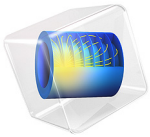

NOx Reduction in a Monolithic Reactor

Introduction

This example illustrates the detailed process modeling of selective catalytic reduction of NO with NH_3, that occurs as flue gases pass through the channels of a monolithic reactor in the exhaust system of a diesel car. The optimal dosing of NH_3 to minimize the NO emission, as found in Analysis of NOx Reaction Kinetics, is utilized.

Figure 1: Catalytic converters reduce the NOx levels in the exhaust gases emitted by combustion engines.

This application is set up in 3D to unravel the full space-dependency of the system.

Model Definition

The single channel model in Analysis of NOx Reaction Kinetics 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 a full reactor monolith, a full 3D reactor model is called for.

MODEL GEOMETRY

The monolithic reactor has a modular structure made up of reactive channel blocks and supporting solid walls. The reactor is 0.36 m long with a 0.1 m radius. Each reactive

channel has a cross-sectional area of 12.6 mm^2, and the void fraction of a channel block is 0.75.

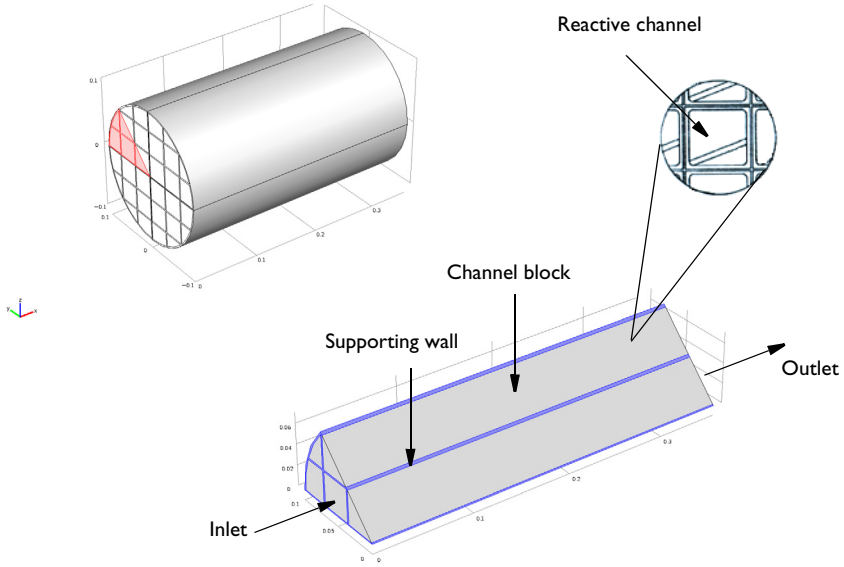

Figure 2: NO reduction chemistry takes place in the channel blocks. Supporting walls hold together the full reactor geometry. Symmetry reduces the modeling domain to one eighth of the full reactor geometry.

MODEL EQUATIONS

The present example takes a pseudo-homogeneous approach to model the hundreds 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 channels, such that the average flow field is proportional to the pressure difference across the reactor. 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 really connects the channels in the reactor structure, turning this into a 3D model.

Mass Transport

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

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

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 x-axis in the 3D geometry used in this example. For the diffusive transport, this is accomplished by setting the y- and z-components of the diffusivity matrix to zero. The pressure-driven flow in the monolith is also defined in the direction of the x-axis, hereby restricting the convective mass transport to the channel direction as well. 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 flow of reacting gas through the monolith is modeled using a Darcy's Law interface with the governing equations:

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

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

The monolith block is treated as a porous matrix with the effective permeability κ (SI unit: m^2). Similarly to the diffusivity, the y- and z-components of the permeability matrix are set to zero. 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 NO and NH_3 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·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, which in this model is calculated in the Darcy's Law interface. Q (SI unit: W/m^3) is the heat source, which is due to exothermic chemical reactions:

$$Q = Q_1 + Q_2 = -r_1 H_1 - r_2 H_2$$

Above, H_1 and H_2 (SI unit: J/(mol·K)) are the heats of 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 supporting walls in the reactor, only heat transfer by conduction applies:

$$-\nabla \cdot (k_s \nabla T) = 0$$

where k_s (SI unit: W/(m·K)) is the thermal conductivity for the solid walls.

