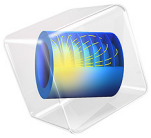

Model created in COMSOL Multiphysics 6.4

NOx and Ammonia Conversion in a Dual-Bed Monolithic Reactor

Introduction

This example illustrates the modeling of a dual bed reactor for exhaust gas treatment in a heavy-duty diesel truck. The reactor consists of two monolithic beds placed in series. In the first bed, selective catalytic reduction (SCR) of NOx (NO and NO_2) with ammonia (NH_3) occurs. Downstream of this catalytic bed, an ammonia-slip catalyst (ASC) is installed. The ASC bed converts the unreacted ammonia into nitrogen. In both beds there are also undesired side-reactions. The complex chemical kinetics is investigated in detail in Analysis of NOx and Ammonia Conversion Kinetics in a Dual-Bed Plug-Flow Reactor. From that study, where a single monolith channel was modeled, it is clear that temperature plays a central role for the selectivity of the system. The current model is set up in 2D with axi-symmetry to unravel the full space-dependency of the system.

Model Definition

The single channel model in Analysis of NOx and Ammonia Conversion Kinetics in a Dual-Bed Plug-Flow Reactor shows that temperature plays a central role in affecting the optimal dosing of NH_3. Because the temperature distribution is sure to vary from channel to channel in monolithic reactor, a space-dependent model is called for.

MODEL GEOMETRY

The modeled reactor consists of a metal shell that protects and insulates the two catalysts placed inside. Each catalytic bed consists of a monolithic support that is loaded with active catalytic material. These two porous domains are modeled as one material in this model. The catalysts are placed in series, wrapped in a porous supportive mat, and contained in a metal can. The supportive mat protects the catalysts from vibrations and holds them in place. Each monolith consists of reactive channels separated by impermeable walls. The first bed in the reactor is 0.4 m long, and the second bed is 0.06 m long. They are placed with a small gap between. Both beds have a diameter of 0.32 m. The void fraction of the catalyst beds are 0.75. A seal is placed at the inlet of the support mat to prevent erosion of the mat, as well as bypassing of reactive gas through the mat. This seal is included as a boundary condition during simulation, and not a detail in the geometry.

An illustration of the modeled system is found in Figure 1 below.

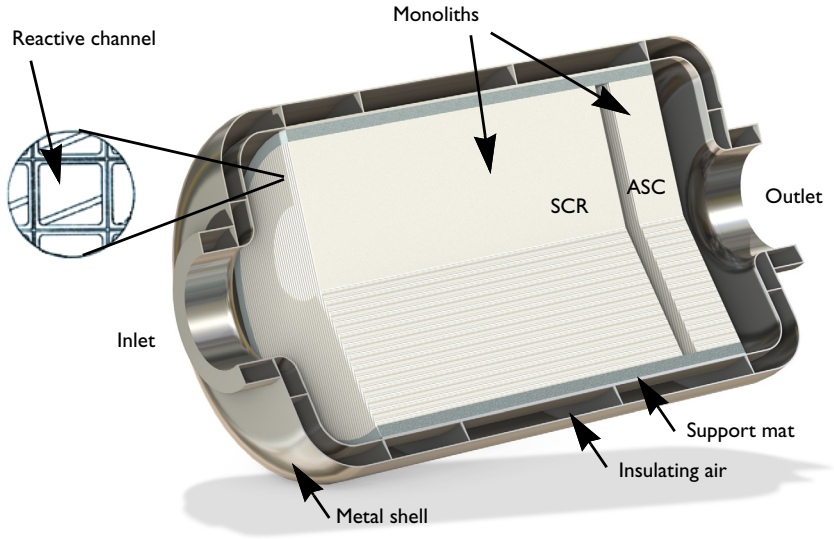

Figure 1: The exhaust gas passes through the channels in the monolithic beds in the reactor.

The reactor is symmetric in its design which gives the geometry seen in Figure 2 below.

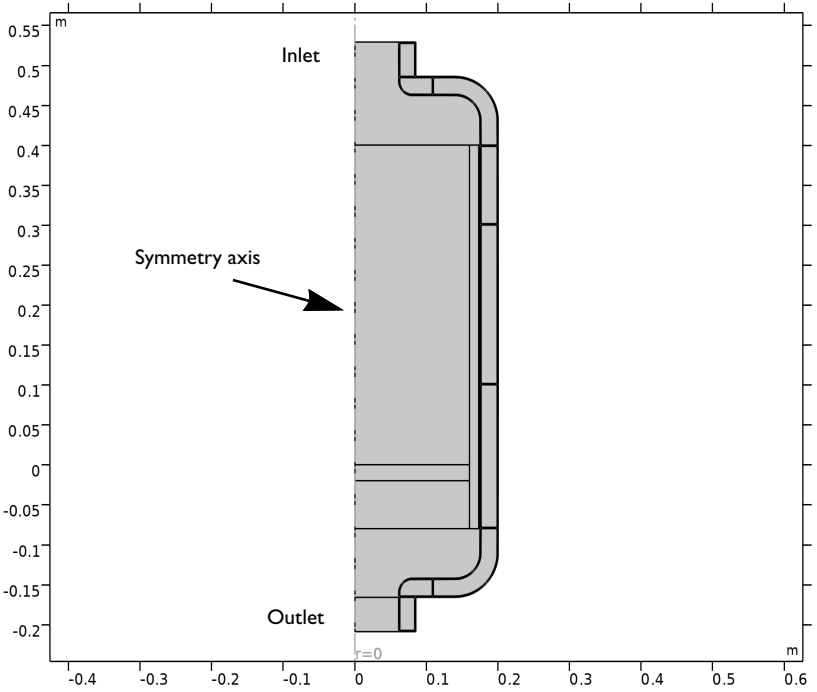

Figure 2: Symmetry reduces the modeling domain.

MODEL EQUATIONS

The present example takes a pseudo-homogeneous approach to model the thousands of channels present in the monolith reactor. No mass is exchanged between channels, so each channel is described by 1D mass-transport equations. Furthermore, assume fully developed laminar flow in the monolith channels, such that the average flow field is proportional to the pressure difference across each bed. The fluid flow transports mass and energy only in the channel direction. The energy equation describes the temperature of the reacting gas in the channels, as well as the conductive heat transfer in the solid parts of the monolith structure. Because the temperature affects not only the reaction kinetics but also the density and viscosity of the reacting gas, the energy equation is what connects the channels in the reactor structure, turning this into a space-dependent model.

Reaction Kinetics

The chemical equations and rate expressions are described in detail in the single channel model Analysis of NOx and Ammonia Conversion Kinetics in a Dual-Bed Plug-Flow Reactor.

Mass Transport

The mass balances describing transport and reaction in the monolith channels are given by diffusion-convection equations at steady state:

$$\nabla \cdot (-D_i \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i \tag{1}$$

Here D_i denotes the diffusion coefficient (SI unit: m^2/s), c_i is the species concentration (SI unit: mol/m^3), and $\mathbf{u}$ equals the velocity vector (SI unit: m/s). The term R_i (SI unit: $mol/(m^3 \cdot s)$) corresponds to the species' rate expression, which is a function of the reaction rates and the reaction stoichiometry.

Mass transport is only allowed in the direction of the channels, corresponding to direction of the z-axis in the 2D-axisymmetric geometry used in this example. For the diffusive transport, this is accomplished by setting the x- and y-components of the diffusivity matrix to zero. The pressure-driven flow in the monolith is also defined in the direction of the z-axis, hereby restricting the convective mass transport to the channel direction. Each monolith channel thus behaves like a 1D plug flow model with included diffusion. These separate channel models are connected through the heat transfer equations for the reactor monolith.

Species concentrations are defined at the reactor inlet boundaries:

$$c = c_{\text{in}}$$

At the outlet, use the Outflow condition:

$$\mathbf{n} \cdot (-D \nabla c) = 0$$

Fluid Flow

The fluid flow in the system is described by the steady-state continuity equation

$$\nabla \cdot (\rho \mathbf{u}) = 0 \,.$$

The flow is modeled as compressible, and a porous slip formulation is used. This formulation ensures a smooth transition between regions with different porosity.

The flow of reacting gas through the monoliths is modeled using Darcy's Law, with the governing equation:

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p$$

The monolith block is treated as a porous matrix with the effective permeability κ (SI unit: m^2). Similarly to the diffusivity, the x- and y-components of the permeability matrix are much lower than that in the axial direction. The density, ρ (SI unit: kg/m^3), and viscosity, μ (SI unit: Pa·s), of the gas are assumed to be well represented by the temperature-dependent properties of nitrogen, as only relatively small concentrations of other gases are present.

Pressure conditions are set at the reactor inlet and outlet boundaries.

Heat Transfer

A single temperature equation describing the heat transfer in the porous monolith reactor can be written as

$$(\rho C_p)_{\text{eff}}\frac{\partial T}{\partial t} + \rho_f C_{pf}\mathbf{u}\cdot\nabla T = \nabla\cdot(k_{\text{eff}}\nabla T) + Q \tag{2}$$

where ρ_f (SI unit: kg/m^3) is the fluid density, C_{pf} (SI unit: J/(kg·K)) is the fluid heat capacity, $(\rho C_p)_{\text{eff}}$ (SI unit: $J/(m^3\cdot K)$) is the effective volumetric heat capacity, and k_{eff} (SI unit: W/(m·K)) is the effective thermal conductivity. Furthermore, $\mathbf{u}$ (SI unit: m/s) is the fluid velocity field, derived by the fluid flow interface. Q (SI unit: W/m^3) is the heat source due to exothermic chemical reactions:

$$Q = -\sum_j H_j r_j$$

Above, H_j is the heat of reaction for reaction j, and r_j is the reaction rate for said reaction.

In the stationary case this implies

$$\rho_f C_{pf}\mathbf{u}\cdot\nabla T = \nabla\cdot(k_{\text{eff}}\nabla T) + Q \tag{3}$$

The effective conductivity of the solid-fluid system, k_{eff}, is related to the conductivity of the solid, k_s, and to the conductivity of the fluid, k_f, by

$$k_{\text{eff}} = \Theta_s k_s + \Theta_f k_f$$

Here Θ_s denotes the solid material's volume fraction, which is related to the volume fraction of the fluid Θ_f (or porosity) by

$$\Theta_f + \Theta_s = 1$$

The Heat Transfer interface sets up Equation 3 for a fluid domain. For the solid monolith walls in the reactor, only heat transfer by conduction applies:

$$-\nabla \cdot (k_s \nabla T) = 0 \tag{4}$$

where k_s (SI unit: W/(m·K)) is the thermal conductivity for the solid walls. For the extruded monolith material, the thermal conductivity is anisotropic.

The heat transfer in the porous support mat is also described by Equation 3 and Equation 4. Contrary to the monoliths, the support mat has isotropic thermal conductivity. The same is true for the solid metal walls in the reactor.

The temperature is specified at the metal walls and the edge of the support mat in the reactor inlet:

$$T = T_0 ,$$

and the Inflow condition, that is

$$-\mathbf{n} \cdot \mathbf{q} = \rho \Delta H \mathbf{u} \cdot \mathbf{n}$$

is assigned to the inlet of the first catalytic bed. ΔH (SI unit: J/(kg)) is the sensible enthalpy.

At the outlet of the second bed, use the Outflow condition

$$\mathbf{n} \cdot (k \nabla T) = 0 .$$

For the external reactor walls, the heat flux through the boundaries is given by

$$\mathbf{q}_m \cdot \mathbf{n} = h(T - T_{amb}) ,$$

where h (SI unit: W/(m^2·K)) denotes the heat transfer coefficient, and T_{amb} (K) equals the ambient temperature.

