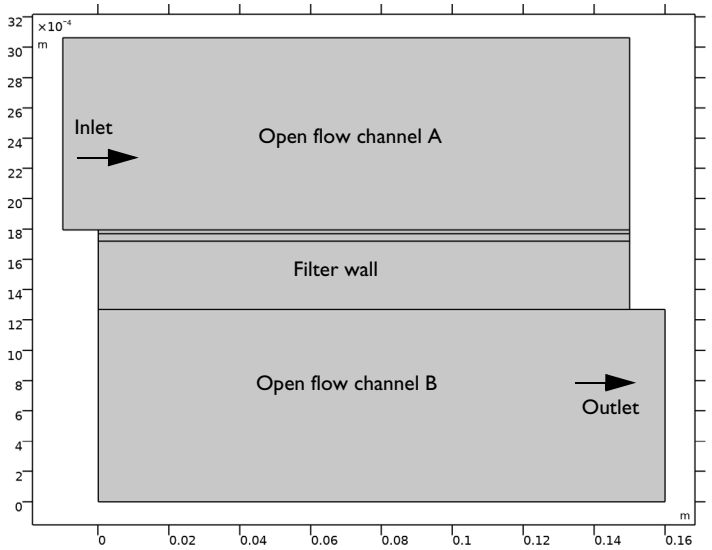

Figure 1: Front view of a channel section in a diesel filter. The A-channels are open while the B-channels are closed (from the left). The channels are separated by porous filter walls. A back view would show the opposite configuration. Gas enters the filter through the A-channels and exits through the B-channels.

This application follows a two-part strategy to investigate the system in which these reactions take place. The first part is setting up an ideal model in the Reaction Engineering interface with the plug-flow reactor feature that assumes stationary conditions and accounts only for variations with reactor volume. This gives a rather qualitative understanding of the reactor system. The second part sets up a space- and time-dependent model in which variations in species composition, soot layer build up, and temperature are investigated in detail.

Model Definition

CHEMICAL REACTIONS

The soot layer in the diesel filter must be removed continuously or at intervals to keep the filter in working condition. Oxygen can react with carbon to form carbon monoxide and carbon dioxide. Further reaction pathways open when the diesel fuel is treated with

additives containing cerium. The soot layer then contains cerium-oxide species that act as catalysts to oxidize the carbon, and oxygen regenerates the catalyst.

This model considers the following five reactions

$$\mathrm{C(s) + O_2 \rightarrow CO_2} \tag{1}$$

$$\mathrm{C(s) + 0.5O_2 \rightarrow CO} \tag{2}$$

$$\mathrm{C(s) + 4CeO_2(s) \rightarrow 2Ce_2O_3(s) + CO_2} \tag{3}$$

$$\mathrm{C(s) + 2CeO_2(s) \rightarrow Ce_2O_3(s) + CO} \tag{4}$$

$$\mathrm{2Ce_2O_3(s) + O_2 \rightarrow 2Ce_2O_3} \tag{5}$$

where (s) indicate a solid phase species.

The reactions are assumed to only occur in the soot layer. The reaction rates (mol/(m^3·s)) are given by:

$$r_1 = k_1 c_{\mathrm{O2}}$$

$$r_2 = k_2 c_{\mathrm{O2}}$$

$$r_3 = k_3 x_{\mathrm{CeO2}}$$

$$r_4 = k_4 x_{\mathrm{CeO2}}$$

$$r_5 = k_5 x_{\mathrm{Ce2O3}} c_{\mathrm{O2}}$$

where c_{O2} is the molar concentration of oxygen (SI unit: mol/m^3), while x_{CeO2} and x_{Ce2O3} are the molar fractions of the different cerium (catalytic) species.

PLUG FLOW MODEL

The Reaction Engineering interface can automatically define the material and energy balances for a plug-flow reactor at steady-state, as shown by the governing equation:

$$\frac{dF_i}{dV} = R_i \tag{6}$$

F_i is the molar flow and R_i includes all the reactions, per unit volume of the channel, in which species i is involved. Equation 6 thus gives a solution of an ideal model system only dependent on the accumulated volume, V, the species pass in the reactor. The plug flow

model is solved for isothermal conditions assuming the reactions have negligible impact on temperature in the system since it contains an excess of nitrogen solvent.

The modeled system is schematically illustrated in Figure 2 and consists of one single cell and one single filter-unit. The exhaust gas enters Channel A and passes through a single filter wall to Channel B (note that a repetitive cell would have a filter wall on all sides). The plug flow model system treats just Channel A, the deposited particles, and the catalyst, and neglects any reaction in Channel B. Along the system boundaries, the filter is a distributed outlet. Because the pressure loss over the filter wall is comparably large, the velocity across the wall along the length of the channel is considered to be constant. This implies that the velocity component along the channel decreases linearly from the inlet to the outlet.

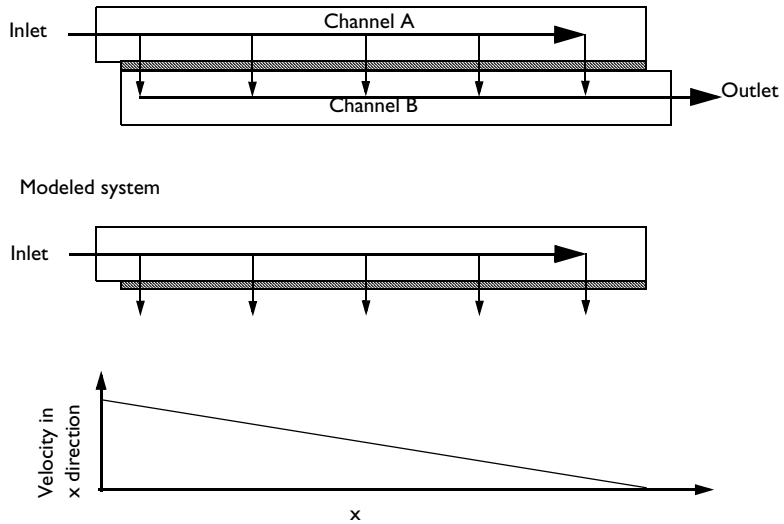

Figure 2: Schematic illustration the plug flow system. The exhaust enters Channel A, goes through the filter wall, and exits through Channel B. Assume the velocity across the filter wall is constant along the x direction in the plug flow model, while the velocity component along the length of the channel decreases linearly with the distance from the inlet.

The general material balance for a small section of Channel A of length Δx gives the following equation for any species i:

$$(N_{i,x+\Delta x} - N_{i,x})A_{cs} + c_i u_f \frac{\Delta V}{L} - R_i A_{cs} \Delta x = 0 \qquad (7)$$

N_i denotes the flux vector (mol/(m^{2}s)), A_{cs} equals the channel's cross-sectional area (m^2), L the reactor length (m), and u_f represents the velocity flow of species toward the filter

(m/s). At ideal conditions, Equation 7 can likewise be set up over the volume element (ΔV) through which the gas passes in Δx:

$$(F_{i,\,V+\Delta V} - F_{i,\,V}) + c_i v_f \frac{\Delta x}{H} - R_i \Delta V = 0 \tag{8}$$

In Equation 8, v_f represents a volumetric flow of species toward the filter (SI unit: m^3/s), H the reactor height (SI unit: m). The reaction is limited to the soot layer on the filter surface. Because the kinetic data is given per unit volume of soot, the volume of soot per unit is estimated to be the same as the volume of the channel. Dividing Equation 8 by ΔV and if ΔV approaches zero gives:

$$\frac{dF_i}{dV} + c_i u_f \frac{1}{H} = R_i \tag{9}$$

From the assumption of a linearly decreasing flow along the channel, the volumetric flow in the reactor is given by:

$$v = k_u V + v_0$$

where k_u (1/s) denotes the proportionality constant and v_0 (m^3/s) equals the inlet flow. V is the accumulated volume the species have passed in the tubular reactor. Note that the cross-sectional area is actually irrelevant; that is, the reactor volume, V, can just as well be interpreted as length and compositions, c_i, as mol per reactor length. The second term on the left-hand side in Equation 9 is added to all species in the model using the Additional Source feature. The compositions of species along the plug-flow reactor are expressed in terms of concentrations with inlet molar flows set as a simplification for all species. Another generalization is that all species are affected by the flow over the filter, even the solid components.

SPACE-DEPENDENT MODEL

This example removes a channel section from the monolith and places it into an experimental setup to study only a single filter unit with a single filter wall. Assuming that only a single filter wall exists and by thermally and mechanically insulating the upper and vertical channel walls, the system can be described with the 2D geometry shown in Figure 3.

