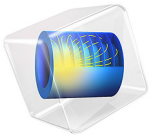

Porous Catalytic Reactor with Injection Needle

Introduction

Heterogeneous catalytic reactors have been widely used in the chemical engineering industry. This type of gas-solid catalytic reactors, where gas phase reactions are catalyzed by a solid catalyst, have widespread applications in the areas such as catalytic oxidation and selective catalytic reduction. This example illustrates the modeling of a porous catalytic reactor for hydrogen oxidation on a noble metal Rh catalyst dispersed on an alumina support (Rh/Al_2O_3). The model investigates the kinetics of the heterogeneous catalytic reaction system, the species concentration distribution (both the species in the bulk gas phase and absorbed on the catalytic surface) and the velocity field in the pore volume.

First, the hydrogen oxidation rate and the rates of adsorption and desorption for all species are studied by using the Reaction Engineering interface, assuming that the chemical system is perfectly mixed. Then, in a space-dependent model of the porous catalytic reactor, the concentration and velocity fields are investigated by using the Transport of Diluted Species in Porous Catalysts interface, which is a combination of Transport of Diluted Species with Porous Catalyst feature and the Brinkman Equation interfaces. The thermodynamic and kinetic properties of the reaction system in the space-dependent model are provided using a Chemistry interface.

Model Definition

HETEROGENEOUS CATALYTIC REACTIONS

For a gas-solid catalytic reaction, the reaction rate (R_s) can be expressed as

$$R_s = \frac{n_{\text{prod}}}{(\text{time})(\text{catalystunit})}$$

where n_{prod} is the number of product moles; `catalystunit` is the measure unit of catalyst amount, which has following different unit bases:

- Active surface area of catalyst (m^2)
- Unit mass of catalyst (kg)
- Unit volume of catalyst (m^3)
- Active metal loading percentage

The reaction-rate unit depends on the measurement unit of the catalyst. In the Porous Catalyst feature in the Transport of Diluted Species and Transport of Concentrated Species interfaces, there are two measure units for the catalyst: one based on the surface area (m^2) and another based on the mass amount (kg).

A general surface reaction can be written as

$$A(ads) + B(ads) \underset{k_r}{\overset{k_f}{\rightleftharpoons}} AB(ads)$$

The reaction rate of this elemental reaction is

$$R_s = k_f\theta_A\theta_B - k_r\theta_{AB}$$

where k_f and k_r are the forward and backward reaction rate constants, respectively, and θ_A, θ_B, and θ_{AB} are the surface coverages of surface species $\mathrm{A(ads)}$, $\mathrm{B(ads)}$, and $\mathrm{AB(ads)}$. The coefficient k_f has the form

$$k_f = AT^{\beta}\exp\left(\frac{-E}{RT}\right)$$

where

- A is a pre-exponential factor
- T is the temperature (K)
- β is the temperature exponent
- E is the activation energy (J/mol)
- R is the gas constant (J/(mol·K))

The rate constant k_r has the same form as that for k_f. Alternatively, it can be obtained from the reaction equilibrium constant (K_0):

$$k_r = \frac{k_f}{K_0}$$

The gas-solid catalytic reaction system of $H_2 + O_2 + H_2O$ on Rh/Al_2O_3 catalyst is investigated using the Reaction Engineering interface. The following reactions are considered:

- Gaseous H_2 being dissociatively adsorbed on two neighboring Rh sites:

$$H_2 + 2Rh(ads) = 2H(ads)$$

- Gaseous O_2 being dissociatively absorbed on two neighboring Rh sites:

$$O_2 + 2Rh(ads) = 2O(ads)$$

- Gaseous H_2O being absorbed on a Rh site:

$$H_2O + Rh(ads) = H_2O(ads)$$

- The surface reactions of the adsorbed species H(ads), O(ads), OH(ads), and H_2O(ads):

$$O(ads) + H(ads) = OH(ads) + Rh(ads)$$

$$OH(ads) + H(ads) = H_2O(ads) + Rh(ads)$$

$$OH(ads) + OH(ads) = O(ads) + H_2O(ads)$$

The thermodynamic and kinetic behaviors of all species and reactions can be simulated provided that the rate constants k_f and k_r are available for these six reactions.

After the initial analysis of the gas-solid reaction system in the Reaction Engineering interface, the reaction system will be exported to a Chemistry interface using the Generate Space-Dependent Model feature. The Chemistry interface will then be used to define the gas-solid reaction system in the space-dependent model.

SPACE-DEPENDENT MODEL OF POROUS CATALYTIC REACTOR

The reactor consists of a tubular structure, with an injection tube whose main axis is perpendicular to the reactor axis. The reactor geometry is shown in Figure 1. The incoming species in the main and injection tubes react in a fixed porous catalyst bed. The model couples the free fluid and porous media flow through the Brinkman equation interface. This physics interface includes two physics features for modeling the fluid flow, one being Porous Medium for porous domain, and the other being Fluid Properties for free flow domain. Because of symmetry, only one half of the reactor is modeled.