The temperature is specified at the reactor inlet walls boundary:

$$T = T_0,$$

and the Inflow condition, i.e.

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

is used at the inlet of the geometry. ΔH (SI unit: J/(kg)) is the sensible enthalpy.

At the outlet, use the Outflow condition:

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

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

$$\mathbf{q}_{\mathrm{m}} \cdot \mathbf{n} = h(T - T_{\mathrm{amb}})$$

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 the 3D 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 the 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

Figure 3 shows the conversion of NO in the monolith channel blocks. The isosurfaces in the plot show how a channel's performance depends on its position in the reactor, clearly pointing to the 3D nature of the problem.

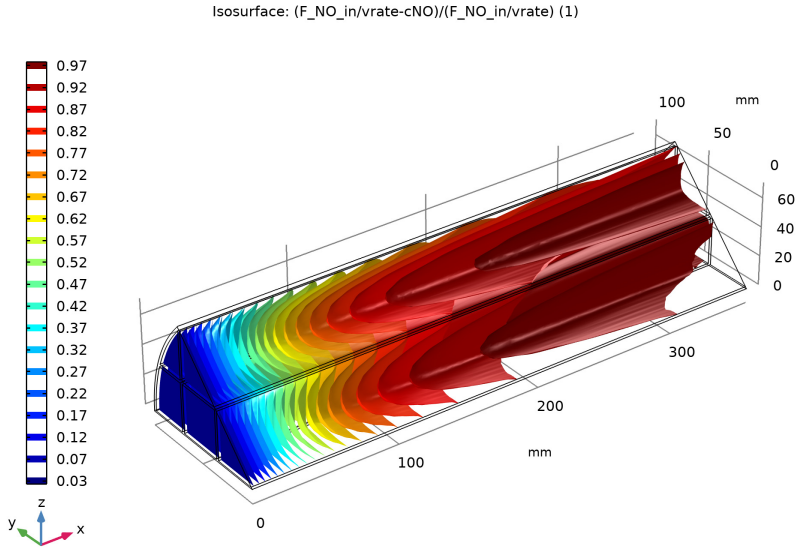

Figure 3: Isosurfaces showing the conversion of NO in the reactor. Fluid flow from left to right.

The average conversion at the outlet is 97% (not seen in Figure 3, see Modeling Instructions, Surface Average, page 25). This is somewhat lower than the 99% conversion predicted by the single channel model (see results from Analysis of NOx Reaction Kinetics).

The individual channels, although they do not exchange mass, are connected through the temperature distribution in the reactor. The temperature affects both the flow velocity of

the reacting gas as well as the reaction rates. Cross sections of the reactor temperature are shown in Figure 4.