As mentioned, the temperature affects not only reaction kinetics but also the density and viscosity of the reacting gas. In this way the heat transfer equation connects the channels in the reactor structure.

THERMODYNAMIC AND TRANSPORT PROPERTIES

Accurate thermodynamic data is required as input to energy balance equations, both in the plug flow model and this 2D axisymmetric monolith model (Equation 2). In addition to thermodynamic properties, the model equations also require transport properties to

accurately describe the space-dependent reactor model. For instance, the mass transport (Equation 1) needs species specific diffusion coefficients as input.

The Thermodynamics feature provides all necessary properties for this simulation. Different models are available for calculation of thermal and transport properties (see *Thermodynamic Models and Theory*). The viscosity of the system is calculated based on the *Brokaw* model. The thermal conductivity and diffusivity are calculated from *Kinetic Theory* and *Fuller–Schettler–Giddings*, respectively.

In this model, to simplify the problem, nitrogen is modeled as a solvent. This means that the gas properties are not composition dependent. Another way to speed up the calculations, also used in this model, is to use *Generate Material* from Thermodynamics. Information about how to efficiently use the Thermodynamics feature is available at *Using Thermodynamic Properties*.

RESULTS

The system conditions used in this model are the same as those in the single channel plug flow system, described in Analysis of NOx and Ammonia Conversion Kinetics in a Dual-Bed Plug-Flow Reactor. Three engine load cases are investigated, with a fixed ammonia-to-NOx ratio of 1.3.

The three engine load cases result in the following inlet gas conditions:

TABLE 1: INLET GAS CONDITIONS FOR EACH ENGINE LOAD CASE STUDIED,

	Low load	Intermediate load	High load
Temperature	523 K	623 K	703 K
Molar fraction of NO	300 ppm	800 ppm	1300 ppm
Mass flow rate	0.086 kg/s	0.110 kg/s	0.160 kg/s

Figure 3 shows the molar fraction of NH_3, NO, and NO_2 in the two catalyst beds for the low engine load case. The effect of the radial temperature gradient is clearly visible as the conversion decreases close to the edge. The temperature for the low engine load case is below the optimal temperature for the SCR reactor, see Analysis of NOx and Ammonia

Conversion Kinetics in a Dual-Bed Plug-Flow Reactor. The low temperature results in low conversion of both NOx and ammonia.

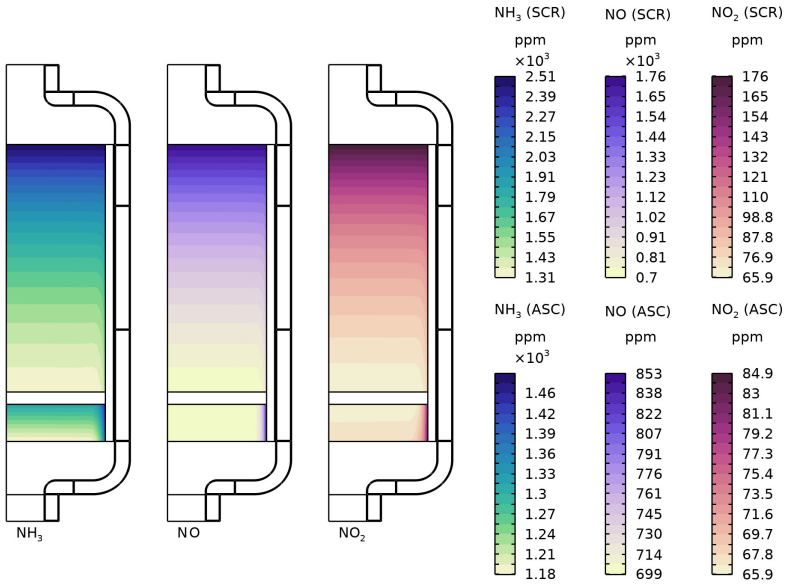

Figure 3: Molar fraction of ammonia, nitrogen monoxide, and nitrogen dioxide in the reactor. Low engine load, and NH_3:NOx equal to 1.3. Fluid flow from top to bottom.

Figure 4 illustrates the result for the intermediate engine load case. At this increased temperature, the conversion increases in the reactor. Higher mass flow rate and higher heat source due to increased conversion, gives smaller radial temperature gradient.

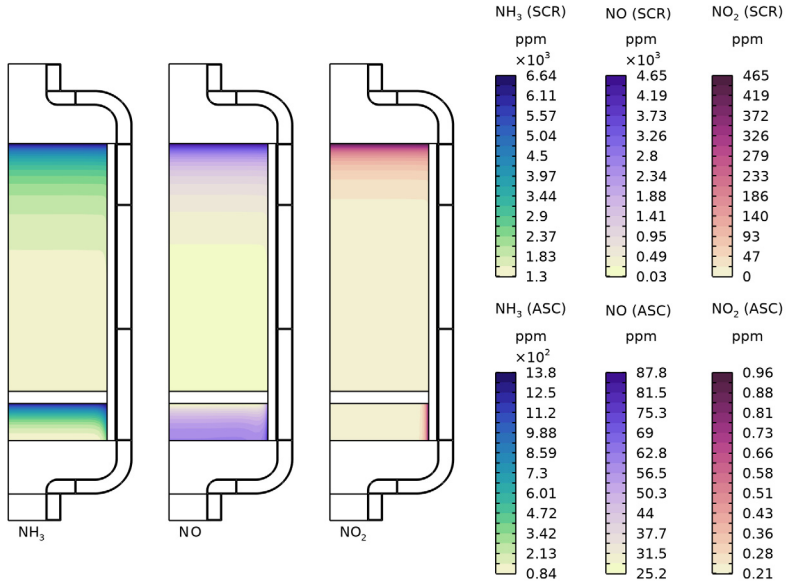

Figure 4: Molar fraction of ammonia, nitrogen monoxide, and nitrogen dioxide in the reactor. Intermediate engine load, and NH_3:NOx equal to 1.3. Fluid flow from top to bottom.

Figure 5 shows the results for the high engine load case.

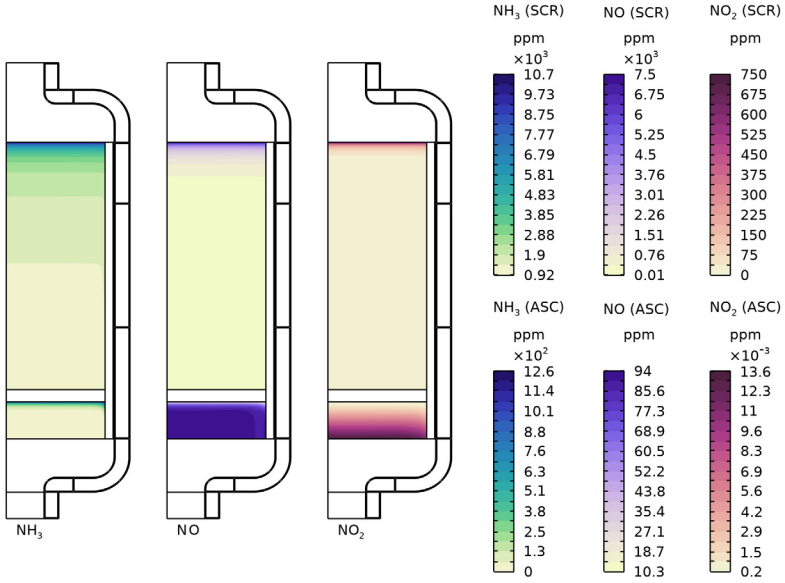

Figure 5: Molar fraction of ammonia, nitrogen monoxide, and nitrogen dioxide in the reactor. High engine load, and NH_3:NOx equal to 1.3. Fluid flow from top to bottom.

The radial temperature gradient has less influence at increased space velocities. For the highest load case, the radial concentration difference is thus lower. Due to the high temperature, the activity of both beds are high. This results in the lowest ammonia emission among the three cases. During oxidation of ammonia in the ASC, the side reactions produce NOx, resulting in a lower NOx conversion than for the intermediate load case. At high engine loads, the ammonia-to-NOx ratio should probably be lower than for the intermediate load.

Figure 6 illustrates the gas velocity, pressure, and temperature in the beds for the highest engine load.

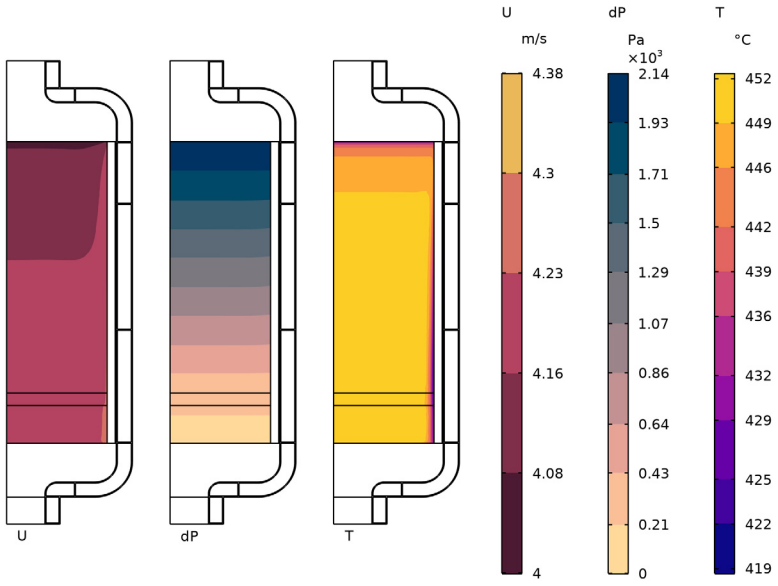

Figure 6: Gas velocity, pressure drop, and temperature in the reactor for the high engine load case. NH_3:NOx equal to 1.3. Fluid flow from top to bottom.

The effect of temperature on conversion is seen in Figure 7. In this figure, the conversion is plotted both along the central symmetry axis, and along the edge of the monoliths. For

a high engine load, the conversion does not vary significantly with the position in the reactor, but for lower engine loads, the conversion differs significantly.

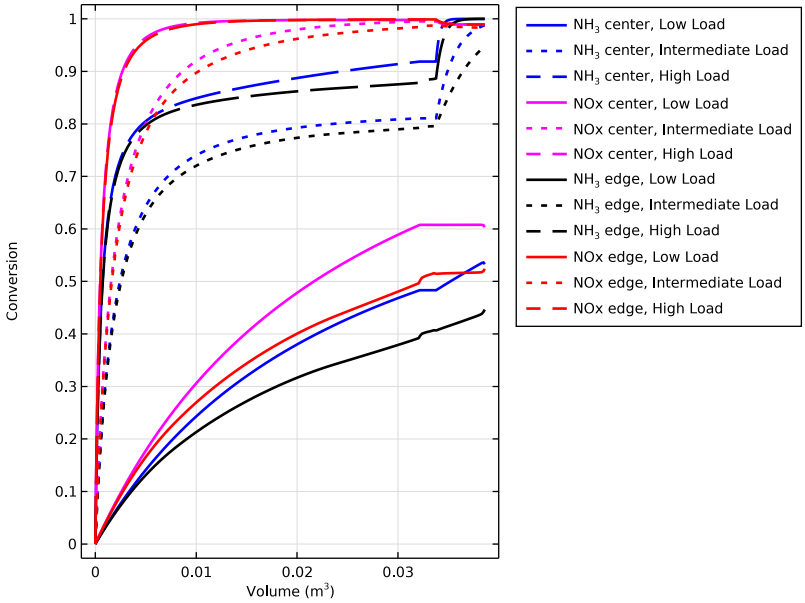

Figure 7: Conversion of ammonia and NOx along the center line, as well as along the monolith edge. All three engine load cases. NH_3:NOx equal to 1.3.