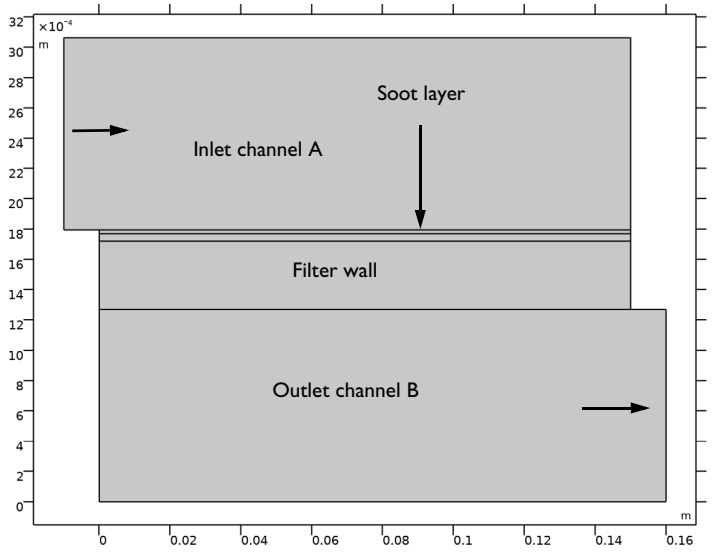

Figure 3: Modeled domain including four sections: the inlet Channel A, soot layer, filter wall, and outlet Channel B. Note that the units on the horizontal and vertical axes are different.

The model includes four model sections: the inlet Channel A, the soot layer on the surface of the filter wall, the filter wall, and the outlet Channel B.

The filter is 15 cm long, and the height of a single channel is 1.27 mm. The filter wall is 0.45 mm thick. Diesel exhaust gas enters the inlet channel, and the gas containing soot particles filters off through the porous SiC filter wall, thereby leaving a soot layer on top of this wall. The exhaust exits the filter through the outlet channel. You must treat the top surface of the soot layer as a moving sub-boundary that grows and shrinks according to the amount of soot.

To solve this model, use the following physics interfaces in the space-dependent model:

- Free and Porous Media Flow
- Transport of Diluted Species (material balance)
- Heat Transfer in Fluids (energy balance)

The position of the top boundary is solved for using the Moving Mesh feature.

In the Free and Porous Media Flow interface, free flow is defined in both the inlet (A) and outlet (B) channels, whereas the Porous Matrix Properties are defined in the soot layer and

the filter wall. The reaction kinetics are defined from the plug flow using the Generate Space-Dependent Model feature. This creates a a Chemistry interface to be used in the space-dependent model.

There are two issues worth mentioning regarding the domain equations and boundary conditions used in the model implementation:

- The Moving Mesh feature needs an expression for the mesh velocity at the top of the soot layer. The expression is given by the following relation which is assumed to hold along the top surface of the soot layer:

$$v_{\mathrm{n}}\rho_{\mathrm{soot}} = -\rho_{\mathrm{part}}(\mathbf{u}\cdot\mathbf{n}) - M_c\delta_{\mathrm{sl}}R_C$$

  Here, v_n is normal velocity of the mesh, ρ_{soot} is the density of the soot layer and ρ_{part} is density of the gas phase particles. The first term on the right hand side corresponds to the transport of soot particles towards the soot layer. The second term represents the removal of soot due to reactions inside the layer. Here M_c equals the molar weight of carbon, R_c is the sum of all carbon-consuming reaction rates, and δ_{sl} is the soot layer thickness. In the model the reaction rates are assumed to be constant throughout the soot layer. This assumption can also be validated from the results.

- Note that the properties of the porous filter wall and soot layer are a combination of those of solids and fluids. For example, in the energy balance, the conduction term should include the conductivities of the solid and the fluid, while the convection term should contain only the properties of the fluid because the solid does not move. The accumulation (time-dependent) term should include a mixture of both properties in the following way:

$$\rho_{\mathrm{mix}} = \rho_{\mathrm{solid}}(1-\varepsilon_{\mathrm{solid}}) + \rho_{\mathrm{gas}}\varepsilon_{\mathrm{solid}}$$

$$C_{p\mathrm{mix}} = C_{p\mathrm{solid}}(1-\varepsilon_{\mathrm{solid}}) + C_{p\mathrm{gas}}\varepsilon_{\mathrm{solid}}$$

$$k_{\mathrm{mix}} = k_{\mathrm{solid}}(1-\varepsilon_{\mathrm{solid}}) + k_{\mathrm{gas}}\varepsilon_{\mathrm{solid}}$$

  where ρ_{mix} is the mixture's density (SI unit: kg/m^3), $C_{p,\mathrm{mix}}$ is its heat capacity (J/(kg·K)), k_{mix} equals its thermal conductivity (W/(m·K)), and $\varepsilon_{\mathrm{solid}}$ the void fraction (porosity).

CHEMICAL REACTIONS AND PLUG FLOW MODEL

Start by looking at the plug flow model for Channel A. Figure 4 and Figure 5 depict the composition of the reacting species along the channel length at two different temperatures, one at 653 K, below "catalyzer ignition" temperature, and one at 705 K where the catalyst is ignited.

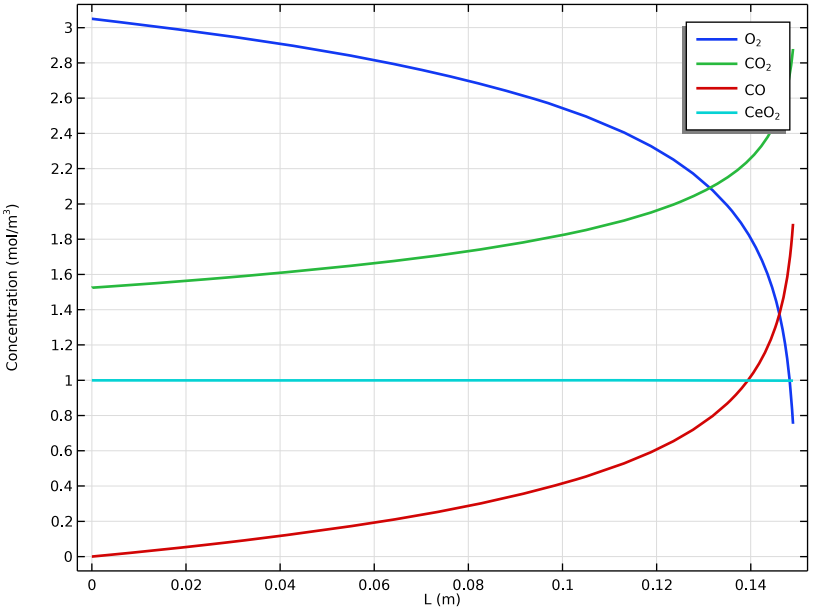

Figure 4: Composition of reacting species along the length of the reactor at 653 K.

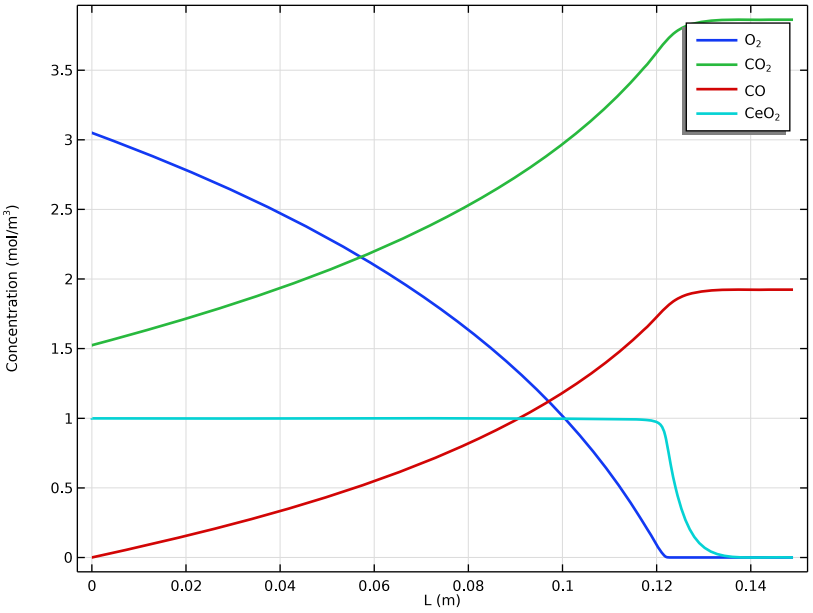

Figure 5: Composition along the length of the reactor at 703 K.