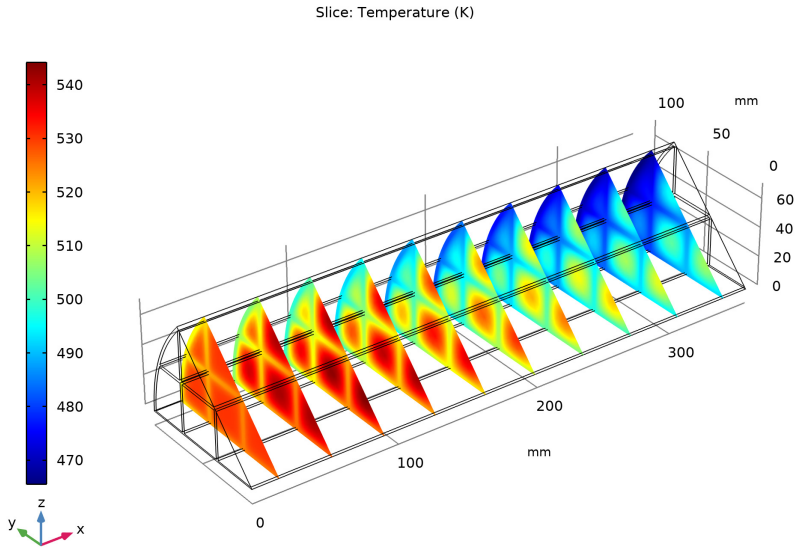

Figure 4: Temperature distribution in cross sections of the reactor. Fluid flow from left to right.

The exothermic reactions increase the temperature in the central parts of the reactor, while the temperature in the outer parts is decreased through heat loss to the surroundings. The maximum temperature calculated for the 3D reactor is 544 K (see Modeling Instructions, Volume Maximum, page 25), which is about 10 K higher than for the single channel model. The effect of the relatively high thermal conductivity of the supporting walls is clearly visible.

A seen from the initial kinetic analysis in Analysis of NOx Reaction Kinetics, elevated temperatures have a detrimental effect on the selectivity, leading to ammonia getting oxidized rather than to be consumed in the desired NO reducing reaction. The connection

between temperature and selectivity is clearly seen in the final plot in Figure 5, where both S and T are shown. Here, symmetry is used to visualize the full monolithic structure.

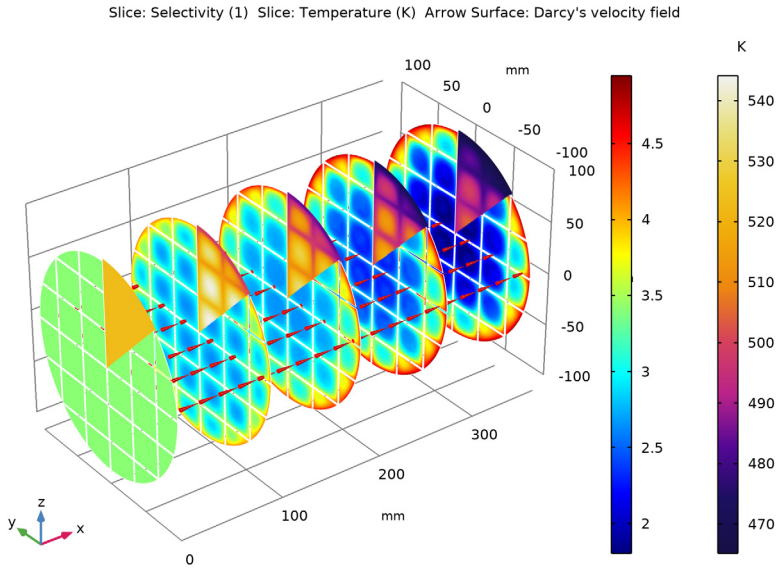

Figure 5: Selectivity and temperature in slices throughout the monolith reactor. Fluid flow from left to right..

Figure 5 shows that channels in the relatively cold region near the reactor outer surface display high selectivity throughout, whereas channels in the region close to the center see selectivity falling off comparatively fast. The fact that r_1/r_2 is greater than 1 throughout the whole reactor means that the desired reducing reaction is favored. The inclusion of Darcy's velocity field aids in showing the flow direction through the reactor.

References

1. G. Schaub, D. Unruh, J. Wang, and T. Turek, "Kinetic analysis of selective catalytic NOx reduction (SCR) in a catalytic filter," *Chem.Eng. and Processing*, vol. 42, no. 5, pp. 365–371, 2003.

Application Library path: `Chemical_Reaction_Engineering_Module/Tutorials/monolith_3d`

Modeling Instructions

ROOT

Open the **Application Library** file monolith_kinetics.mph in the following way:

1. From the **File** menu, choose **Open**.
2. From the Application Libraries root, browse to the folder `Chemical_Reaction_Engineering_Module/Tutorials` and double-click the file `monolith_kinetics.mph`.