The temperature differences along the reactor axis, at the center of the reactor, and at the edge of the beds, are seen in Figure 8. Close to the inlet of the first bed, the temperature increases both at the center and along the SCR edge. This is due to the exothermic reactions. After the first rapid temperature increase, the increase in temperature is slower, and at the edge of the first bed, the temperature instead decreases due to heat flux to the surroundings. For the high and intermediate engine load cases, the slip of ammonia from the first bed creates a significant temperature increase when this ammonia is oxidized in the second bed. For the low engine case, the activity is too low to create a temperature increase. At the bed edge, the heat flux to the surrounding decreases the temperature in

the first bed, decreasing the ammonia conversion rate, which creates an even larger temperature increased during ammonia oxidation in the second bed.

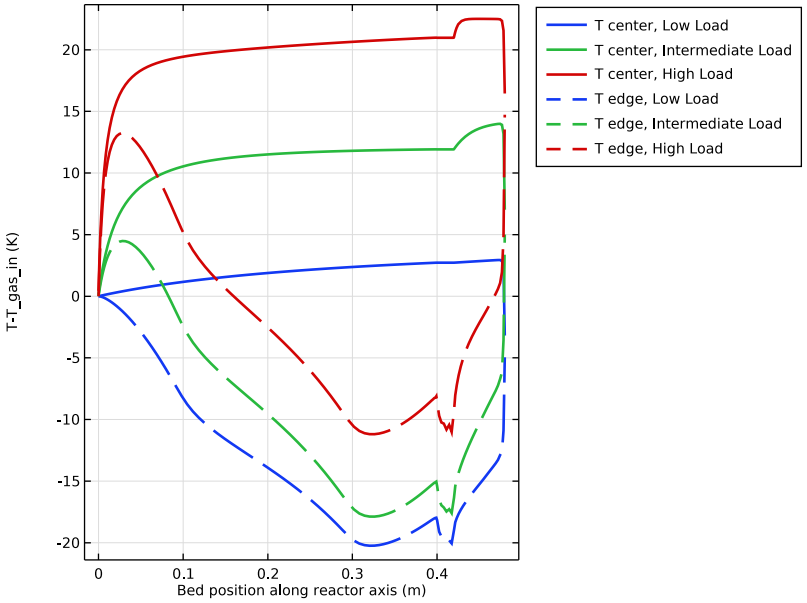

Figure 8: Temperature difference along the reactor axis, both at the center of the reactor, and at the edge of the monoliths. All three engine load cases. NH_3:NOx equal to 1.3.

Finally, the average values of ammonia and NOx molar fractions were derived both along the outlet of the first bed, as well as along the outlet of the second bed. The values are found in Table 2.

TABLE 2: MOLAR FRACTIONS FOR AMMONIA AND NOX OUT FROM EACH BED, FOR EACH ENGINE LOAD CASE STUDIED.

	Low load	**Intermediate load**	**High load**
y_NH3 out from first bed	1320 ppm	1299 ppm	932 ppm
y_NH3 out from second bed	1190 ppm	99 ppm	0 ppm
y_NOx out from first bed	774 ppm	24 ppm	15 ppm
y_NOx out from second bed	775 ppm	54 ppm	78 ppm

From the results in Table 2 it is clear that for an ammonia-to-NOx ratio of 1.3, the exhaust gases from the truck will contain the least ammonia at high load, and the least NOx at intermediate load.

With this model we have shown that in order get low exhaust levels for both ammonia and NOx, the injected amount of ammonia needs to be adjusted as a function of engine load.

Application Library path: `Chemical_Reaction_Engineering_Module/Tutorials/monolith_reactor`

Note: This model is included in the booklet *Introduction to the Chemical Reaction Engineering Module*.

Modeling Instructions

This space dependent model of an exhaust gas cleaning catalytic reactor is built from the **Application Library** model monolith_kinetics. Begin by opening that model.

APPLICATION LIBRARIES

1 From the **File** menu, choose **Application Libraries**.

2 In the **Application Libraries** window, select **Chemical Reaction Engineering Module** > **Tutorials** > **monolith_kinetics** in the tree.

3 Click **Open**.

Start by loading some parameters from a file.

GLOBAL DEFINITIONS

Parameters: Temperature and Monolith Parameters

1 In the **Model Builder** window, under **Global Definitions** click **Parameters: Temperature and Monolith Parameters**.

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 `monolith_reactor_temperature_monolith_parameters.txt`.

COMPONENT 1 (COMP1)

In the **Model Builder** window, expand the **Component 1 (comp1)** node.

SELECTIVE CATALYTIC REDUCTION CATALYST (SCR) (RE)

To simplify the problem of calculating the transport properties, nitrogen is set as the solvent from here on.

Species: N2

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Selective Catalytic Reduction Catalyst (SCR) (re)** node, then click **Species: N2**.

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

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

AMMONIA SLIP CATALYST (ASC) (RE2)

In the **Model Builder** window, expand the **Component 1 (comp1)** > **Ammonia Slip Catalyst (ASC) (re2)** node.

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Ammonia Slip Catalyst (ASC) (re2)** > **Species: N2** node, then click **Species: N2**.

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

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

SINGLE CHANNEL MODEL

1 In the **Model Builder** window, click **Component 1 (comp1)**.

2 In the **Settings** window for **Component**, type `Single Channel Model` in the **Label** text field.

SELECTIVE CATALYTIC REDUCTION CATALYST (SCR) (RE)

In the next phase of this example, set up a space dependent 2D axi-symmetric model of the monolithic reactor, including mass transport and reaction, heat transfer, and fluid flow.

The **Generate Space-Dependent Model** feature creates a link between the single channel model and the space dependent monolith model. It allows you to transfer reaction kinetics, thermodynamics, and transport properties set up in the **Reaction Engineering** interfaces to the physics interfaces describing space and time-dependent systems.

1 In the **Model Builder** window, under **Single Channel Model (comp1)** click **Selective Catalytic Reduction Catalyst (SCR) (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 **2Daxi: New**.

4 Locate the **Physics Interfaces** section. Find the **Chemical species transport** subsection. From the list, choose **Transport of Diluted Species in Porous Media: New**.

5 Find the **Fluid flow** subsection. From the list, choose **Laminar Flow: New**.

6 Find the **Heat transfer** subsection. From the list, choose **Heat Transfer in Porous Media: New**.

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

MONOLITH REACTOR MODEL

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

2 In the **Settings** window for **Component**, type `Monolith Reactor Model` in the **Label** text field.

GEOMETRY 1(2DAXI)

Now import a file with the reactor geometry. Symmetry reduces the modeling domain.

1 In the **Model Builder** window, expand the **Monolith Reactor Model (comp2)** node.

2 Right-click **Monolith Reactor Model (comp2)** > **Geometry 1(2Daxi)** and choose **Insert Sequence**.

3 Browse to the model's Application Libraries folder and double-click the file `monolith_reactor_geom_sequence.mph`.

4 In the **Geometry** toolbar, click **Build All**.

Import some variables from a file. The variables in the variable expressions have not yet been created and this is indicated with yellow text in the expression fields.

DEFINITIONS (COMP2)

Variables: SCR Kinetics

1 In the **Model Builder** window, expand the **Monolith Reactor Model (comp2)** > **Definitions** node.

2 Right-click **Monolith Reactor Model (comp2)** > **Definitions** and choose **Variables**.

3 In the **Settings** window for **Variables**, locate the **Geometric Entity Selection** section.

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

5 From the **Selection** list, choose **SCR Catalyst**.

6 Locate the **Variables** section. Click **Load from File**.

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

8 In the **Label** text field, type `Variables: SCR Kinetics`.

Variables: ASC Kinetics

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables: ASC Kinetics` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **ASC Catalyst**.

5 Locate the **Variables** section. Click **Load from File**.

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

Variables: Postprocessing

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables: Postprocessing` in the **Label** text field.

3 Locate the **Variables** section. Click **Load from File**.

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

CHEMISTRY: SCR

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

2 In the **Settings** window for **Chemistry**, type `Chemistry: SCR` in the **Label** text field.

Use **Generate Space Dependent Model** again to set up a **Chemistry** interface for the Ammonia Slip Catalyst.

AMMONIA SLIP CATALYST (ASC) (RE2)

In the **Model Builder** window, under **Single Channel Model (comp1)** click **Ammonia Slip Catalyst (ASC) (re2)**.

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 **Monolith Reactor Model (2Daxi)**.

4 Locate the **Physics Interfaces** section. Find the **Chemical species transport** subsection. From the list, choose **None**.

5 Find the **Fluid flow** subsection. From the list, choose **None**.

6 Find the **Heat transfer** subsection. From the list, choose **None**.

7 Locate the **Study Type** section. From the **Study type** list, choose **None**.

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

CHEMISTRY: ASC

1 In the **Model Builder** window, under **Monolith Reactor Model (comp2)** click **Chemistry 2 (chem2)**.

2 In the **Settings** window for **Chemistry**, type `Chemistry: ASC` in the **Label** text field.

GLOBAL DEFINITIONS

Transport properties need to be calculated for the space-dependent monolith reactor model. Assuming nitrogen as the solvent, generate a material node from **Thermodynamics**.

Gas System 1 (pp1)

1 In the **Model Builder** window, expand the **Global Definitions** > **Thermodynamics** node.

2 Right-click **Global Definitions** > **Thermodynamics** > **Gas System 1 (pp1)** and choose **Generate Material**.

SELECT PHASE

1 Go to the **Select Phase** window.

2 Click the **Next** button in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.

2 Click **Add All**.

3 Find the **Material composition** subsection. In the table, enter the following settings:

Species	Mole fraction
ammonia	0
nitrogen	1
nitrogen oxide	0
NO2	0
oxygen	0
water	0

4 Click the **Mass fraction** button.

5 Click the **Next** button in the window toolbar.

SELECT PROPERTIES

1 Go to the **Select Properties** window.

2 In the list box, select **Diffusion coefficient at infinite dilution (m^2/s)**.

3 Click + **Add Selected**.

4 Find the **Select solvent** subsection. From the **Select solvent** list, choose **nitrogen**.

5 Click the **Next** button in the window toolbar.

DEFINE MATERIAL

1 Go to the **Define Material** window.

Add the material to the global **Materials** node. This is needed in order to use it in a **Porous Material** feature. Additionally, create interpolation functions for the material properties. This provides faster property evaluations.

2 From the **Component** list, choose **Global**.

3 From the **Function type** list, choose **Interpolation**.

4 In row **Temperature**, set **High** to 733.

5 Click the **Finish** button in the window toolbar.

GLOBAL DEFINITIONS

Gas: Nitrogen Solvent

1 In the **Model Builder** window, expand the **Global Definitions** > **Materials** node, then click **Gas: ammonia(0)-nitrogen(1)-nitrogen oxide(0)-NO2(0)-oxygen(0)-water(0) 1 (pp1mat1)**.