At 703 K oxygen becomes depleted at approximately 0.12 m into the reactor. As the temperature increases, the rate of oxidation increases until the depletion of oxygen in the reactor. This decreases the rate of CeO_2 regeneration substantially and Ce_2O_3 becomes the dominating cerium-containing species.

The impact of temperature can also be investigated with the ratio of the non-catalyzed to the catalyzed reaction rates for the carbon monoxide and carbon dioxide producing reactions. In the following figures the reaction rate ratios r_1/r_3, carbon dioxide

production, and r_2/r_4, carbon monoxide production, rates are depicted for the two different temperatures.

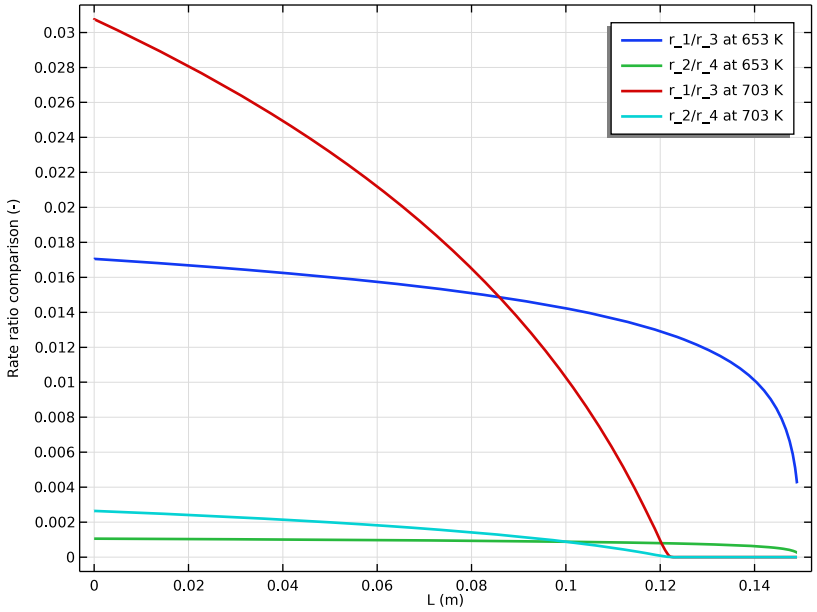

Figure 6: Relationship between the non-catalytic and catalytic carbon-oxidation reactions.

Figure 6 shows that the catalytic reactions by far dominate the oxidation of carbon. This is expected at these relatively moderate temperatures. The oxidation of carbon to carbon dioxide has a higher fraction of non-catalyzed oxidation than that of carbon to carbon monoxide. The dominance of the catalytic reactions decreases with temperature.

SPACE-DEPENDENT MODEL

Figure 7 shows the velocity distribution in the channel unit cell at the last time step. The flow is shown to exhibit a laminar behavior.

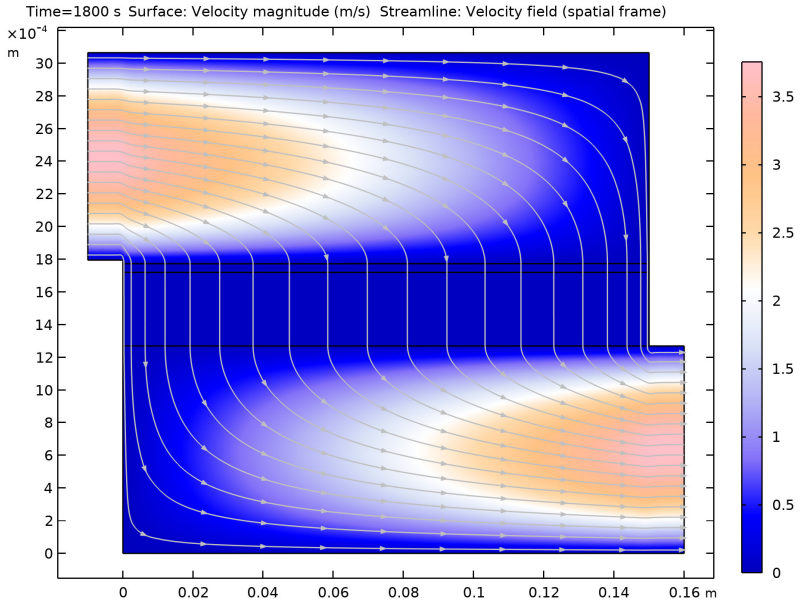

Figure 7: Velocity magnitude in a filter unit cell.

Figure 8 shows the pressure distribution across the channel pair. The main pressure drop is observed across the soot layer deposited on top of the porous membrane.

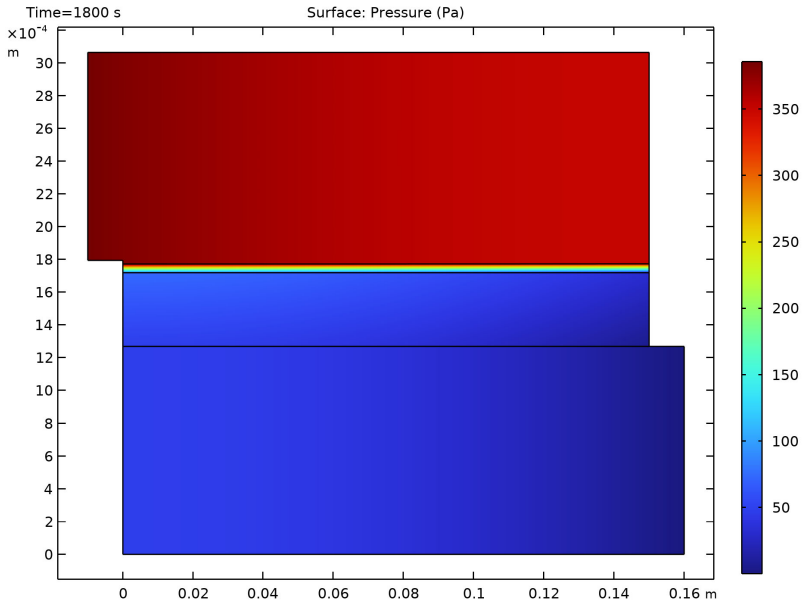

Figure 8: Pressure distribution in a filter unit cell.

The oxidation of carbon is overall an exothermic reaction, although the catalytic steps are endothermic. The regeneration of the catalyst is heavily exothermic and makes up for the endothermic properties of the catalytic oxidation reaction. Figure 9 shows the temperature distribution in the system after 1800 s for an inlet temperature of 550 K. The exhaust gases leave the filter at somewhat slightly reduced temperatures due to the net endothermicity of the reactions.

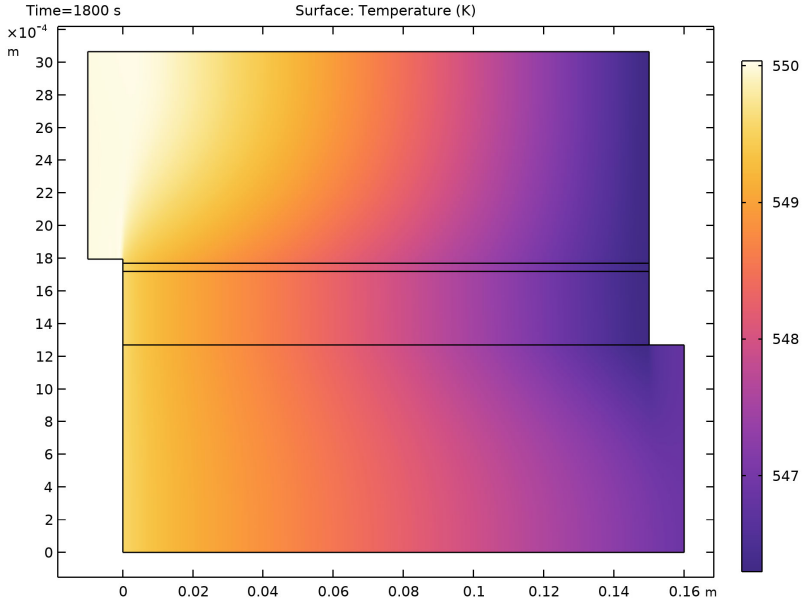

Figure 9: Temperature distribution in the filter for an inlet temperature of 550 K.

The following illustration (Figure 10) shows the soot layer along the length of the reactor at an inlet temperature of 550 K. The base-line corresponds to the initial soot layer thickness of 50 µm. Under the present conditions, carbon oxidation is not sufficient to

keep the soot layer from growing. It is also seen that the soot layer build-up is slightly faster at the far end of the filter.