Start by changing the molar NH_3:NO ratio, X0, to the optimal value found in the investigation of the reaction kinetics. Continue by adding the model geometry settings to the table.

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. In the table, enter the following settings:

Name	Expression	Value	Description
X0	1.35	1.35	Ratio NH3 to NO at inlet
por	0.75	0.75	Gas phase volume fraction
d_N2_in	0.65[kg/m^3]	0.65 kg/m³	Density of nitrogen at T_in
A_in	3359.9 [mm^2]	0.0033599 m²	Inlet cross sectional area
M0_in	v_av*por*A_in* d_N2_in	4.9139E-4 kg/s	Mass flow inlet

COMPONENT 1 (COMP1)

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

REACTION ENGINEERING (RE)

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

Species: N2

1. In the **Model Builder** window, expand the **Component 1 (comp1)> Reaction Engineering (re)** node, then click **Species: N2**.
2. In the **Settings** window for **Species**, locate the **Species Type** section.
3. From the list, choose **Solvent**.

In the next phase of the example you prepare to set up a 3D model of the monolithic reactor, including mass transport and reaction, heat transfer, and fluid flow.

Generate Space-Dependent Model 1

The **Generate Space-Dependent Model** feature creates a link between the plug flow channel model and the full 3D monolith model. It allows you to transfer reaction kinetics, thermodynamics, and transport properties set up in the **Reaction Engineering** feature to the physics interfaces describing space and time-dependent systems.

1. In the **Reaction Engineering** toolbar, click **Generate Space-Dependent Model**.
2. In the **Settings** window for **Generate Space-Dependent Model**, locate the **Physics Interfaces** section.
3. Find the **Chemical species transport** subsection. From the list, choose **Transport of Diluted Species in Porous Media: New**.
4. Find the **Fluid flow** subsection. From the list, choose **Darcy's Law: New**.
5. Find the **Heat transfer** subsection. From the list, choose **Heat Transfer in Porous Media: New**.
6. Locate the **Space-Dependent Model Generation** section. Click **Create/Refresh**.

3D MODEL

1. In the **Model Builder** window, click **Component 2 (comp2)**.
2. In the **Settings** window for **Component**, type `3D Model` in the **Label** text field.

DEFINITIONS (COMP2)

Variables 2

1 In the **Model Builder** window, expand the **3D Model (comp2)** node.

2 Right-click **3D Model (comp2)>Definitions** and choose **Variables**.

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

4 In the table, enter the following settings:

Name	Expression	Unit	Description
S	chem.r_1/chem.r_2		Selectivity
a	a0*exp(-E0/(R_const* chem.T))	m³/mol	Concentration correction

GEOMETRY 1 (3D)

Now import a file with the reactor geometry. Symmetry reduces the modeling domain to one eighth of the full monolith.

1 In the **Geometry** toolbar, click  **Insert Sequence**.

2 Browse to the model's Application Libraries folder and double-click the file `monolith_3d_geom_sequence.mph`.

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

GLOBAL DEFINITIONS

Transport properties need to be calculated for the space-dependent 3D model. Assuming nitrogen as 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 **Next** 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
oxygen	0
water	0

4 Click the **Mass fraction** button.

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

SELECT PROPERTIES

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

2 In the list, 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 **Next** 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. 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 673.

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

GLOBAL DEFINITIONS

Gas: Nitrogen

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

2 In the **Settings** window for **Material**, type `Gas: Nitrogen` 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 **Property Group**, locate the **Output Properties** section.