2 In the **Settings** window for **Material**, type `Gas: Nitrogen Solvent` in the **Label** text field.

Solid: Monolith Material

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

2 In the **Model Builder** window, expand the **Material 1 (mat1)** node, then click **Basic (def)**.

3 In the **Settings** window for **Basic**, locate the **Output Properties** section.

4 Click + **Select Quantity**.

5 In the **Physical Quantity** dialog, type `density` in the text field.

6 In the tree, select **General** > **Density (kg/m^3)**.

7 Click **OK**.

8 In the **Settings** window for **Basic**, locate the **Output Properties** section.

9 Click + **Select Quantity**.

10 In the **Physical Quantity** dialog, type `heatcapacity` in the text field.

11 In the tree, select **Transport** > **Heat capacity at constant pressure (J/(kg*K))**.

12 Click **OK**.

13 In the **Settings** window for **Basic**, locate the **Output Properties** section.

14 Click + **Select Quantity**.

15 In the **Physical Quantity** dialog, type `thermalconductivity` in the text field.

16 In the tree, select **Transport** > **Thermal conductivity (W/(m*K))**.

17 Click **OK**.

18 In the **Settings** window for **Basic**, locate the **Output Properties** section.

19 In the table, enter the following settings:

Property	Variable	Expression	Unit	Size
Density	rho	`2970[kg/m^3]`	kg/m³	1x1
Heat capacity at constant pressure	Cp	`975[J/kg/K]`	J/(kg·K)	1x1
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	`35[W/m/K]`	W/(m·K)	3x3

20 In the **Model Builder** window, right-click **Material 1 (mat1)** and choose **Rename**.

21 In the **Rename Material** dialog, type `Solid: Monolith Material` in the **New label** text field.

22 Click **OK**.

Now add a **Porous Material** node.

MATERIALS

Porous Material 1 (pmat1)

1 In the **Materials** toolbar, click **More Materials** and choose **Local** > **Porous Material**.

2 Select Domains 3, 5, and 14 only.

Fluid 1 (pmat1.fluid1)

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

Note that the global nitrogen material is used by this node.

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 From the **Material** list, choose **Solid: Monolith Material (mat1)**.

4 In the θ_s text field, type `1-por`.

Add a material for the metal parts of the reactor.

ADD MATERIAL FROM LIBRARY

In the **Home** toolbar, click **Windows** and choose **Add Material from Library**.

ADD MATERIAL

1 Go to the **Add Material** window.

2 In the tree, select **Built-in** > **Structural steel**.

3 Click the **Add to Component** button in the window toolbar.

MATERIALS

Structural steel (mat2)

1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

2 From the **Selection** list, choose **Metal Shell Domain**.

Add a material for the insulating air in the reactor wall.

ADD MATERIAL FROM LIBRARY

In the **Home** toolbar, click **Windows** and choose **Add Material from Library**.

ADD MATERIAL

1 Go to the **Add Material** window.

2 In the tree, select **Built-in** > **Air**.

3 Click the **Add to Component** button in the window toolbar.

4 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Air (mat3)

1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

2 From the **Selection** list, choose **Insulating Gas**.

Add a **Material Link** to the nitrogen gas to create a material for the free flowing gas between the two catalysts.

Free Flow Domain Material

1 In the **Model Builder** window, right-click **Materials** and choose **More Materials** > **Material Link**.

2 In the **Settings** window for **Material Link**, locate the **Geometric Entity Selection** section.

3 From the **Selection** list, choose **Free Flow Domain**.

4 In the **Label** text field, type `Free Flow Domain Material`.

Complete the settings for the two **Chemistry** interfaces by setting the concentration of nitrogen and coupling the ammonia slip catalyst chemistry to the mass transfer interface.

CHEMISTRY: SCR (CHEM)

1 In the **Model Builder** window, under **Monolith Reactor Model (comp2)** click **Chemistry: SCR (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)	From Thermodynamics
H2O	Variable	cH2O	Solved for	H2O
N2	Solvent	User defined	`cN2_in`	N2
NH3	Variable	cNH3	Solved for	H3N
NO	Variable	cNO	Solved for	NO

Species	Type	Molar concentration	Value (mol/m^3)	From Thermodynamics
NO2	Variable	cNO2	Solved for	NO2
O2	Variable	cO2	Solved for	O2

CHEMISTRY: ASC (CHEM2)

1 In the **Model Builder** window, under **Monolith Reactor Model (comp2)** click **Chemistry: ASC (chem2)**.

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

3 Find the **Bulk species** subsection. From the **Species solved for** list, choose **Transport of Diluted Species in Porous Media**.

4 In the table, enter the following settings:

Species	Type	Molar concentration	Value (mol/m^3)	From Thermodynamics
H2O	Variable	cH2O	Solved for	H2O
N2	Solvent	User defined	`cN2_in`	N2
NH3	Variable	cNH3	Solved for	H3N
NO	Variable	cNO	Solved for	NO
NO2	Variable	cNO2	Solved for	NO2
O2	Variable	cO2	Solved for	O2

Before setting up the heat, mass, and momentum physics, add selections that can be used for these physics interfaces.

GEOMETRY 1 (2DAXI)

Porous and Free Flow Domains

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

2 In the **Settings** window for **Union Selection**, type `Porous and Free Flow Domains` in the **Label** text field.

3 Locate the **Input Entities** section. Click **Add**.

4 In the **Add** dialog, in the **Selections to add** list, choose **SCR Catalyst**, **ASC Catalyst**, and **Free Flow Domain**.

5 Click **OK**.

Heat Transfer Domains

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

2 In the **Settings** window for **Union Selection**, type `Heat Transfer Domains` in the **Label** text field.

3 Locate the **Input Entities** section. Click **Add**.

4 In the **Add** dialog, in the **Selections to add** list, choose **SCR Catalyst**, **ASC Catalyst**, **Mat Domain**, **Metal Shell Domain**, **Free Flow Domain**, and **Insulating Gas**.

5 Click **OK**.

In the next stage of the modeling process you will set up the physics interfaces describing the mass transport, heat transfer, and fluid flow in the monolithic reactor.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

1 In the **Model Builder** window, under **Monolith Reactor Model (comp2)** click **Transport of Diluted Species in Porous Media (tds)**.

2 In the **Settings** window for **Transport of Diluted Species in Porous Media**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Porous and Free Flow Domains**.

Since we would like to model the gas as compressible, change to the conservative form of the mass balance equation.

4 Click the **Show More Options** button in the **Model Builder** toolbar.

5 In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics** > **Advanced Physics Options**.

6 Click **OK**.

7 In the **Settings** window for **Transport of Diluted Species in Porous Media**, click to expand the **Advanced Settings** section.

8 From the **Material balance form** list, choose **Conservative**.

Porous Medium 1

In the **Model Builder** window, expand the **Transport of Diluted Species in Porous Media (tds)** node.

Fluid 1

The mass transport model for the monolith channels assumes that there is only diffusive mass transport in the axial direction of the reactor, here along the z-axis. This can be accomplished by specifying the diffusivity only in the first element of the diagonal diffusion matrix. This may be difficult to converge though, and a more robust alternative is to set the radial diffusivity to a very low value.

1 In the **Model Builder** window, expand the **Porous Medium 1** node, then click **Fluid 1**.

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

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

4 From the **Fluid material** list, choose **Gas: Nitrogen Solvent (pp1mat1)**.

For each species, change from Isotropic to Diagonal, for the Fluid diffusion coefficient.

5 From the list, choose **Diagonal**.

6 Specify the $D_{\mathrm{F,cH2O}}$ matrix as

pp1mat1.df5.D11*0.0001	0
0	pp1mat1.df5.D11

7 From the list, choose **Diagonal**.

8 Specify the $D_{\mathrm{F,cNH3}}$ matrix as

pp1mat1.df1.D11*0.0001	0
0	pp1mat1.df1.D11

9 From the list, choose **Diagonal**.

10 Specify the $D_{\mathrm{F,cNO}}$ matrix as

pp1mat1.df2.D11*0.0001	0
0	pp1mat1.df2.D11

11 From the list, choose **Diagonal**.

12 Specify the $D_{\mathrm{F,cNO2}}$ matrix as

pp1mat1.df3.D11*0.0001	0
0	pp1mat1.df3.D11

13 From the list, choose **Diagonal**.

14 Specify the $D_{\mathrm{F,cO2}}$ matrix as

pp1mat1.df4.D11*0.0001	0
0	pp1mat1.df4.D11

The entered expressions were set up by the **Generate Material** wizard and they can be found under the **Global Definitions** > **Materials** > **Gas: Nitrogen (pp1mat1)** node. D11 represents the zz-component in the diffusivity matrix.

Porous Matrix 1

The porosity is by default defined by the **Porous Material** node.

This model is highly nonlinear due to the reaction kinetics. In this case, starting from a nonreacting system leads to a more robust simulation. To achieve this set the initial concentration to zero.

Initial Values 1

Features defining reaction rates and inlet concentrations have also been set up during the model generation procedure. Definitions correspond to the reactor conditions specified for the single channel model. Make sure that the **Inlet** and **Outlet** features are assigned to the proper domains and boundaries in the monolith reactor.

Reactions SCR

1. In the **Model Builder** window, under **Monolith Reactor Model (comp2)** > **Transport of Diluted Species in Porous Media (tds)** click **Reactions 1**.
2. In the **Settings** window for **Reactions**, type `Reactions SCR` in the **Label** text field.
3. Locate the **Domain Selection** section. From the **Selection** list, choose **SCR Catalyst**.

Reactions ASC

1. In the **Physics** toolbar, click **Domains** and choose **Reactions**.
2. In the **Settings** window for **Reactions**, type `Reactions ASC` in the **Label** text field.
3. Locate the **Domain Selection** section. From the **Selection** list, choose **ASC Catalyst**.
4. Locate the **Reaction Rates** section. From the **Chemistry** list, choose **Chemistry: ASC (chem2)**.
5. Click to expand the **Reacting Volume** section. From the list, choose **Pore volume**.
6. Drag and drop below **Reactions SCR**.

Inflow 1

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 **Flow Inlet**.
4. Locate the **Concentration** section. In the $c_{0,\mathrm{cH2O}}$ text field, type `cH2O_in`.
5. In the $c_{0,\mathrm{cNH3}}$ text field, type `cNH3_in`.
6. In the $c_{0,\mathrm{cNO}}$ text field, type `cNO_in`.
7. In the $c_{0,\mathrm{cNO2}}$ text field, type `cNO2_in`.
8. In the $c_{0,\mathrm{cO2}}$ text field, type `cO2_in`.

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 **Flow Outlet**.

Fluid 1

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

Next, add a **Fluid** feature to model the mass transfer in the free-flowing domain between the two catalysts. Use the diffusion coefficients defined by the nitrogen material.

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

3 From the **Selection** list, choose **Free Flow Domain**.

4 Locate the **Diffusion** section. From the **Material** list, choose **Gas: Nitrogen Solvent (pp1mat1)**.

5 From the D_{cH2O} list, choose **Diffusion coefficient, water in nitrogen (solvent) 5 (df5)**.

6 From the D_{cNH3} list, choose **Diffusion coefficient, ammonia in nitrogen (solvent) 1 (df1)**.

7 From the D_{cNO} list, choose **Diffusion coefficient, nitrogen oxide in nitrogen (solvent) 2 (df2)**.

8 From the D_{cNO2} list, choose **Diffusion coefficient, no2 in nitrogen (solvent) 3 (df3)**.

9 From the D_{cO2} list, choose **Diffusion coefficient, oxygen in nitrogen (solvent) 4 (df4)**.

Next, set up the **Heat Transfer in Porous Media** interface.

HEAT TRANSFER IN POROUS MEDIA (HT)

1 In the **Model Builder** window, under **Monolith Reactor Model (comp2)** click **Heat Transfer in Porous Media (ht)**.

2 In the **Settings** window for **Heat Transfer in Porous Media**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Heat Transfer Domains**.