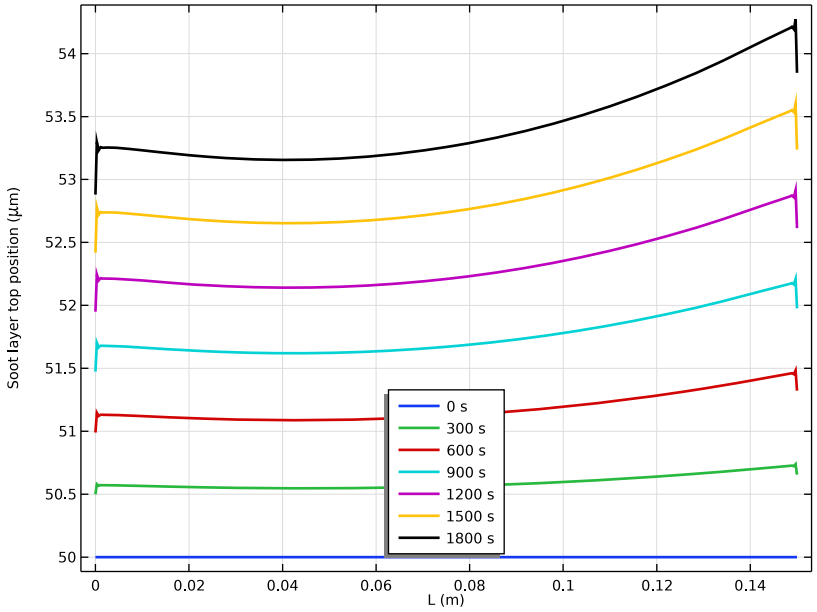

Figure 10: The soot layer's thickness at 0 to 1800 s in 300 s intervals for an inlet temperature of 550 K.

A fixed outlet pressure is used in the simulation. Figure 10 shows the development of the average inlet pressure. As was seen in Figure 8, the main pressure drop occurs in the compact soot layer. Consequently, the required inlet pressure also increases over time.

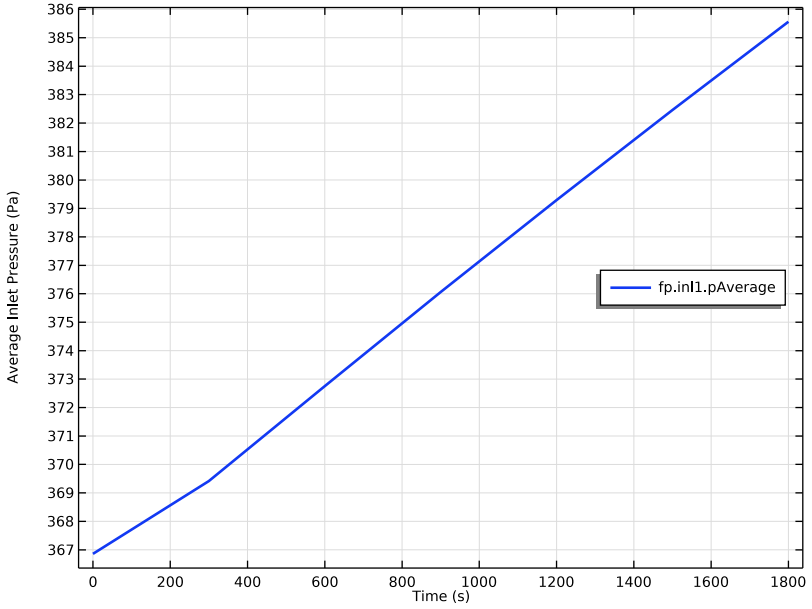

Figure 11: Average inlet pressure as a function of time for an inlet temperature of 550 K.

Reference

1. G. Konstantas and A.M. Stamatelos, "Computer Aided Engineering of Diesel Filter Systems," *Joint Meeting of the Greek and Italian Sections of the Combustion Institute*, http://www.mie.uth.gr/labs/ltte/pubs/Combust_Inst_Corfou_013.pdf.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/diesel_filter`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **0D**.

2 In the **Select Physics** tree, select **Chemical Species Transport>Reaction Engineering (re)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Stationary Plug Flow**.

6 Click **Done**.

GLOBAL DEFINITIONS

Load model parameters from a text file.

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `diesel_filter_parameters.txt`.

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

Add the variable for the volumetric flow in the tubular reactor.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
v1	v_inlet+ku*re.Vr	m^3/s	Volumetric flow field in tubular reactor

REACTION ENGINEERING (RE)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering (re)**.

2 In the **Settings** window for **Reaction Engineering**, locate the **Reactor** section.

3 From the **Reactor type** list, choose **Plug flow**.

4 Locate the **Energy Balance** section. In the T text field, type `T0`.

In order to be able to prescribe the volumetric flow rate, select to compute pressure from the ideal gas law.

5 Locate the **Mixture Properties** section. From the **Reactor pressure** list, choose **Ideal gas law**.

6 Click to expand the **Calculate Transport Properties** section. Select the **Calculate mixture properties** check box.

7 Locate the **Reactor** section. Find the **Mass balance** subsection. In the v text field, type `v1`.

Reaction 1

1 In the **Reaction Engineering** toolbar, click  **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `C(s)+O2=>CO2`.

4 Click **Apply**.

Modify the reaction rates in order to take the difference in domain thickness between the catalyzing layer (0.05 mm thick) and the channel (1.27 mm) into account. This is achieved by multiplying all reaction rates with the constant `Sa`. Alternatively, edit the Arrhenius parameter for the Frequency factor by multiplying the value with the constant `Sa`.

5 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

6 In the A^{f} text field, type `1e13[m/s]*Sa`.

7 In the E^{f} text field, type `165e3[J/mol]`.

8 Locate the **Reaction Rate** section. From the list, choose **User defined**.

9 In the r_j text field, type `re.kf_1*re.c_O2`.

10 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `1`.

In this model, user-defined reaction rate expressions are used.

Reaction 2

1 In the **Reaction Engineering** toolbar, click  **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `C(s)+0.5O2=>CO`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

6 In the A^{f} text field, type `5.5e10[m/s]*Sa`.

7 In the E^f text field, type `150e3[J/mol]`.

8 Locate the **Reaction Rate** section. In the r_j text field, type `re.kf_2*re.c_O2`.

9 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `1`.

Reaction 3

1 In the **Reaction Engineering** toolbar, click  **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `C(s)+4CeO2(s)=>2Ce2O3(s)+CO2`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

6 In the A^f text field, type `4.5e11[m/s]*Sa`.

7 In the E^f text field, type `120e3[J/mol]`.

8 Locate the **Reaction Rate** section. From the list, choose **User defined**.

9 In the r_j text field, type `re.kf_3*re.c_CeO2_solid`.

10 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `1`.

Reaction 4

1 In the **Reaction Engineering** toolbar, click  **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `C(s)+2CeO2(s)=>Ce2O3(s)+CO`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

6 In the A^f text field, type `4e8[m/s]*Sa`.

7 In the E^f text field, type `80e3[J/mol]`.

8 Locate the **Reaction Rate** section. From the list, choose **User defined**.

9 In the r_j text field, type `re.kf_4*re.c_CeO2_solid`.

10 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `1`.

Reaction 5

1 In the **Reaction Engineering** toolbar, click  **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `Ce2O3(s)+0.5O2=>2CeO2(s)`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

6 In the A^f text field, type `1e12[m^4/(mol*s)]*Sa`.

7 In the E^f text field, type `80e3[J/mol]`.

8 Locate the **Reaction Rate** section. In the r_j text field, type `re.kf_5*re.c_O2*re.c_Ce2O3_solid`.

9 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `2`.

Species: C(s)

The carbon composition is locked in the model.

1 In the **Model Builder** window, click **Species: C(s)**.

2 In the **Settings** window for **Species**, click to expand the **Species Concentration/Activity** section.

3 Select the **Constant concentration/activity** check box.

Note that the molar mass of carbon has been set, since we have named the Species using its chemical formula.

Nitrogen is also present in the gas as an inert.

Species 1

1 In the **Reaction Engineering** toolbar, click **Species**.

Constant pressure in channel A is assumed. N2 is simply inert and does not act as a solvent in the first part of the model.

2 In the **Settings** window for **Species**, locate the **Species Name** section.

3 In the text field, type `N2`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Volumetric Species Initial Values** section.