4 Click + **Select Quantity**.

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

6 Click **Filter**.

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

8 Click **OK**.

9 In the **Settings** window for **Property Group**, locate the **Output Properties** section.

10 Click + **Select Quantity**.

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

12 Click **Filter**.

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

14 Click **OK**.

15 In the **Settings** window for **Property Group**, locate the **Output Properties** section.

16 Click + **Select Quantity**.

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

18 Click **Filter**.

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

20 Click **OK**.

21 In the **Settings** window for **Property Group**, locate the **Output Properties** section.

22 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

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

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

25 Click **OK**.

Now add a Porous Material to be used in the monolith channels.

MATERIALS

Porous Material 1 (poromat1)

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

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

3 From the **Selection** list, choose **Channel blocks**.

Fluid 1 (poromat1.fluid1)

Right-click **Porous Material 1 (poromat1)** and choose **Fluid**.

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

Solid 1 (poromat1.solid1)

1 In the **Model Builder** window, right-click **Porous Material 1 (poromat1)** 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 monolith walls by linking to the global monolith material.

Walls

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

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

3 From the **Selection** list, choose **Supporting walls**.

4 Locate the **Link Settings** section. From the **Material** list, choose **Solid: Monolith Material (mat1)**.

5 In the **Label** text field, type `Walls`.

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 **3D 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 **Channel blocks**.

Porous Medium 1

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

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 **Convection** section.

3 From the **u** list, choose **Darcy's velocity field (dl)**.

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 x-axis. This can be accomplished by specifying the diffusivity only in the first element of the diagonal diffusion matrix. This is done in the following way:

4 Locate the **Diffusion** section. From the **Source** list, choose **Material**.

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

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

6 In the $D_{\mathrm{F,cH2O}}$ table, enter the following settings:

pp1mat1.df4.D11	0	0
0	0	0
0	0	0

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

8 In the $D_{\mathrm{F,cNH3}}$ table, enter the following settings:

pp1mat1.df1.D11	0	0
0	0	0
0	0	0

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

10 In the $D_{\mathrm{F,cNO}}$ table, enter the following settings:

pp1mat1.df2.D11	0	0

0	0	0
0	0	0

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

12 In the $D_{\mathrm{F,cO2}}$ table, enter the following settings:

pp1mat1.df3.D11	0	0
0	0	0
0	0	0

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

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 xx-component in the diffusivity matrix.

Porous Matrix 1

The porosity is by default defined from the Porous Material.

This model is highly nonlinear due to the reaction kinetics. In this case, to solve all the physics simultaneously, starting from a non-reacting system leads to a more robust simulation. To achieve this set the initial concentration to zero.

Initial Values 1

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

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

3 In the $cH2O$ text field, type 0.

4 In the $cNH3$ text field, type 0.

5 In the cNO text field, type 0.

6 In the $cO2$ text field, type 0.

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 plug flow channel model. Make sure that the **Inlet** and **Outlet** features are assigned to the proper domains and boundaries in the 3D reactor.

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 **Inlet**.

Outflow 1

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

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

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

HEAT TRANSFER IN POROUS MEDIA 1 (HT)

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

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 Convection** section.

3 From the $\mathbf{u}$ list, choose **Darcy's velocity field (dl)**.

4 Locate the **Heat Conduction, Fluid** section. From the k_f list, choose **From material**.

5 Locate the **Thermodynamics, Fluid** section. From the ρ_f list, choose **From material**.

6 From the $C_{p,f}$ list, choose **From material**.

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

Note that the fluid properties are now 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 channel blocks.

5 In the k_s table, enter the following settings:

0.13[W/m/K]	0	0
0	0.25[W/m/K]	0
0	0	0.25[W/m/K]

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

Initial Values 1

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

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

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

Heat Source 1

Associate the **Heat Source** to the exothermic chemistry within the channel blocks. Note that the feature and the expressions describing the heat source are generated by the **Generate Space-Dependent Model** feature, linking the 3D monolith model to the plug flow model.

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

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

3 From the **Selection** list, choose **Channel blocks**.

Temperature 1

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

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

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

Outflow 1

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

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

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

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 **Supporting walls**.