Fluid 1

1 In the **Model Builder** window, expand the **Porous Medium 1** node, then click **Fluid 1**.

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

3 From the k_{f} list, choose **From material**.

4 Locate the **Thermodynamics, Fluid** section. From the ρ_{f} list, choose **From material**.

5 From the $C_{p,\mathrm{f}}$ list, choose **From material**.

6 From the γ list, choose **From material**.

Note that the fluid properties are defined by the corresponding node of the **Porous Material**.

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.

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

3 From the **Define** list, choose **Solid phase properties**.

4 Locate the **Heat Conduction, Porous Matrix** section. From the k_s list, choose **User defined**. From the list, choose **Diagonal**.

Specifying the diagonal thermal conductivity elements allows you to represent anisotropic conductive heat transfer in the monolith channels.

5 Specify the k_s matrix as

`ks_radial`	`0`
`0`	`ks_axial`

Note that apart from the conductivity, the matrix properties are defined by the **Solid** node added to the **Porous Material** feature.

Next, set up the **Heat Transfer** interface.

Initial Values 1

1 In the **Model Builder** window, under **Monolith Reactor Model (comp2)** > **Heat Transfer in Porous Media (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 `T_gas_in`.

Temperature 1

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

2 Select Boundary 18 only.

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 **Flow Outlet**.

Heat Source 1

Couple the **Heat Source** to the heat source defined by the **Transport of Diluted Species in Porous Media** interface. The heat source defined in this interface already accounts for the porosity and various chemical reactions on the different catalyst domains. For this coupling, it is important that the domain selections match.

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

2 In the **Settings** window for **Heat Source**, locate the **Material Type** section.

3 From the **Material type** list, choose **From material**.

4 Locate the **Domain Selection** section. From the **Selection** list, choose **Porous and Free Flow Domains**.

5 Locate the **Heat Source** section. From the Q_0 list, choose **Heat source (tds)**.

Continue by adding the features needed to describe the inflow boundary condition, the fluid domains, temperature boundary conditions, solid domains, porous domain, and the heat flux boundary conditions.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

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

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

4 Locate the **Upstream Properties** section. In the T_{ustr} text field, type `T_gas_in`.

Fluid 1

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

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

3 From the **Selection** list, choose **Free Flow Domain**.

4 Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Gas/Liquid**.

Fluid 2

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

2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

3 In the **Settings** window for **Fluid**, locate the **Domain Selection** section.

4 From the **Selection** list, choose **Insulating Gas**.

Next, add a temperature boundary condition at the metal wall of the reactor upstream of the SCR catalyst. We assume that the temperature is the same as that of the inlet gas.

Temperature 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Temperature**.

2 Select Boundaries 17, 48, and 51 only.

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

4 In the T_0 text field, type `T_gas_in`.

We also have to define the temperature for the reactor wall downstream of the ASC catalyst. We assume that the temperature is that of the gas exiting the ASC catalyst. Add a feature to derive the average temperature of the outlet gas, and assign it to the boundary.

DEFINITIONS (COMP2)

Average 1 (aveop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Average**.

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

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

4 Select Boundaries 6 and 45 only.

HEAT TRANSFER IN POROUS MEDIA (HT)

Temperature 3

1 In the **Physics** toolbar, click **Boundaries** and choose **Temperature**.

2 Select Boundaries 14, 16, 45, and 50 only.

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

4 In the T_0 text field, type `aveop1(T)`.

Add a **Solid** feature to describe the heat transfer in the metal shell.

Solid 1

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

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

3 From the **Selection** list, choose **Metal Shell Domain**.

Add a **Heat Flux** feature to describe the heat transfer from the reactor exterior surface to the surrounding air.

Heat Flux 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Heat Flux**.

2 Select Boundaries 31–34 and 70 only.

3 In the **Settings** window for **Heat Flux**, locate the **Material Type** section.

4 From the **Material type** list, choose **From material**.

5 Locate the **Heat Flux** section. From the **Flux type** list, choose **Convective heat flux**.

6 In the h text field, type `h_conv`.

7 In the T_{ext} text field, type `T_amb`.

Add another **Heat Flux** feature to describe the heat transfer from the reactor outlet surface to the surrounding air.

Heat Flux 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Heat Flux**.

2 Select Boundary 15 only.

3 In the **Settings** window for **Heat Flux**, locate the **Material Type** section.

4 From the **Material type** list, choose **Solid**.

5 Locate the **Heat Flux** section. From the **Flux type** list, choose **Convective heat flux**.

6 In the h text field, type `1[W/(m^2*K)]`.

7 In the T_{ext} text field, type `T_amb`.

The final feature that is needed to describe the heat transfer in the system is a **Porous Medium** feature for the supportive mat domain. The fluid in the mat is, for the simplicity of this example, assumed to be exhaust gas. This is a fair assumption, and this way we can take the fluid properties from the material.

Porous Medium 2

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

Fluid 1

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

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

3 From the γ list, choose **From material**.

Porous Medium 2

1 In the **Model Builder** window, click **Porous Medium 2**.

2 Select Domain 14 only.

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.

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

3 From the ε_p list, choose **User defined**. In the associated text field, type `0.5`.

4 Locate the **Heat Conduction, Porous Matrix** section. From the k_b list, choose **User defined**. In the associated text field, type `0.1`.

5 Locate the **Thermodynamics, Porous Matrix** section. From the ρ_b list, choose **User defined**. In the associated text field, type `0.63[g/cm^3]`.

6 From the $C_{p,b}$ list, choose **User defined**. In the associated text field, type `1.1[J/g/degC]`.

Having finished setting up the heat transfer physics, proceed to set up the **Laminar Flow** interface. Model the fluid as compressible, and assume that the flow is laminar both inside the channels and in the free-flow domain between the catalysts.

LAMINAR FLOW (SPF)

1 In the **Model Builder** window, under **Monolith Reactor Model (comp2)** click **Laminar Flow (spf)**.

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

3 From the **Selection** list, choose **Porous and Free Flow Domains**.

4 Locate the **Physical Model** section. From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

5 Select the **Enable porous media domains** checkbox.

Fluid Properties 1

1 In the **Model Builder** window, expand the **Laminar Flow (spf)** node, then click **Fluid Properties 1**.

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

3 From the μ list, choose **From material**.

Wall 1

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

2 In the **Settings** window for **Wall**, locate the **Boundary Condition** section.

3 From the **Wall condition** list, choose **Slip**.

Inlet 1

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

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

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

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

5 Locate the **Mass Flow** section. In the *m* text field, type `m_tot_in`.

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 **Flow Outlet**.

Porous Medium 1

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

2 Select Domains 3 and 5 only.

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.

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

3 From the κ list, choose **User defined**. From the list, choose **Diagonal**.

4 Specify the κ matrix as

`kappa_radial`	`0`
`0`	`kappa_axial`

This completes the setup of the model equations describing the reacting flow and heat transfer in the reactor. Before solving the problem, the geometry needs to be meshed.

MESH 1

Use a **Free Triangular** mesh for the supportive mat, the metal shell, and the insulating air, and use a mapped mesh for the monoliths. Finally, add a boundary layer mesh to the monoliths, the mat, and the free flow domain.

1 In the **Model Builder** window, under **Monolith Reactor Model (comp2)** click **Mesh 1**.

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

3 From the list, choose **User-controlled mesh**.

Size

1 In the **Model Builder** window, under **Monolith Reactor Model (comp2)** > **Mesh 1** click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Coarser**.

Size 1

1 In the **Mesh** toolbar, click **Sizing** and choose **Size**.

2 Drag and drop below **Size**.

3 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

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

5 Select Domain 4 only.

6 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

7 From the **Predefined** list, choose **Finer**.

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 From the **Selection** list, choose **ASC Catalyst**.

5 Click  **Clear Selection**.

6 Select Domains 3 and 5 only.

Distribution 1

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

2 Select Boundaries 6, 8, 10, 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 20.

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

Distribution 2

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

2 Select Boundaries 9 and 47 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 80.

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

7 Select the **Symmetric distribution** checkbox.

Distribution 3

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

2 Select Boundaries 5 and 44 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 20.

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

7 Select the **Symmetric distribution** checkbox.

Distribution 4

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

Size 1

1 In the **Model Builder** window, right-click **Free Triangular 1** and choose **Size**.

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

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

4 Select Domain 7 only.

Boundary Layers 1

1 In the **Mesh** toolbar, click **Boundary Layers**.

2 Drag and drop below **Boundary Layers 1**.

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

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

5 Select Domains 3–5 and 14 only.

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.

2 Select Boundaries 8, 10, 44, 46, and 47 only.

3 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.

4 In the **Number of layers** text field, type 6.

5 In the **Stretching factor** text field, type 1.3.

Boundary Layers 1

1 In the **Model Builder** window, click **Boundary Layers 1**.

2 Drag and drop below **Free Triangular 1**.

3 In the **Settings** window for **Boundary Layers**, click **Build All**.

Set up the study to solve for each of the engine load cases using a **Parametric Sweep** study step.

STUDY 5: MONOLITH REACTOR MODEL

1 In the **Model Builder** window, click **Study 5**.

2 In the **Settings** window for **Study**, type `Study 5: Monolith Reactor Model` in the **Label** text field.

Step 1: Stationary

1 In the **Model Builder** window, expand the **Study 5: Monolith Reactor Model** node, then click **Step 1: Stationary**.

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

3 In the **Solve for** column of the table, under **Monolith Reactor Model (comp2)**, clear the checkboxes for **Chemistry: SCR (chem)**, **Chemistry: ASC (chem2)**, **Transport of Diluted Species in Porous Media (tds)**, and **Heat Transfer in Porous Media (ht)**.

4 In the **Solve for** column of the table, under **Monolith Reactor Model (comp2)** > **Multiphysics**, clear the checkboxes for **Reacting Flow, Diluted Species 1 (rfd1)** and **Nonisothermal Flow 1 (nitf1)**.

5 Click to expand the **Study Extensions** section.

Step 2: Stationary 2

In the **Study** toolbar, click **Stationary**.

Parametric Sweep

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

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

3 From the **Sweep type** list, choose **Parameter switch**.

4 Click **Add**.

5 In the table, enter the following settings:

Switch	Cases	Case numbers
Cases	All	range(1,1,3)

6 In the **Model Builder** window, click **Study 5: Monolith Reactor Model**.

7 In the **Settings** window for **Study**, locate the **Study Settings** section.

8 Clear the **Generate default plots** checkbox.

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

The following steps generate Figure 3, Figure 4, and Figure 5. Using a **Result Template** is an efficient way to create plots. Add the template and then modify it if necessary.

RESULT TEMPLATES

1 In the **Results** toolbar, click **Result Templates** to open the **Result Templates** window.

2 Go to the **Result Templates** window.

3 In the tree, select **Study 5: Monolith Reactor Model/Solution 23 (12) (sol23)** > **Transport of Diluted Species in Porous Media** > **Plot array: Concentrations, H2O, NH3, NO, NO2 (tds)**.

4 Click the **Add Result Template** button in the window toolbar.

RESULTS

Nitrogen Species Molar Fractions

1 In the **Settings** window for **2D Plot Group**, type `Nitrogen Species Molar Fractions` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 5: Monolith Reactor Model/Parametric Solutions 5 (16) (sol25)**.

3 From the **Cases** list, choose **Low Load**.

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

5 Click to expand the **Plot Array** section. In the **Relative padding** text field, type `0.3`.

6 In the **Model Builder** window, expand the **Nitrogen Species Molar Fractions** node.

H2O, Surface, H2O, Total Flux, H2O, Total Flux, NH3, Total Flux, NO, Total Flux, NO2

1 In the **Model Builder** window, under **Results** > **Nitrogen Species Molar Fractions**, Ctrl-click to select **Surface, H2O**, **Total Flux, H2O**, **H2O**, **Total Flux, NH3**, **Total Flux, NO**, and **Total Flux, NO2**.