3 In the table, enter the following settings:

Species	Molar flow rate (mol/s)
C(s)	C_inlet*v_inlet
CO	F_CO_inlet
CO2	F_CO2_inlet
Ce2O3(s)	Ce2O3_inlet*v_inlet
CeO2(s)	CeO2_inlet*v_inlet

Species	Molar flow rate (mol/s)
N2	F_N2_inlet
O2	F_O2_inlet

Additional Source 1

1 In the **Reaction Engineering** toolbar, click **Additional Source**.

All species are driven toward or through the filter as a simplification.

2 In the **Settings** window for **Additional Source**, locate the **Additional Rate Expression** section.

3 In the **Volumetric species** table, enter the following settings:

Species	Additional rate expression (mol/(m^3*s))
CO	-uf/H*re.c_CO
CO2	-uf/H*re.c_CO2
Ce2O3(s)	-uf/H*re.c_Ce2O3_solid
CeO2(s)	-uf/H*re.c_CeO2_solid
N2	-uf/H*re.c_N2
O2	-uf/H*re.c_O2

STUDY 1

Step 1: Stationary Plug Flow

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary Plug Flow**.

2 In the **Settings** window for **Stationary Plug Flow**, locate the **Study Settings** section.

3 In the **Output volumes** text field, type `0.149`.

Using `0.149` avoids describing the stagnant zone close to the dead-end of the tubular reactor.

To study the model at two different temperatures, use a parametric sweep to vary `T0`.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
T0 (Initial temperature)	653 703	K

5 In the **Study** toolbar, click **Compute**.

RESULTS

Concentrations plug flow model

To produce the plots shown in Figure 4, Figure 5, and Figure 6 follow these steps.

1 In the **Settings** window for **1D Plot Group**, type `Concentrations plug flow model` in the **Label** text field.

2 Click to expand the **Title** section. From the **Title type** list, choose **None**.

3 Locate the **Plot Settings** section. In the **x-axis label** text field, type `L (m)`.

Global 1

1 In the **Model Builder** window, expand the **Concentrations plug flow model** node, then click **Global 1**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`re.c_O2`	`mol/m^3`	`Concentration`
`re.c_CO2`	`mol/m^3`	`Concentration`
`re.c_CO`	`mol/m^3`	`Concentration`
`re.c_CeO2_solid`	`mol/m^3`	`Concentration`
`re.c_Ce2O3_solid`	`mol/m^3`	`Concentration`

5 Click to select row number 5 in the table.

6 Click **Delete**.

7 Click **Delete**.

8 Click to expand the **Coloring and Style** section. In the **Width** text field, type `2`.

9 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

10 In the table, enter the following settings:

Legends
O₂
CO₂
CO
CeO₂
Ce₂O₃

11 Locate the **Data** section. From the **Parameter selection (T0)** list, choose **First**.

12 In the **Concentrations plug flow model** toolbar, click **Plot**.

13 From the **Parameter selection (T0)** list, choose **Last**.

14 In the **Concentrations plug flow model** toolbar, click **Plot**.

Rate comparison plug flow model

1 In the **Model Builder** window, right-click **Concentrations plug flow model** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Rate comparison plug flow model` in the **Label** text field.

3 Locate the **Plot Settings** section. Select the **y-axis label** check box.

4 In the associated text field, type `Rate ratio comparison (-)`.

Global 1

1 In the **Model Builder** window, expand the **Rate comparison plug flow model** node, then click **Global 1**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Parameter selection (T0)** list, choose **First**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.r_1 - Reaction rate - mol/(m³·s)**.

5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
re.r_1/re.r_3	1	
re.r_2/re.r_4	1	

6 Locate the **Legends** section. In the table, enter the following settings:

Legends
r_1/r_3 at 653 K
r_2/r_4 at 653 K

Global 2

1 Right-click **Results>Rate comparison plug flow model>Global 1** and choose **Duplicate**.

Use the **Generate Space-Dependent Model** feature to generate a 2D model that solves mass, energy, and momentum balances within the system.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Parameter selection (T0)** list, choose **Last**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
r_1/r_3 at 703 K
r_2/r_4 at 703 K

5 In the **Rate comparison plug flow model** toolbar, click **Plot**.

REACTION ENGINEERING (RE)

Generate Space-Dependent Model 1

1 In the **Reaction Engineering** toolbar, click **Generate Space-Dependent Model**.

2 In the **Settings** window for **Generate Space-Dependent Model**, locate the **Component Settings** section.

3 From the **Component to use** list, choose **2D: New**.

4 Locate the **Physics Interfaces** section. Find the **Heat transfer** subsection. From the list, choose **Heat Transfer in Fluids: New**.

5 Find the **Fluid flow** subsection. From the list, choose **Free and Porous Media Flow: New**.

6 Locate the **Space-Dependent Model Generation** section. Click **Create/Refresh**.

COMPONENT 2 (COMP2)

Also add multiphysics coupling features. These ensure that the coupled interfaces are set up in consistent manner.

MULTIPHYSICS

In the **Model Builder** window, expand the **Component 2 (comp2)** node, then click **Multiphysics**.

Nonisothermal Flow 1 (nitf1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain> Nonisothermal Flow**.

Reacting Flow, Diluted Species 1 (rfd1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain>Reacting Flow, Diluted Species**.

The geometry to be used has a high aspect ratio. The length of the geometry is about 50 time the height. In this case using an automatic scaling of the view makes it easier to setup the model. This is since the entire geometry is fitted in the **Graphics** window.

DEFINITIONS (COMP2)

In the **Model Builder** window, expand the **Component 2 (comp2)>Definitions** node.

Axis

1. In the **Model Builder** window, expand the **Component 2 (comp2)>Definitions>View 1** node, then click **Axis**.
2. In the **Settings** window for **Axis**, locate the **Axis** section.
3. From the **View scale** list, choose **Automatic**.

GEOMETRY 1 (2D)

Start by drawing the Outlet Channel, B, as shown in Figure 3.

Rectangle 1 (r1)

1. In the **Geometry** toolbar, click **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `L+1[cm]`.
4. In the **Height** text field, type `H`.

Next, draw the soot layer and filter wall as follows.

Rectangle 2 (r2)

1. In the **Geometry** toolbar, click **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `L`.

4 In the **Height** text field, type `Hf+dHs`.

5 Locate the **Position** section. In the **y** text field, type `H`.

6 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
`Layer 1`	`Hf`

7 Click **Build Selected**.

Rectangle 3 (r3)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `L`.

4 In the **Height** text field, type `0.5*dHs`.

5 Locate the **Position** section. In the **y** text field, type `H+Hf+dHs`.

6 Click **Build Selected**.

Finally move the **Rectangle 1** as shown below to create the inlet channel.

Move 1 (mov1)

1 In the **Geometry** toolbar, click **Transforms** and choose **Move**.

2 Click the **Zoom Extents** button in the **Graphics** toolbar.

3 Select the object **r1** only.

4 In the **Settings** window for **Move**, locate the **Input** section.

5 Select the **Keep input objects** check box.

6 Locate the **Displacement** section. In the **x** text field, type `-1[cm]`.

7 In the **y** text field, type `H+Hf+1.5*dHs`.

Form Union (fin)

1 In the **Model Builder** window, click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, click **Build Selected**.

3 Click the **Zoom Extents** button in the **Graphics** toolbar.

Make geometry selections.

Inlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Inlet` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 1 only.

Outlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Outlet` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 18 only.

Channel A

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Channel A` in the **Label** text field.

3 On the object **fin**, select Domains 1 and 5 only.

Soot layer

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Soot layer` in the **Label** text field.

3 On the object **fin**, select Domain 4 only.

Filter wall

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Filter wall` in the **Label** text field.

3 On the object **fin**, select Domain 3 only.

Soot and filter wall

1 In the **Geometry** toolbar, click **Selections** and choose **Union Selection**.

2 In the **Settings** window for **Union Selection**, locate the **Input Entities** section.

3 Click **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Soot layer** and **Filter wall**.

5 Click **OK**.

6 In the **Settings** window for **Union Selection**, type `Soot and filter wall` in the **Label** text field.

Channel B

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Channel B` in the **Label** text field.

3 On the object **fin**, select Domain 2 only.

GLOBAL DEFINITIONS

Material 1 (mat1)

In the **Model Builder** window, under **Global Definitions** right-click **Materials** and choose **Blank Material**.

Material 2 (mat2)

Right-click **Materials** and choose **Blank Material**.

MATERIALS

Porous Material 1 (pmat1)

1 In the **Model Builder** window, under **Component 2 (comp2)** right-click **Materials** and choose **More Materials>Porous Material**.