Heat Flux 1

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

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

3 From the **Selection** list, choose **Reactor surface**.

4 Locate the **Heat Flux** section. Click the **Convective heat flux** button.

5 In the h text field, type `10[W/(m^2*K)]`.

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

Heat Flux 2

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

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

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

4 Locate the **Heat Flux** section. Click the **Convective heat flux** button.

5 In the h text field, type `1`.

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

Symmetry 1

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

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

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

Inflow 1

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

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

3 In the T_{ustr} text field, type `T_in`.

4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Inlet**.

DARCY'S LAW 1 (DL)

1 In the **Model Builder** window, under **3D Model (comp2)** click **Darcy's Law 1 (dl)**.

2 In the **Settings** window for **Darcy's Law**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Channel blocks**.

Fluid and Matrix Properties 1

1 In the **Model Builder** window, expand the **Darcy's Law 1 (dl)** node, then click **Fluid and Matrix Properties 1**.

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

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

4 From the ρ list, choose **From material**.

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

6 Locate the **Matrix Properties** section. From the **Porous material** list, choose **Solid: Monolith Material (mat1)**.

7 From the ε_p list, choose **User defined**. In the associated text field, type `1-por`.

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

9 In the κ table, enter the following settings:

3.3e-7[m^2]	0	0
0	0	0
0	0	0

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 **Inlet**.

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

5 Locate the **Mass Flow** section. In the M_0 text field, type `M0_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 **Outlet**.

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

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

MESH 1

First create a **Free Triangular** mesh at the reactor inlet and then, complete the mesh by sweeping in the axial direction of the reactor.

Free Triangular 1

1 In the **Mesh** toolbar, click  **Boundary** and choose **Free Triangular**.

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

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

Size 1

1 Right-click **Free Triangular 1** and choose **Size**.

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

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

4 Locate the **Element Size** section. Click the **Custom** button.

5 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

6 In the associated text field, type `2.2`.

7 Select the **Resolution of narrow regions** check box.

8 In the associated text field, type `0.85`.

9 Click **Build All**.

Size 2

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 **Edge**.

4 Select Edges 5 and 17 only.

5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

7 In the associated text field, type `5`.

8 Click **Build All**.

Swept 1

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

Distribution 1

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

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

3 In the **Number of elements** text field, type `50`.

4 Click **Build All**.

STUDY 2

1 In the **Model Builder** window, click **Study 2**.

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

3 Clear the **Generate default plots** check box.

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

Follow these instruction to generate Figure 3 through Figure 5.

RESULTS

Follow these instruction to generate Figure 3.

Conversion 3D Model

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Conversion 3D Model` in the **Label** text field.

3 Locate the **Color Legend** section. From the **Position** list, choose **Left**.

Isosurface 1

1 Right-click **Conversion 3D Model** and choose **Isosurface**.

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

3 In the **Expression** text field, type `(F_NO_in/vrate-cNO)/(F_NO_in/vrate)`.

4 Locate the **Levels** section. In the **Total levels** text field, type `20`.

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

6 In the **Conversion 3D Model** toolbar, click  **Plot**.

Follow these instruction to generate Figure 4.

Temperature 3D Model

1 In the **Home** toolbar, click  **Add Plot Group** and choose **3D Plot Group**.

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

3 Locate the **Color Legend** section. From the **Position** list, choose **Left**.

Slice 1

1 Right-click **Temperature 3D Model** and choose **Slice**.

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

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

4 Locate the **Plane Data** section. In the **Planes** text field, type `10`.

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

6 In the **Temperature 3D Model** toolbar, click  **Plot**.

To plot the full monolithic structure seen in Figure 5, complete the following steps.