2 Right-click and choose **Delete**.

Surface, NH3 (SCR)

1 In the **Settings** window for **Surface**, type `Surface, NH3 (SCR)` in the **Label** text field.

2 Locate the **Expression** section. In the **Expression** text field, type `yNH3`.

3 From the **Unit** list, choose **ppm**.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Cynanthus**.

5 In the **Color legend title** text field, type `NH<sub>3</sub> (SCR)`.

6 From the **Color table type** list, choose **Discrete**.

7 In the **Number of bands** text field, type `20`.

Selection 1

1 Right-click **Surface, NH3 (SCR)** and choose **Selection**.

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

3 Select Domain 5 only.

Surface, NH3 (ASC)

1 Right-click **Surface, NH3 (SCR)** and choose **Duplicate**.

2 In the **Settings** window for **Surface**, type `Surface, NH3 (ASC)` in the **Label** text field.

3 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `NH<sub>3</sub> (ASC)`.

Selection 1

1 In the **Model Builder** window, expand the **Surface, NH3 (ASC)** node, then click **Selection 1**.

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

3 Click to select the  **Activate Selection** toggle button.

4 Select Domain 3 only.

Surface, NO (SCR)

1 In the **Model Builder** window, under **Results** > **Nitrogen Species Molar Fractions** click **Surface, NO**.

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

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

4 From the **Unit** list, choose **ppm**.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Baptisia**.

6 In the **Color legend title** text field, type `NO (SCR)`.

7 From the **Color table type** list, choose **Discrete**.

8 In the **Number of bands** text field, type `20`.

9 In the **Label** text field, type `Surface, NO (SCR)`.

Selection 1

1 Right-click **Surface, NO (SCR)** and choose **Selection**.

2 Select Domain 5 only.

Surface, NO (ASC)

1 Right-click **Surface, NO (SCR)** and choose **Duplicate**.

2 In the **Settings** window for **Surface**, type `Surface, NO (ASC)` in the **Label** text field.

3 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `NO (ASC)`.

Selection 1

1 In the **Model Builder** window, expand the **Surface, NO (ASC)** node, then click **Selection 1**.

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

3 Click to select the **Activate Selection** toggle button.

4 Select Domain 3 only.

Surface, NO2 (SCR)

1 In the **Model Builder** window, under **Results** > **Nitrogen Species Molar Fractions** click **Surface, NO2**.

2 In the **Settings** window for **Surface**, type `Surface, NO2 (SCR)` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `yNO2`.

4 From the **Unit** list, choose **ppm**.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Arctium**.

6 In the **Color legend title** text field, type `NO<sub>2</sub> (SCR)`.

7 From the **Color table type** list, choose **Discrete**.

8 In the **Number of bands** text field, type `20`.

Selection 1

1 Right-click **Surface, NO2 (SCR)** and choose **Selection**.

2 Select Domain 5 only.

Surface, NO2 (ASC)

1 Right-click **Surface, NO2 (SCR)** and choose **Duplicate**.

2 In the **Settings** window for **Surface**, type `Surface, NO2 (ASC)` in the **Label** text field.

3 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `NO<sub>2</sub> (ASC)`.

Surface, NH3 (ASC)

1 In the **Model Builder** window, expand the **Surface, NO2 (ASC)** node, then click **Surface, NH3 (ASC)**.

2 Drag and drop below **NH3**.

Surface, NO (ASC)

1 In the **Model Builder** window, click **Surface, NO (ASC)**.

2 Drag and drop below **NO**.

Nitrogen Species Molar Fractions

Optionally, edit the plot array indices to start from zero instead of from one.

Surface, NH3 (SCR)

1 In the **Model Builder** window, expand the **Results** > **Nitrogen Species Molar Fractions** node, then click **Surface, NH3 (SCR)**.

2 In the **Settings** window for **Surface**, click to expand the **Plot Array** section.

3 In the **Index** text field, type `0`.

Surface, NH3 (ASC)

1 In the **Model Builder** window, click **Surface, NH3 (ASC)**.

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

3 In the **Index** text field, type `0`.

Surface, NO (SCR)

1 In the **Model Builder** window, click **Surface, NO (SCR)**.

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

3 In the **Index** text field, type `1`.

Surface, NO (ASC)

1 In the **Model Builder** window, click **Surface, NO (ASC)**.

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

3 In the **Index** text field, type `1`.

Surface, NO2 (SCR)

1 In the **Model Builder** window, click **Surface, NO2 (SCR)**.

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

3 In the **Index** text field, type `2`.

Surface, NO2 (ASC)

1 In the **Model Builder** window, click **Surface, NO2 (ASC)**.

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

3 In the **Index** text field, type `2`.

NH3

1 In the **Model Builder** window, click **NH3**.

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

3 In the **Text** text field, type `NH$_3$`.

4 Select the **LaTeX markup** checkbox.

5 Click to expand the **Plot Array** section. In the **Index** text field, type `0`.

NO

1 In the **Model Builder** window, click **NO**.

2 In the **Settings** window for **Annotation**, locate the **Plot Array** section.

3 In the **Index** text field, type `1`.

NO2

1 In the **Model Builder** window, click **NO2**.

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

3 In the **Text** text field, type `NO$_2$`.

4 Select the **LaTeX markup** checkbox.

5 Locate the **Plot Array** section. In the **Index** text field, type `2`.

Selection 1

1 In the **Model Builder** window, under **Results** > **Nitrogen Species Molar Fractions** > **Surface, NO2 (ASC)** click **Selection 1**.

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

3 Click to select the **Activate Selection** toggle button.

4 Select Domain 3 only.

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

6 In the **Nitrogen Species Molar Fractions** toolbar, click **Plot**.

7 Click the **Show Grid** button in the **Graphics** toolbar.

Nitrogen Species Molar Fractions

Switch between the cases to see the different results.

1 In the **Model Builder** window, under **Results** click **Nitrogen Species Molar Fractions**.

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

3 From the **Cases** list, choose **Intermediate Load**.

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

5 In the **Nitrogen Species Molar Fractions** toolbar, click **Plot**.

6 From the **Cases** list, choose **High Load**.

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

8 In the **Nitrogen Species Molar Fractions** toolbar, click **Plot**.

The following steps generate Figure 6.

Drive Cases, ANR = 1.3, T, U, and dP

1 In the **Results** toolbar, click **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Drive Cases, ANR = 1.3, T, U, and dP` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 5: Monolith Reactor Model/ Parametric Solutions 5 (16) (sol25)**.

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

5 Locate the **Color Legend** section. Select the **Show titles** checkbox.

6 Select the **Show units** checkbox.

7 Click to expand the **Plot Array** section. From the **Array type** list, choose **Linear**.

Surface 1

In the **Results** toolbar, click **More Datasets** and choose **Surface**.

Drive Cases, ANR = 1.3, T, U, and dP

In the **Model Builder** window, under **Results** click **Drive Cases, ANR = 1.3, T, U, and dP**.

Velocity

1 In the **Drive Cases, ANR = 1.3, T, U, and dP** toolbar, click **Surface**.

2 In the **Settings** window for **Surface**, type `Velocity` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `spf.U`.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Metasepia**.

5 In the **Color legend title** text field, type `U`.

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

7 From the **Color table type** list, choose **Discrete**.

8 In the **Number of bands** text field, type `5`.

Drive Cases, ANR = 1.3, T, U, and dP

In the **Drive Cases, ANR = 1.3, T, U, and dP** toolbar, click **Annotation**.

U

1 In the **Settings** window for **Annotation**, type `U` in the **Label** text field.

2 Locate the **Annotation** section. In the **Text** text field, type `U`.

3 Locate the **Position** section. In the **z** text field, type `-0.21`.

4 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

5 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Drive Cases, ANR = 1.3, T, U, and dP

In the **Drive Cases, ANR = 1.3, T, U, and dP** toolbar, click **Surface**.

Pressure

1. In the **Settings** window for **Surface**, type `Pressure` in the **Label** text field.
2. Locate the **Expression** section. In the **Expression** text field, type `p`.
3. Locate the **Coloring and Style** section. From the **Color table** list, choose **Agama**.
4. In the **Color legend title** text field, type `dP`.
5. From the **Color table type** list, choose **Discrete**.

Drive Cases, ANR = 1.3, T, U, and dP

In the **Drive Cases, ANR = 1.3, T, U, and dP** toolbar, click **Annotation**.

dP

1. In the **Settings** window for **Annotation**, type `dP` in the **Label** text field.
2. Locate the **Annotation** section. In the **Text** text field, type `dP`.
3. Locate the **Position** section. In the **z** text field, type `-0.21`.
4. Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
5. Locate the **Plot Array** section. Select the **Manual indexing** checkbox.
6. In the **Index** text field, type `1`.

Drive Cases, ANR = 1.3, T, U, and dP

In the **Drive Cases, ANR = 1.3, T, U, and dP** toolbar, click **Surface**.

Temperature

1. In the **Settings** window for **Surface**, type `Temperature` in the **Label** text field.
2. Locate the **Expression** section. In the **Expression** text field, type `T`.
3. From the **Unit** list, choose **°C**.
4. Locate the **Coloring and Style** section. From the **Color table** list, choose **Plasma**.
5. In the **Color legend title** text field, type `T`.
6. From the **Color table type** list, choose **Discrete**.

Selection 1

1. In the **Drive Cases, ANR = 1.3, T, U, and dP** toolbar, click **Selection**.
2. In the **Settings** window for **Selection**, locate the **Selection** section.
3. From the **Selection** list, choose **Porous and Free Flow Domains**.

Drive Cases, ANR = 1.3, T, U, and dP

In the **Drive Cases, ANR = 1.3, T, U, and dP** toolbar, click **Annotation**.

T

1. In the **Settings** window for **Annotation**, type `T` in the **Label** text field.
2. Locate the **Annotation** section. In the **Text** text field, type `T`.
3. Locate the **Position** section. In the **z** text field, type `-0.21`.
4. Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
5. Locate the **Plot Array** section. Select the **Manual indexing** checkbox.
6. In the **Index** text field, type `2`.
7. Click the **Zoom Extents** button in the **Graphics** toolbar.
8. In the **Drive Cases, ANR = 1.3, T, U, and dP** toolbar, click **Plot**.

The following steps generate Figure 7.

Conversions, NH3 and NOx

1. In the **Results** toolbar, click **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Conversions, NH3 and NOx` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 5: Monolith Reactor Model/ Parametric Solutions 5 (16) (sol25)**.
4. Click to expand the **Title** section. From the **Title type** list, choose **None**.
5. Locate the **Plot Settings** section.
6. Select the **y-axis label** checkbox. In the associated text field, type `Conversion`.

NH3 center

1. In the **Conversions, NH3 and NOx** toolbar, click **Line Graph**.
2. In the **Settings** window for **Line Graph**, type `NH3 center` in the **Label** text field.
3. Select Boundaries 5, 7, and 9 only.
4. Locate the **y-Axis Data** section. In the **Expression** text field, type `X_NH3`.
5. Select the **Description** checkbox. In the associated text field, type `Conversion`.
6. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
7. In the **Expression** text field, type `(0.4-z)*pi*d_cat^2/4`.
8. Select the **Description** checkbox. In the associated text field, type `Volume`.
9. Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle**.

10 From the **Color** list, choose **Blue**.

11 From the **Width** list, choose **2**.

12 Click to expand the **Legends** section. Select the **Show legends** checkbox.

13 Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `NH<sub>3</sub> center, `.