2 Select Domain 4 only.

Fluid 1 (pmat1.fluid1)

1 Right-click **Porous Material 1 (pmat1)** and choose **Fluid**.

2 In the **Settings** window for **Fluid**, locate the **Fluid Properties** section.

3 From the **Material** list, choose **Locally defined**.

Solid 1 (pmat1.solid1)

1 In the **Model Builder** window, right-click **Porous Material 1 (pmat1)** and choose **Solid**.

2 In the **Settings** window for **Solid**, locate the **Solid Properties** section.

3 In the θ_s text field, type `1-poro`.

Porous Material 2 (pmat2)

1 Right-click **Porous Material 1 (pmat1)** and choose **Duplicate**.

2 Select Domain 3 only.

Solid 1 (pmat2.solid1)

1 In the **Model Builder** window, expand the **Porous Material 2 (pmat2)** node, then click **Solid 1 (pmat2.solid1)**.

2 In the **Settings** window for **Solid**, locate the **Solid Properties** section.

3 From the **Material** list, choose **Material 2 (mat2)**.

Most reaction kinetics definitions were set up in the **Reaction Engineering** interface, but some changes need to be done directly in the **Chemistry** interface.

CHEMISTRY 1 (CHEM)

Adjust the reaction kinetics.

1: C(s)+O2=>CO2

1. In the **Model Builder** window, expand the **Component 2 (comp2)>Chemistry 1 (chem)** node, then click **1: C(s)+O2=>CO2**.
2. In the **Settings** window for **Reaction**, locate the **Rate Constants** section.
3. In the A^{f} text field, type `1e13`.
4. Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.
5. In the H text field, type `-3.96e5[J/mol]`.

Set the parameters necessary to compute mixture transport properties. Also, the additional source should be inactivated here, since the filter is now included in the model geometry.

Species: O2

1. In the **Model Builder** window, click **Species: O2**.
2. In the **Settings** window for **Species**, click to expand the **Additional Source** section.
3. Clear the **Additional source** check box.
4. Click to expand the **Species Transport Expressions** section. In the σ text field, type `3.467[angstrom]`.
5. In the $\varepsilon/k_{\mathrm{b}}$ text field, type `106.7[K]`.

Species: CO2

1. In the **Model Builder** window, click **Species: CO2**.
2. In the **Settings** window for **Species**, locate the **Additional Source** section.
3. Clear the **Additional source** check box.
4. Locate the **Species Transport Expressions** section. In the σ text field, type `3.941[angstrom]`.
5. In the $\varepsilon/k_{\mathrm{b}}$ text field, type `195.2[K]`.

2: C(s)+0.5O2=>CO

1. In the **Model Builder** window, click **2: C(s)+0.5O2=>CO**.
2. In the **Settings** window for **Reaction**, locate the **Rate Constants** section.
3. In the A^{f} text field, type `5.5e10`.

4 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

5 In the H text field, type `-1.1e5[J/mol]`.

Species: CO

1 In the **Model Builder** window, click **Species: CO**.

2 In the **Settings** window for **Species**, locate the **Additional Source** section.

3 Clear the **Additional source** check box.

4 Locate the **Species Transport Expressions** section. In the σ text field, type `3.69[angstrom]`.

5 In the ε/k_b text field, type `91.7[K]`.

3: C(s)+4CeO2(s)=>2Ce2O3(s)+CO2

1 In the **Model Builder** window, click **3: C(s)+4CeO2(s)=>2Ce2O3(s)+CO2**.

2 In the **Settings** window for **Reaction**, locate the **Rate Constants** section.

3 In the A^f text field, type `4.5e11`.

4 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

5 In the H text field, type `6.72e4[J/mol]`.

The concentration of the cerium additatives are assumed to be constant in the space-dependent model.

Species: CeO2(s)

1 In the **Model Builder** window, click **Species: CeO2(s)**.

2 In the **Settings** window for **Species**, click to expand the **Species Concentration/Activity** section.

3 Select the **Constant concentration/activity** check box.

Species: Ce2O3(s)

1 In the **Model Builder** window, click **Species: Ce2O3(s)**.

2 In the **Settings** window for **Species**, locate the **Species Concentration/Activity** section.

3 Select the **Constant concentration/activity** check box.

4: C(s)+2CeO2(s)=>Ce2O3(s)+CO

1 In the **Model Builder** window, click **4: C(s)+2CeO2(s)=>Ce2O3(s)+CO**.

2 In the **Settings** window for **Reaction**, locate the **Rate Constants** section.

3 In the A^f text field, type `4e8`.

4 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

5 In the H text field, type `1.21e5[J/mol]`.

5: Ce2O3(s)+0.5O2=>2CeO2(s)

1 In the **Model Builder** window, click **5: Ce2O3(s)+0.5O2=>2CeO2(s)**.

2 In the **Settings** window for **Reaction**, locate the **Rate Constants** section.

3 In the A^{f} text field, type `1e12`.

4 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

5 In the H text field, type `-2.24e5[J/mol]`.

Select nitrogen as a solvent. When a species has been selected as solvent, the physical properties of the mixture will be defined from the solvent. This fits the **Transport in Diluted Species** interface particularly well.

Additionally, add the thermodynamic properties for the solvent.

Species: N2

1 In the **Model Builder** window, click **Species: N2**.

2 In the **Settings** window for **Species**, locate the **Species Type** section.

3 From the list, choose **Solvent**.

4 Locate the **Species Transport Expressions** section. In the σ text field, type `3.798[angstrom]`.

5 In the $\varepsilon/k_{\mathrm{b}}$ text field, type `71.4[K]`.

6 Click to expand the **Species Thermodynamic Expressions** section. In the T_{mid} text field, type `3000[K]`.

7 In the T_{hi} text field, type `3000[K]`.

8 In the $a_{\mathrm{low},1}$ text field, type `3.298677`.

9 In the $a_{\mathrm{low},2}$ text field, type `0.14082404e-2`.

10 In the $a_{\mathrm{low},3}$ text field, type `-0.03963222e-4`.

11 In the $a_{\mathrm{low},4}$ text field, type `0.05641515e-7`.

12 In the $a_{\mathrm{low},5}$ text field, type `-0.02444854e-10`.

13 In the $a_{\mathrm{low},6}$ text field, type `-0.10208999e4`.

14 In the $a_{\mathrm{low},7}$ text field, type `3.950372`.

Move on to the rest of the interfaces.

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Transport of Diluted Species (tds)**.

2 In the **Settings** window for **Transport of Diluted Species**, locate the **Transport Mechanisms** section.

3 Select the **Mass transfer in porous media** check box.

Remove the species that are not involved in the mass transport: the solid phase species and the solvent.

4 Click to expand the **Dependent Variables** section. In the **Number of species** text field, type 3.

5 In the **Concentrations** table, enter the following settings:

c02
cC02
cC0

Last, set the concentrations of the species not solved for.

CHEMISTRY 1 (CHEM)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Chemistry 1 (chem)**.

2 In the **Settings** window for **Chemistry**, locate the **Species Matching** section.

3 Find the **Bulk species** subsection. In the table, enter the following settings:

Species	Type	Molar concentration	Value (mol/m^3)
CO	Variable	cCO	Solved for
CO2	Variable	cCO2	Solved for
N2	Solvent	User defined	`F_N2_inlet/v_inlet`
O2	Variable	cO2	Solved for

4 Find the **Solid species** subsection. In the table, enter the following settings:

Species	Species concentration type	Molar concentration (mol/m^3)
C(s)	Constant	`C_inlet`
Ce2O3(s)	Constant	`Ce2O3_inlet`
CeO2(s)	Constant	`CeO2_inlet`

Transport Properties 1

1 In the **Model Builder** window, expand the **Component 2 (comp2)> Transport of Diluted Species (tds)** node, then click **Transport Properties 1**.

2 In the **Settings** window for **Transport Properties**, locate the **Diffusion** section.

3 From the **Source** list, choose **Chemistry**.

4 From the D_{cO2} list, choose **Diffusion coefficient , O2 in N2 (solvent) (chem)**.

5 From the D_{cCO2} list, choose **Diffusion coefficient , CO2 in N2 (solvent) (chem)**.

6 From the D_{cCO} list, choose **Diffusion coefficient , CO in N2 (solvent) (chem)**.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $cO2$ text field, type `0`.

4 In the $cCO2$ text field, type `0`.

5 In the cCO text field, type `0`.

The reactions should only take place in the soot layer.