Monolith

1 In the **Results** toolbar, click  **More Datasets** and choose **Sector 3D**.

2 In the **Settings** window for **Sector 3D**, type `Monolith` in the **Label** text field.

3 Locate the **Axis Data** section. In row **Point 2**, set **X** to `1`.

4 In row **Point 2**, set **Z** to `0`.

5 Locate the **Symmetry** section. In the **Number of sectors** text field, type `8`.

6 From the **Sectors to include** list, choose **Manual**.

7 From the **Transformation** list, choose **Rotation and reflection**.

8 Find the **Radial direction of reflection plane** subsection. In the **X** text field, type `0`.

9 In the **Z** text field, type `1`.

10 Click to expand the **Advanced** section. Select the **Define variables** check box.

Temperature sector

1 Right-click **Monolith** and choose **Duplicate**.

2 In the **Settings** window for **Sector 3D**, type `Temperature sector` in the **Label** text field.

3 Locate the **Symmetry** section. In the **Start sector** text field, type `2`.

4 In the **Number of sectors to include** text field, type `1`.

Monolith view

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

2 In the **Settings** window for **3D Plot Group**, type `Monolith view` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Monolith**.

4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

5 Locate the **Color Legend** section. Select the **Show units** check box.

Selectivity

1 Right-click **Monolith view** and choose **Slice**.

2 In the **Settings** window for **Slice**, type `Selectivity` in the **Label** text field.

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

4 Select the **Description** check box.

5 Locate the **Plane Data** section. From the **Entry method** list, choose **Coordinates**.

6 Click  **Range**.

7 In the **Range** dialog box, choose **Number of values** from the **Entry method** list.

8 In the **Start** text field, type `0`.

9 In the **Stop** text field, type `L`.

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

11 Click **Replace**.

12 In the **Monolith view** toolbar, click  **Plot**.

Temperature

1 Right-click **Selectivity** and choose **Duplicate**.

2 In the **Settings** window for **Slice**, type `Temperature` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Temperature sector**.

4 Locate the **Expression** section. In the **Expression** text field, type `T`.

5 In the **Description** text field, type `Temperature`.

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

Selectivity

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

2 In the **Settings** window for **Slice**, click to expand the **Quality** section.

3 From the **Smoothing** list, choose **None**.

Filter 1

1 Right-click **Selectivity** and choose **Filter**.

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

3 In the **Logical expression for inclusion** text field, type `sec1number!=2`.

4 In the **Monolith view** toolbar, click **Plot**.

Cut Plane 1

1 In the **Results** toolbar, click **Cut Plane**.

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

3 From the **Dataset** list, choose **Monolith**.

4 Locate the **Plane Data** section. From the **Plane** list, choose **YX-planes**.

5 In the **Z-coordinate** text field, type `2`.

6 Click **Plot**.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Monolith view** and choose **Arrow Surface**.

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

3 From the **Dataset** list, choose **Cut Plane 1**.

4 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **3D Model (comp2)>Darcy's Law 1>Velocity and pressure>dl.u,dl.v,dl.w - Darcy's velocity field**.

5 Locate the **Coloring and Style** section. From the **Arrow type** list, choose **Cone**.

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

7 In the associated text field, type `80`.

8 In the **Monolith view** toolbar, click **Plot**.

Monolith view

Click the  **Go to Default View** button in the **Graphics** toolbar.

The final step is to derive values for the outlet average conversion, as well as the highest temperature reached in the reactor.

Surface Average 1

1. In the **Results** toolbar, click  **More Derived Values** and choose **Average> Surface Average**.
2. In the **Settings** window for **Surface Average**, locate the **Selection** section.
3. From the **Selection** list, choose **Outlet**.
4. Locate the **Expressions** section. Click  **Clear Table**.
5. In the table, enter the following settings:

Expression	Unit	Description
`(F_NO_in/vrate-chem.c_NO)/(F_NO_in/vrate)`	1	`Conversion`

6. Click  **Evaluate**.

Volume Maximum 1

1. In the **Results** toolbar, click  **More Derived Values** and choose **Maximum> Volume Maximum**.
2. In the **Settings** window for **Volume Maximum**, locate the **Selection** section.
3. From the **Selection** list, choose **All domains**.
4. Click **Evaluate**.