NOx center

1 Right-click **NH3 center** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type `NOx center` in the **Label** text field.

3 Select Boundaries 5, 7, and 9 only.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `X_NOx`.

5 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle (reset)**.

6 From the **Color** list, choose **Magenta**.

7 Locate the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `NOx center, `.

NH3 center, NOx center

1 In the **Model Builder** window, under **Results** > **Conversions, NH3 and NOx**, Ctrl-click to select **NH3 center** and **NOx center**.

2 Right-click and choose **Duplicate**.

NH3 edge

1 In the **Settings** window for **Line Graph**, type `NH3 edge` in the **Label** text field.

2 Locate the **Selection** section. Click  **Clear Selection**.

3 Select Boundaries 44, 46, and 47 only.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle (reset)**.

5 From the **Color** list, choose **Black**.

6 Locate the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `NH<sub>3</sub> edge, `.

NOx edge

1 In the **Model Builder** window, under **Results** > **Conversions, NH3 and NOx** click **NOx center 1**.

2 In the **Settings** window for **Line Graph**, type `NOx edge` in the **Label** text field.

3 Locate the **Selection** section. Click **Clear Selection**.

4 Select Boundaries 44, 46, and 47 only.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Red**.

6 Locate the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `NOx edge,` .

Conversions, NH3 and NOx

1 In the **Model Builder** window, click **Conversions, NH3 and NOx**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Window Settings** section.

3 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

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

5 In the **Conversions, NH3 and NOx** toolbar, click **Plot**.

The following steps generate Figure 8.

Temperature Difference Along Reactor Axis

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

2 In the **Settings** window for **1D Plot Group**, type `Temperature Difference Along Reactor Axis` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 5: Monolith Reactor Model/ Parametric Solutions 5 (16) (sol25)**.

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

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** checkbox. In the associated text field, type `Bed position along reactor axis (m)`.

7 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

Temperature At Reactor Center

1 Right-click **Temperature Difference Along Reactor Axis** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Temperature At Reactor Center` in the **Label** text field.

3 Select Boundaries 5, 7, and 9 only.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `T-T_gas_in`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Reversed arc length**.

6 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

7 Locate the **Legends** section. Select the **Show legends** checkbox.

8 Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `T center, `.

Temperature At Bed Edge

1 Right-click **Temperature At Reactor Center** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type `Temperature At Bed Edge` in the **Label** text field.

3 Locate the **Selection** section. Click  **Clear Selection**.

4 Select Boundaries 44, 46, and 47 only.

5 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

6 From the **Color** list, choose **Cycle (reset)**.

7 From the **Width** list, choose **2**.

8 Locate the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `T edge, `.

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

10 In the **Temperature Difference Along Reactor Axis** toolbar, click  **Plot**.

As a final evaluation, derive the average molar fraction of NH_3 and NOx out from the first bed, as well as out from the reactor.

Line Average SCR Outlet

1 In the **Results** toolbar, click  **More Derived Values** and choose **Average** > **Line Average**.

2 In the **Settings** window for **Line Average**, type `Line Average SCR Outlet` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 5: Monolith Reactor Model/ Parametric Solutions 5 (16) (sol25)**.

4 Select Boundary 10 only.

5 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
yNH3	ppm	Molar Fraction NH3
yNOx	ppm	Molar Fraction NOx

6 Click next to  **Evaluate**, then choose **New Table**.

Line Average Reactor Outlet

1 Right-click **Line Average SCR Outlet** and choose **Duplicate**.

2 In the **Settings** window for **Line Average**, type `Line Average Reactor Outlet` in the **Label** text field.

3 Select Boundary 6 only.

4 Click ▼ next to **Evaluate**, then choose **New Table**.

The following steps generate the thumbnail for this model.

Concentration and Temperature Profiles

1 In the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Concentration and Temperature Profiles` in the **Label** text field.

Revolution 2D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Revolution 2D**.

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

3 From the **Dataset** list, choose **Study 5: Monolith Reactor Model/ Parametric Solutions 5 (16) (sol25)**.

4 Click to expand the **Revolution Layers** section. In the **Start angle** text field, type `-90`.

5 In the **Revolution angle** text field, type `200`.

Concentration and Temperature Profiles

1 In the **Model Builder** window, under **Results** click **Concentration and Temperature Profiles**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Revolution 2D 1**.

4 From the **Cases** list, choose **Low Load**.

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

6 Locate the **Plot Settings** section. From the **View** list, choose **View 3D 4**.

7 Clear the **Plot dataset edges** checkbox.

8 Locate the **Color Legend** section. Clear the **Show legends** checkbox.

Surface 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Surface**.

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

3 In the **Expression** text field, type `1`.

Selection 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Selection**.

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

3 From the **Selection** list, choose **Metal Shell Domain**.

Surface 1

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

Material Appearance 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Material Appearance**.

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

3 From the **Appearance** list, choose **Custom**.

4 From the **Material type** list, choose **Tungsten**.

Concentration and Temperature Profiles

In the **Concentration and Temperature Profiles** toolbar, click **Surface**.

Surface 2

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

2 In the **Expression** text field, type `T`.

3 Locate the **Coloring and Style** section. From the **Color table** list, choose **HeatCameraLight**.

Selection 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Selection**.

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

3 From the **Selection** list, choose **Insulating Gas**.

Surface 2

In the **Model Builder** window, click **Surface 2**.

Material Appearance 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Material Appearance**.

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

3 From the **Material** list, choose **Air (mat3)**.

4 Locate the **Color** section. Select the **Use the plot's color** checkbox.

Concentration and Temperature Profiles

In the **Concentration and Temperature Profiles** toolbar, click **Surface**.

Surface 3

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

2 In the **Expression** text field, type `T`.

3 Locate the **Coloring and Style** section. From the **Color table** list, choose **HeatCameraLight**.

Selection 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Selection**.

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

3 From the **Selection** list, choose **Mat Domain**.

Surface 3

In the **Model Builder** window, click **Surface 3**.

Material Appearance 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Material Appearance**.

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

3 From the **Appearance** list, choose **Custom**.

4 From the **Material type** list, choose **Rock**.

5 Locate the **Color** section. Select the **Use the plot's color** checkbox.

Concentration and Temperature Profiles

In the **Concentration and Temperature Profiles** toolbar, click **Surface**.

Surface 4

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

2 In the **Expression** text field, type `cNO+cNO2`.

3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Cerinthe**.

Selection 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Selection**.

2 Select Domains 3 and 5 only.

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

4 Clear the **Evaluate the end cap** checkbox.

Surface 4

In the **Model Builder** window, click **Surface 4**.

Material Appearance 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Material Appearance**.

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

3 From the **Appearance** list, choose **Custom**.

4 From the **Material type** list, choose **Rock**.

5 Locate the **Color** section. Select the **Use the plot's color** checkbox.

Contour 1

1 In the **Model Builder** window, right-click **Concentration and Temperature Profiles** and choose **Contour**.

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

3 In the **Expression** text field, type `cNO+cNO2`.

4 Locate the **Levels** section. In the **Total levels** text field, type `15`.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prionace**.

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

Selection 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Selection**.

2 Select Domain 5 only.

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

4 Clear the **Evaluate the mantle** checkbox.

Concentration and Temperature Profiles

In the **Concentration and Temperature Profiles** toolbar, click **Surface**.

Surface 5

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

2 In the **Expression** text field, type `1`.

Selection 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Selection**.

2 Select Domains 3 and 5 only.

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

4 Clear the **Evaluate the end cap** checkbox.

5 Clear the **Evaluate the start cap** checkbox.

Surface 5

In the **Model Builder** window, click **Surface 5**.

Material Appearance 1

1 In the **Concentration and Temperature Profiles** toolbar, click **Material Appearance**.

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

3 From the **Appearance** list, choose **Custom**.

4 From the **Material type** list, choose **Custom**.

5 Click **Define custom colors**.

6 Set the RGB values to 250, 240, and 230, respectively.

7 Click **Add to custom colors**.

8 Click **Show color palette only** or **OK** on the cross-platform desktop.

9 From the **Diffuse color** list, choose **Custom**.

10 Click **Define custom colors**.

11 Set the RGB values to 189, 201, and 216, respectively.

12 Click **Add to custom colors**.

13 Click **Show color palette only** or **OK** on the cross-platform desktop.

14 From the **Edit** menu, choose **Undo Material Appearance 1: Custom Color**.

15 From the **Ambient color** list, choose **Custom**.

16 Click **Define custom colors**.

17 Set the RGB values to 230, 225, and 204, respectively.

18 Click **Add to custom colors**.

19 Click **Show color palette only** or **OK** on the cross-platform desktop.

20 Select the **Custom basis for brush lines** checkbox.

21 In the **Scale** text field, type 2.

22 In the **Origin** text field, type 1.

23 Select the **Specify ym-axis** checkbox.

24 Select the **Normal mapping** checkbox.

25 From the **Noise type** list, choose **Simplex noise**.

26 In the **Normal vector noise scale** text field, type 50.

27 In the **Normal vector noise frequency** text field, type 50.

28 From the **Brush lines** list, choose **Brush lines orthogonal to xm-axis**.

29 In the **Surface roughness** text field, type 1.

30 In the **Diffuse wrap** text field, type 0.

31 In the **Reflectance** text field, type 0.05.

Surface 6

1 Right-click **Surface 5** and choose **Duplicate**.

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

3 In the **Expression** text field, type `cNH3`.

Selection 1

1 In the **Model Builder** window, expand the **Surface 6** node, then click **Selection 1**.

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

3 Clear the **Evaluate the mantle** checkbox.

4 Select the **Evaluate the end cap** checkbox.

Material Appearance 1

1 In the **Model Builder** window, click **Material Appearance 1**.

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

3 Select the **Use the plot's color** checkbox.

Surface 6

1 In the **Model Builder** window, click **Surface 6**.

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

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

4 In the **Concentration and Temperature Profiles** toolbar, click  **Plot**.

Add the result plots from Study 5 in a group.

Concentration and Temperature Profiles, Conversions, NH3 and NOx, Drive Cases, ANR = 1.3, T, U, and dP, Nitrogen Species Molar Fractions, Temperature Difference Along Reactor Axis

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Nitrogen Species Molar Fractions**, **Drive Cases, ANR = 1.3, T, U, and dP**, **Conversions, NH3 and NOx**, **Temperature Difference Along Reactor Axis**, and **Concentration and Temperature Profiles**.

2 Right-click and choose **Group**.

Monolith Reactor Model

In the **Settings** window for **Group**, type `Monolith Reactor Model` in the **Label** text field.

Appendix — Geometry Modeling Instructions

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

NEW

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

GLOBAL DEFINITIONS

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 `monolith_reactor_geometry_parameters.txt`.

ADD COMPONENT

In the **Home** toolbar, click **Add Component** and choose **2D Axisymmetric**.

GEOMETRY 1

SCR (selective catalytic reduction) monolith

1. In the **Geometry** toolbar, click **Rectangle**.
2. In the **Settings** window for **Rectangle**, type `SCR (selective catalytic reduction) monolith` in the **Label** text field.
3. Locate the **Size and Shape** section. In the **Width** text field, type `d_cat/2`.
4. In the **Height** text field, type `l_SCR`.
5. Click to expand the **Layers** section.