Reactions 1

1 In the **Model Builder** window, click **Reactions 1**.

2 In the **Settings** window for **Reactions**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Soot layer**.

4 Locate the **Reaction Rates** section. From the R_{cO2} list, choose **Reaction rate for species O2 (chem)**.

5 From the R_{cCO} list, choose **Reaction rate for species CO (chem)**.

6 Click to expand the **Reacting Volume** section. From the list, choose **Pore volume**.

Inflow 1

Set the concentrations at the inflow boundary to be same as the initial concentrations.

1 In the **Model Builder** window, click **Inflow 1**.

2 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Concentration** section. In the $c_{0,\mathrm{cO2}}$ text field, type `F_O2_inlet/v_inlet`.

5 In the $c_{0,\mathrm{cCO2}}$ text field, type `F_CO2_inlet/v_inlet`.

6 In the $c_{0,cCO}$ text field, type `F_CO_inlet/v_inlet`.

Outflow 1

1 In the **Model Builder** window, click **Outflow 1**.

2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

Porous Medium 1

1 In the **Physics** toolbar, click **Domains** and choose **Porous Medium**.

2 Select Domains 3 and 4 only.

Fluid 1

1 In the **Model Builder** window, click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Diffusion** section.

3 From the **Source** list, choose **Chemistry**.

4 From the D_{cO2} list, choose **Diffusion coefficient , O2 in N2 (solvent) (chem)**.

5 From the D_{cCO2} list, choose **Diffusion coefficient , CO2 in N2 (solvent) (chem)**.

6 From the D_{cCO} list, choose **Diffusion coefficient , CO in N2 (solvent) (chem)**.

7 From the **Effective diffusivity model** list, choose **No correction**.

Continue with the **Heat Transfer in Fluids** interface. Note that several properties are available from the **Chemistry** interface.

HEAT TRANSFER IN FLUIDS 1 (HT)

Initial Values 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Heat Transfer in Fluids 1 (ht)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the T text field, type `Tin`.

Heat Source 1

1 In the **Model Builder** window, click **Heat Source 1**.

2 In the **Settings** window for **Heat Source**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Soot layer**.

Temperature 1

1 In the **Model Builder** window, click **Temperature 1**.

2 In the **Settings** window for **Temperature**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Temperature** section. In the T_0 text field, type `Tin`.

Outflow 1

1 In the **Model Builder** window, click **Outflow 1**.

2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

Porous Medium 1

1 In the **Physics** toolbar, click **Domains** and choose **Porous Medium**.

2 Select Domains 3 and 4 only.

Fluid 1

1 In the **Model Builder** window, click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Heat Conduction, Fluid** section.

3 From the k_f list, choose **Thermal conductivity (chem)**.

4 Locate the **Thermodynamics, Fluid** section. From the ρ_f list, choose **Density (chem)**.

5 From the $C_{p,f}$ list, choose **Heat capacity at constant pressure (chem)**.

6 From the γ list, choose **User defined**.

GLOBAL DEFINITIONS

Material 1 (mat1)

1 In the **Model Builder** window, under **Global Definitions>Materials** click **Material 1 (mat1)**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	`k_s`	W/(m·K)	Basic
Density	rho	`rho_s`	kg/m³	Basic
Heat capacity at constant pressure	Cp	`Cp_s`	J/(kg·K)	Basic

Material 2 (mat2)

1 In the **Model Builder** window, click **Material 2 (mat2)**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	k_m	W/(m·K)	Basic
Density	rho	rho_m	kg/m³	Basic
Heat capacity at constant pressure	Cp	Cp_m	J/(kg·K)	Basic

FREE AND POROUS MEDIA FLOW 1 (FP)

Inlet 1

1 In the **Model Builder** window, expand the **Component 2 (comp2)> Free and Porous Media Flow 1 (fp)** node, then click **Inlet 1**.

2 In the **Settings** window for **Inlet**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Boundary Condition** section. From the list, choose **Fully developed flow**.

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `2.5[m/s]`.

Outlet 1

1 In the **Model Builder** window, click **Outlet 1**.

2 In the **Settings** window for **Outlet**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

4 Locate the **Pressure Conditions** section. Select the **Normal flow** check box.

Porous Medium 1

1 In the **Physics** toolbar, click **Domains** and choose **Porous Medium**.

2 In the **Settings** window for **Porous Medium**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Soot layer**.

Fluid 1

1 In the **Model Builder** window, click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Fluid Properties** section.

3 From the μ list, choose **Dynamic viscosity (chem)**.

Porous Medium 2

1 In the **Model Builder** window, under **Component 2 (comp2)>**
Free and Porous Media Flow 1 (fp) right-click **Porous Medium 1** and choose **Duplicate**.

2 In the **Settings** window for **Porous Medium**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Filter wall**.

MATERIALS

Porous Material 1 (pmat1)

1 In the **Model Builder** window, under **Component 2 (comp2)>Materials** click **Porous Material 1 (pmat1)**.

2 In the **Settings** window for **Porous Material**, locate the **Homogenized Properties** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Permeability	kappa_iso ; kappaii = kappa_iso, kappaij = 0	kappa_s	m²	Basic

Porous Material 2 (pmat2)

1 In the **Model Builder** window, click **Porous Material 2 (pmat2)**.

2 In the **Settings** window for **Porous Material**, locate the **Homogenized Properties** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Permeability	kappa_iso ; kappaii = kappa_iso, kappaij = 0	kappa_m	m²	Basic

The soot layer changes in size and the model takes this into account using a **Moving Mesh** feature. The top of the soot layer (boundary 11) is prescribed to move in accordance with the soot build-up, and the adjacent domains are allowed to change shape.

COMPONENT 2 (COMP2)

In the **Definitions** toolbar, click  **Moving Mesh** and choose **Domains>Deforming Domain**.

MOVING MESH

Deforming Domain 1

Select Domains 4 and 5 only.

Prescribed Normal Mesh Velocity 1

1 In the **Definitions** toolbar, click  **Moving Mesh** and choose **Boundaries> Prescribed Normal Mesh Velocity**.

2 Select Boundary 11 only.

The soot layer build-up is controlled by the transport of carbon particles to the layer, as well as the consumption of soot particles inside the layer.

3 In the **Settings** window for **Prescribed Normal Mesh Velocity**, locate the **Prescribed Normal Mesh Velocity** section.

4 In the $\mathbf{v}_n$ text field, type `(-paco*(u*fp.nx+v*fp.ny)-Mc*((y-Y)+dHsoot)*(comp2.chem.r_1+comp2.chem.r_2+comp2.chem.r_3+ comp2.chem.r_4))/rho_s`.

Prescribed Normal Mesh Displacement 1

1 In the **Definitions** toolbar, click  **Moving Mesh** and choose **Boundaries> Prescribed Normal Mesh Displacement**.

2 Select Boundaries 8, 10, 15, and 16 only.

3 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Next step is to build a suitable mesh. Due to the regular structure of the geometry, a mapped mesh both captures the physics and keeps the number of elements to a minimum.

MESH 1

Mapped 1

1 In the **Mesh** toolbar, click  **Mapped**.

2 In the **Settings** window for **Mapped**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domains 1 and 3–5 only.

5 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 1 and 17 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 25.

6 In the **Element ratio** text field, type 3.

7 Select the **Symmetric distribution** check box.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 10.

6 In the **Element ratio** text field, type 3.

Distribution 3

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 7, 9, 11, and 12 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 90.

6 In the **Element ratio** text field, type 10.

7 Select the **Symmetric distribution** check box.

Distribution 4

1 Right-click **Mapped 1** and choose **Distribution**.

2 Click the  **Zoom Extents** button in the **Graphics** toolbar.

3 In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.

4 Click  **Paste Selection**.

5 In the **Paste Selection** dialog box, type `8, 10, 15, 16` in the **Selection** text field.

6 Click **OK**.

Distribution 5

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 6 and 13 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 In the **Number of elements** text field, type 15.

5 Click **Build Selected**.

Mapped 2

In the **Mesh** toolbar, click **Mapped**.

Distribution 1

1 Right-click **Mapped 2** and choose **Distribution**.

2 Select Boundaries 4 and 18 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 25.

6 In the **Element ratio** text field, type 3.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 2** and choose **Distribution**.

2 Select Boundary 14 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 10.

6 In the **Element ratio** text field, type 3.

7 Click **Build All**.

8 Click the **Zoom Extents** button in the **Graphics** toolbar.

Hide the internal boundary just above the soot layer. This was kept in the model to simplify the mesh generation.

DEFINITIONS (COMP2)

Hide for Physics 1

1 In the **Model Builder** window, right-click **View 1** and choose **Hide for Physics**.

2 In the **Settings** window for **Hide for Physics**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 12 only.

In a model described by a strongly coupled system of equations, it is often a good practice to solve the problem sequentially to avoid convergence issues. Start by solving for the

stationary flow. After that, solve the full time-dependent system, with the dynamic nature of the soot layer handled by the **Moving Mesh** feature.

STUDY 2

Step 1: Stationary

1 In the **Model Builder** window, expand the **Study 2** node, then click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, enter the following settings:

Physics interface	Solve for	Equation form
Reaction Engineering (re)		Automatic (Time dependent)
Chemistry 1 (chem)		Automatic (Stationary)
Transport of Diluted Species (tds)		Automatic (Stationary)
Heat Transfer in Fluids 1 (ht)		Automatic (Stationary)
Free and Porous Media Flow 1 (fp)	√	Automatic (Stationary)
Moving mesh (Component 2)		

Time Dependent

1 In the **Study** toolbar, click **Study Steps** and choose **Time Dependent> Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Reaction Engineering (re)**.

4 Locate the **Study Settings** section. In the **Output times** text field, type `range(0,300, 1800)`.

Set up proportional **Scale** values for **Dependent Variables 2**.

Solution 5 (sol5)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 5 (sol5)** node.

3 In the **Model Builder** window, expand the **Study 2>Solver Configurations> Solution 5 (sol5)>Dependent Variables 2** node, then click **Concentration (comp2.cCO)**.

4 In the **Settings** window for **Field**, locate the **Scaling** section.

5 From the **Method** list, choose **Manual**.

6 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 5 (sol5)> Dependent Variables 2** click **Concentration (comp2.cO2)**.

7 In the **Settings** window for **Field**, locate the **Scaling** section.

8 From the **Method** list, choose **Manual**.

9 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 5 (sol5)> Dependent Variables 2** click **Concentration (comp2.cO2)**.

10 In the **Settings** window for **Field**, locate the **Scaling** section.

11 From the **Method** list, choose **Manual**.

12 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 5 (sol5)> Dependent Variables 2** click **Temperature (comp2.T)**.

13 In the **Settings** window for **Field**, locate the **Scaling** section.

14 From the **Method** list, choose **Initial value based**.

To avoid discontinuities at the inlet for the **Time Dependent** study, add a step function to gradually increase the **Inflow** concentration

DEFINITIONS (COMP2)

Step 1 (step1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Step**.

2 In the **Settings** window for **Step**, locate the **Parameters** section.

3 In the **Location** text field, type `0.5`.

4 Click to expand the **Smoothing** section. In the **Size of transition zone** text field, type `1`.

TRANSPORT OF DILUTED SPECIES (TDS)

Inflow 1

1 In the **Model Builder** window, under **Component 2 (comp2)> Transport of Diluted Species (tds)** click **Inflow 1**.

2 In the **Settings** window for **Inflow**, locate the **Concentration** section.

3 In the $c_{0,cO2}$ text field, type `F_O2_inlet/v_inlet*step1(t[1/s])`.

4 In the $c_{0,cCO2}$ text field, type `F_CO2_inlet/v_inlet*step1(t[1/s])`.

5 In the $c_{0,cCO}$ text field, type `F_CO_inlet/v_inlet*step1(t[1/s])`.

STUDY 2

In the **Home** toolbar, click = **Compute**.

RESULTS

Streamline 1

1 In the **Model Builder** window, expand the **Results>Concentration, O2 (tds)** node, then click **Streamline 1**.

2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

3 From the **Positioning** list, choose **On selected boundaries**.

4 In the **Number** text field, type `15`.

5 Locate the **Selection** section. Click to select the **Activate Selection** toggle button.

6 Select Boundary 1 only.

7 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Arrow length** list, choose **Normalized**.

8 Select the **Scale factor** check box.

9 In the associated text field, type `6e-4`.

10 In the **Concentration, O2 (tds)** toolbar, click **Plot**.

Streamline 1

1 In the **Model Builder** window, expand the **Results>Concentration, CO2 (tds)** node, then click **Streamline 1**.

2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

3 From the **Positioning** list, choose **On selected boundaries**.

4 In the **Number** text field, type `15`.

5 Locate the **Selection** section. Click to select the **Activate Selection** toggle button.

6 Select Boundary 1 only.

7 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Arrow length** list, choose **Normalized**.

8 Select the **Scale factor** check box.

9 In the associated text field, type `1.4e-3`.

10 In the **Concentration, CO2 (tds)** toolbar, click **Plot**.

Streamline 1

1 In the **Model Builder** window, expand the **Results>Concentration, CO (tds)** node, then click **Streamline 1**.

2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

3 From the **Positioning** list, choose **On selected boundaries**.

4 In the **Number** text field, type `15`.

5 Locate the **Selection** section. Click to select the **Activate Selection** toggle button.

6 Select Boundary 18 only.

7 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Arrow length** list, choose **Normalized**.

8 Select the **Scale factor** check box.

9 In the associated text field, type `0.13`.

10 In the **Concentration, CO (tds)** toolbar, click **Plot**.

To produce the plots shown in Figures 7-11 follow these steps.

Surface

1 In the **Model Builder** window, expand the **Results>Velocity (fp1)** node, then click **Surface**.

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **Twilight**.

4 From the **Color table transformation** list, choose **Reverse**.

5 In the **Velocity (fp1)** toolbar, click **Plot**.

Streamline 1

1 In the **Model Builder** window, right-click **Velocity (fp1)** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 2 (comp2)> Free and Porous Media Flow 1>Velocity and pressure>u,v - Velocity field (spatial frame)**.

3 Select Boundary 1 only.

4 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **Gray**.

5 From the **Type** list, choose **Arrow**.

6 Select the **Scale factor** check box.

7 In the associated text field, type `0.002`.

8 In the **Velocity (fp1)** toolbar, click **Plot**.

9 Click the **Zoom Extents** button in the **Graphics** toolbar.

Contour

1 In the **Model Builder** window, expand the **Pressure (fp1)** node.

2 Right-click **Contour** and choose **Disable**.

Surface 1

1 In the **Model Builder** window, right-click **Pressure (fp1)** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `p`.

4 In the **Pressure (fp1)** toolbar, click **Plot**.

Temperature (ht1)

1 In the **Model Builder** window, under **Results** click **Temperature (ht1)**.

2 In the **Temperature (ht1)** toolbar, click **Plot**.

3 Click the **Zoom Extents** button in the **Graphics** toolbar.

Soot layer thickness

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Soot layer thickness` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 5 (sol5)**.

4 Locate the **Title** section. From the **Title type** list, choose **None**.

5 Locate the **Plot Settings** section. Select the **x-axis label** check box.

6 In the associated text field, type `L (m)`.

7 Select the **y-axis label** check box.

8 In the associated text field, type `Soot layer top position (\mu m)`.

9 Locate the **Legend** section. From the **Position** list, choose **Lower middle**.

Line Graph 1

1 Right-click **Soot layer thickness** and choose **Line Graph**.

2 Click the **Zoom Extents** button in the **Graphics** toolbar.

3 Select Boundary 11 only.

4 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

5 In the **Expression** text field, type `y-Y+dHsoot`.

6 From the **Unit** list, choose **µm**.

7 Click to expand the **Coloring and Style** section. In the **Width** text field, type `2`.

8 Click to expand the **Legends** section. Select the **Show legends** check box.

9 In the **Soot layer thickness** toolbar, click **Plot**.

10 Click the **Zoom Extents** button in the **Graphics** toolbar.

1D Plot Group 11

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 5 (sol5)**.

Global 1

1 Right-click **1D Plot Group 11** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 2 (comp2)> Free and Porous Media Flow 1>Auxiliary variables>fp.inl1.pAverage - Pressure average over feature selection - Pa**.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`fp.inl1.pAverage`	`Pa`	`Average Inlet Pressure`

4 Locate the **Coloring and Style** section. In the **Width** text field, type 2.

5 In the **1D Plot Group 11** toolbar, click **Plot**.

Inlet pressure

1 In the **Model Builder** window, under **Results** click **1D Plot Group 11**.

2 In the **Settings** window for **1D Plot Group**, type `Inlet pressure` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.

For future use of **Study 1** disable the interfaces that are used in the space-dependent model.

STUDY 1

Step 1: Stationary Plug Flow

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary Plug Flow**.

2 In the **Settings** window for **Stationary Plug Flow**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check boxes for **Chemistry 1 (chem)**, **Transport of Diluted Species (tds)**, **Heat Transfer in Fluids 1 (ht)**, **Free and Porous Media Flow 1 (fp)**, and **Moving mesh (Component 2)**.