Mat

1. In the **Geometry** toolbar, click **Rectangle**.
2. In the **Settings** window for **Rectangle**, type `Mat` in the **Label** text field.
3. Locate the **Size and Shape** section. In the **Width** text field, type `matThickness+shellThickness`.
4. In the **Height** text field, type `l_SCR+freeFlowHeight+l_ASC`.
5. Locate the **Position** section. In the **r** text field, type `d_cat/2`.
6. In the **z** text field, type `-freeFlowHeight-l_ASC`.
7. Locate the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	shellThickness

8 Select the **Layers to the right** checkbox.

9 Clear the **Layers on bottom** checkbox.

Free Flow

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

2 In the **Settings** window for **Rectangle**, type `Free Flow` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `d_cat/2+ shellThickness-shellThickness`.

4 In the **Height** text field, type `freeFlowHeight`.

5 Locate the **Position** section. In the **z** text field, type `-0.02`.

ASC (ammonia slip catalyst)

1 Right-click **Free Flow** and choose **Duplicate**.

2 In the **Settings** window for **Rectangle**, type `ASC (ammonia slip catalyst)` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `d_cat/2`.

4 In the **Height** text field, type `l_ASC`.

5 Locate the **Position** section. In the **z** text field, type `-freeFlowHeight-l_ASC`.

Thicken 1 (thi1)

1 In the **Geometry** toolbar, click **Conversions** and choose **Thicken**.

2 In the **Settings** window for **Thicken**, locate the **Input** section.

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

4 On the object **r2**, select Boundary 7 only.

5 Select the **Keep input objects** checkbox.

6 Locate the **Options** section. From the **Offset** list, choose **Asymmetric**.

7 In the **Upside thickness** text field, type `shellThickness`.

8 From the **Convex corner handling** list, choose **Tangent lines**.

Union 1 (uni1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

2 Select the object **thi1** only.

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

4 Click the **Remove from Selection** button for **Input objects**.

5 Clear the **Keep interior boundaries** checkbox.

Gas Box

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

2 In the **Settings** window for **Rectangle**, type `Gas Box` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `boxThickness`.

4 In the **Height** text field, type `l_ASC+freeFlowHeight+l_SCR`.

5 Locate the **Position** section. In the **r** text field, type `d_cat/2+matThickness+shellThickness+shellThickness`.

6 In the **z** text field, type `-l_ASC-freeFlowHeight`.

7 Locate the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	shellThickness

8 Select the **Layers to the right** checkbox.

9 Select the **Layers on top** checkbox.

Inlet

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

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

3 Locate the **Size and Shape** section. In the **Width** text field, type `inletInnerD`.

4 In the **Height** text field, type `inletHeight`.

5 Locate the **Position** section. In the **z** text field, type `l_SCR+inletHeight*2`.

Inlet Box

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

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

3 Locate the **Size and Shape** section. In the **Width** text field, type `boxThickness`.

4 In the **Height** text field, type `inletHeight`.

5 Locate the **Position** section. In the **r** text field, type `inletInnerD`.

6 In the **z** text field, type `l_SCR+inletHeight*2`.

7 Locate the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	shellThickness

8 Select the **Layers to the left** checkbox.

9 Select the **Layers to the right** checkbox.

10 Select the **Layers on top** checkbox.

Help Rectangle Top

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

2 In the **Settings** window for **Rectangle**, type `Help Rectangle Top` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `totalWidth-inletInnerD`.

4 In the **Height** text field, type `inletHeight*2`.

5 Locate the **Position** section. In the **r** text field, type `inletInnerD`.

6 In the **z** text field, type `l_SCR`.

7 Locate the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	shellThickness

8 Select the **Layers to the left** checkbox.

9 Select the **Layers to the right** checkbox.

10 Clear the **Layers on bottom** checkbox.

11 Select the **Layers on top** checkbox.

Help Rectangle Horizontal Small Top

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

2 In the **Settings** window for **Rectangle**, type `Help Rectangle Horizontal Small Top` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `totalWidth - inletInnerD`.

4 In the **Height** text field, type `boxThickness`.

5 Locate the **Position** section. In the **r** text field, type `inletInnerD`.

6 In the **z** text field, type `l_SCR+inletHeight*2-boxThickness`.

7 Locate the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	shellThickness

Help Rectangle Vertical Top

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

2 In the **Settings** window for **Rectangle**, type `Help Rectangle Vertical Top` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `boxThickness+shellThickness`.

4 In the **Height** text field, type `inletHeight*2`.

5 Locate the **Position** section. In the **r** text field, type `d_cat/2+matThickness+shellThickness`.

6 In the **z** text field, type `l_SCR`.

7 Locate the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	shellThickness

8 Select the **Layers to the left** checkbox.

9 Select the **Layers to the right** checkbox.

10 Clear the **Layers on bottom** checkbox.

Quadratic Bézier 1 (qb1)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Quadratic Bézier**.

2 In the **Settings** window for **Quadratic Bézier**, locate the **Control Points** section.

3 In row **1**, set **r** to `0.14`.

4 In row **1**, set **z** to `0.462`.

5 In row **2**, set **r** to `0.174651`.

6 In row **2**, set **z** to `0.462`.

7 In row **3**, set **r** to `0.1746619234313964`.

8 In row **3**, set **z** to `0.4301309883594513`.

Quadratic Bézier 2 (qb2)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Quadratic Bézier**.

2 In the **Settings** window for **Quadratic Bézier**, locate the **Control Points** section.

3 In row **1**, set **r** to `0.14`.

4 In row **1**, set **z** to `0.463651`.

5 In row **2**, set **r** to `0.176302`.

6 In row **2**, set **z** to `0.463651`.

7 In row **3**, set **r** to `0.17631292343140004`.

8 In row **3**, set **z** to `0.4301309883594513`.

Quadratic Bézier 3 (qb3)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Quadratic Bézier**.

2 In the **Settings** window for **Quadratic Bézier**, locate the **Control Points** section.

3 In row **1**, set **r** to `0.14`.

4 In row **1**, set **z** to `0.484349`.

5 In row **2**, set **r** to `0.198651`.

6 In row **2**, set **z** to `0.48448984122275995`.

7 In row **3**, set **r** to `0.198651`.

8 In row **3**, set **z** to `0.4301309883594513`.

Quadratic Bézier 4 (qb4)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Quadratic Bézier**.

2 In the **Settings** window for **Quadratic Bézier**, locate the **Control Points** section.

3 In row **1**, set **r** to `0.14`.

4 In row **1**, set **z** to `0.486`.

5 In row **2**, set **r** to `0.200302`.

6 In row **2**, set **z** to `0.48614084122275997`.

7 In row **3**, set **r** to `0.200302`.

8 In row **3**, set **z** to `0.4301309883594513`.

Quadratic Bézier 5 (qb5)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Quadratic Bézier**.

2 In the **Settings** window for **Quadratic Bézier**, locate the **Control Points** section.

3 In row **1**, set **r** to `0.062738`.

4 In row **1**, set **z** to `0.48`.

5 In row **2**, set **r** to `0.062738`.

6 In row **2**, set **z** to `0.463651`.

7 In row **3**, set **r** to `0.08`.

8 In row **3**, set **z** to `0.463651`.

Quadratic Bézier 6 (qb6)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Quadratic Bézier**.

2 In the **Settings** window for **Quadratic Bézier**, locate the **Control Points** section.

3 In row **1**, set **r** to `0.061087`.

4 In row **1**, set **z** to `0.48`.

5 In row **2**, set **r** to `0.061087`.

6 In row **2**, set **z** to `0.462`.

7 In row **3**, set **r** to `0.08`.

8 In row **3**, set **z** to `0.462`.

Mirror 1 (mir1)

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

2 In the **Settings** window for **Mirror**, locate the **Input** section.

3 Select the **Keep input objects** checkbox.

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

5 In the **Graphics** window toolbar, click next to **Select Objects**, then choose **Select Objects**.

6 Select the objects **qb1**, **qb2**, **qb3**, **qb4**, **qb5**, **qb6**, **r10**, **r6**, **r7**, **r8**, and **r9** only.

7 In the list box, select **r6**.

8 Locate the **Line of Reflection** section. From the **Specify** list, choose **Edge**.

9 On the object **r8**, select Boundary 7 only.

10 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

Move 1 (mov1)

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

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

3 From the **Input objects** list, choose **Mirror 1**.

4 Locate the **Displacement** section. From the **Specify** list, choose **Positions**.

5 Click to select the **Activate Selection** toggle button for **Vertex to move**.

6 On the object **mir1(10)**, select Point 10 only.

7 Click to select the **Activate Selection** toggle button for **Vertices to move to**.

8 On the object **r5**, select Point 9 only.

Rectangle 11 (r11)

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 `totalWidth`.

4 In the **Height** text field, type `l_SCR+inletHeight*2+freeFlowHeight+l_ASC+inletHeight*2`.

5 Locate the **Position** section. In the **z** text field, type `-freeFlowHeight-l_ASC-inletHeight*2`.

Shell Support Top

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

2 In the **Settings** window for **Rectangle**, type `Shell Support Top` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `shellThickness`.

4 In the **Height** text field, type `boxThickness`.

5 Locate the **Position** section. In the **r** text field, type `0.108`.

6 In the **z** text field, type `0.462`.

Shell Support Bottom

1 Right-click **Shell Support Top** and choose **Duplicate**.

2 In the **Settings** window for **Rectangle**, type `Shell Support Bottom` in the **Label** text field.

3 Locate the **Position** section. In the **z** text field, type `-0.166`.

Shell Support Side Top

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

2 In the **Settings** window for **Rectangle**, type `Shell Support Side Top` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `boxThickness`.

4 In the **Height** text field, type `shellThickness`.

5 Locate the **Position** section. In the **r** text field, type `0.1763`.

6 In the **z** text field, type `0.3`.

Shell Support Side Bottom

1 Right-click **Shell Support Side Top** and choose **Duplicate**.

2 In the **Settings** window for **Rectangle**, type `Shell Support Side Bottom` in the **Label** text field.

3 Locate the **Position** section. In the **r** text field, type `0.17465`.

4 In the **z** text field, type `0.1`.

Partition Edges 1 (pare1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Partition Edges**.

2 On the object **r5**, select Boundary 10 only.

3 In the **Settings** window for **Partition Edges**, locate the **Positions** section.

4 From the **Type of specification** list, choose **Vertex projection**.

5 On the object **r15**, select Points 2 and 3 only.

Ignore Edges 1 (ige1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Ignore Edges**.

2 On the object **fin**, select Boundaries 14, 19, 21, 23, 25–30, 32, 34–37, 40, 42, 44, 46, 48, 53, 54, 58–63, 65, 67–71, 73, 78, 79, 82, 83, 88, 91, 93, 94, 96, 98–100, 110, 113–115, 117, 120–122, 124, 128, 131, 135, 138–141, 143–150, 159–169, 172, 174, 175, 177, 179–191, 194–203, 205, 209, 213, 217, 221–247, 249, 250, 252–254, 256, 257, 259–261, 263–277, 283–286, 313, 314, 320, and 321 only.

SCR Catalyst

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

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

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

4 On the object **ige1**, select Domain 5 only.

ASC Catalyst

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

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

3 On the object **ige1**, select Domain 3 only.

Mat Domain

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

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

3 On the object **ige1**, select Domain 14 only.

Metal Shell Domain

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

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

3 On the object **ige1**, select Domains 7 and 15 only.

Flow Inlet

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

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

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

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

5 On the object **ige1**, select Boundary 12 only.

Flow Outlet

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

2 In the **Settings** window for **Explicit Selection**, type `Flow 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 **ige1**, select Boundary 6 only.

Free Flow Domain

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

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

3 On the object **ige1**, select Domain 4 only.

Insulating Gas

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

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

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

4 On the object **ige1**, select Domains 8–13 and 16–18 only.