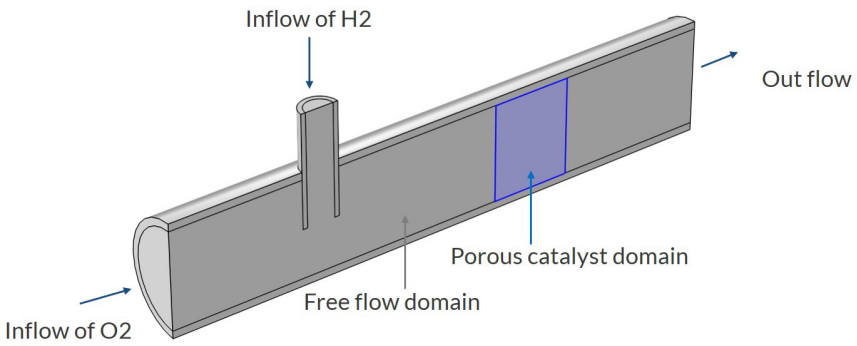

Figure 1: The species O_2 and H_2 enter the reactor from the main and injection tubes, respectively, and react in a fixed porous catalyst bed to produce H_2O.

In the porous catalyst domain, the hydrogen oxidation on the Rh/Al_2O_3 catalyst takes place. The net reaction of the gas phase species is $2H_2 + O2 \rightarrow 2H_2O$.

Governing Equations

The Navier–Stokes equations describe the fluid flow in the free-flow regions. In the porous domain, the Brinkman equations for porous media apply.

As the modeled species are present in low concentrations, diffusion is assumed to take place according to Fick's law. The mass transport for the three species H_2, O_2, and H_2O can therefore be modeled with the following convection-diffusion equation

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

In this equation, c_i denotes the concentration (SI unit: mol/m^3), D_i the diffusivity (SI unit: m^2/s), and R_i the reaction rate for species i (SI unit: $mol/(m^3 \cdot s)$). Because the reaction takes place in the porous bed only, the reaction term is zero in the free-flow regions. The reaction rate R_i is contributed by the surface reaction, which takes place inside the porous catalyst material.

The bulk transport species H_2, O_2, and H_2O adsorb onto the active sites on the Rh catalyst surface. The adsorption of H_2, O_2, and H_2O is described using the Langmuir adsorption isotherm:

$$c_{\mathrm{P,\,e,}\,i} = \frac{K_{\mathrm{L,}\,i} c_{\mathrm{Pmax,}\,i} c_i}{1 + K_{\mathrm{L,}\,i} c_i}$$

Here, for species i,

- $c_{\mathrm{P,e},i}$ is the equilibrium amount adsorbed on the catalyst (mol/kg),
- $\mathrm{K_{L,i}}$ is the Langmuir constant ($\mathrm{m^3/mol}$),
- $\mathrm{c_{Pmax,i}}$ is the maximum adsorbed amount (mol/kg), and
- c_i is the species molar concentration in the gas phase ($\mathrm{mol/m^3}$)

In the Langmuir isotherm, the equilibrium adsorbed amount is dependent both on the maximum possible amount adsorbed ($\mathrm{c_{Pmax,i}}$), and the bulk concentration of species i (c_i). If the bulk concentration is zero, the equilibrium concentration is also zero.

The equilibrium molar concentration ($c_{\mathrm{eq},i}$, $\mathrm{mol/m^3}$) for adsorbed species i is given by

$$c_{\mathrm{eq,}\,i} = \rho_{\mathrm{b}} c_{\mathrm{P,\,e,}\,i} \tag{2}$$

where ρ_{b} is the catalyst bulk density.

For the adsorbed species concentration $c_{\mathrm{ads},i}$ ($\mathrm{mol/m^2}$), its corresponding volumetric concentration $c_{\mathrm{vol},i}$ ($\mathrm{mol/m^3}$) is

$$c_{\mathrm{vol},i} = S_{\mathrm{area,cat}} c_{\mathrm{ads},i} \tag{3}$$

Using Equation 2 and Equation 3, the adsorption/desorption rate $R_{\mathrm{ads},i}$ ($\mathrm{mol/(m^3 \cdot s)}$) is defined as

$$R_{\mathrm{ads,}\,i} = h_{\mathrm{LDF},i}(c_{\mathrm{vol},i} - c_{\mathrm{eq},i})$$

where $h_{\mathrm{LDF},i}$ is the mass transfer coefficient (1/s), which is based on a linear driving force. The adsorption rate is a mass source term and contributes to the bulk reaction rate R_i in Equation 1. With this definition, a positive $R_{\mathrm{ads},i}$ corresponds to desorption of species i, that is, a positive source term of species i in Equation 1.

For the adsorbed species, the governing equation is

$$\frac{dc_{\mathrm{ads},i}}{dt} = R_{\mathrm{s,\,ads,}\,i}$$

and for other surface species (without mass transfer between the bulk and the catalyst surface)

$$\frac{dc_{\text{surf},i}}{dt} = R_{\text{s, surf, } i}$$

where $R_{\text{s,ads},i}$ and $R_{\text{s,surf},i}$ are the surface reaction rates for adsorbed and surface species, respectively.

Boundary Conditions

In the Brinkman Equations interface, a constant velocity profile is assumed at the inlet boundaries:

$$\mathbf{u} = u_{\text{in}}$$

For the outlet, a zero pressure condition is applied.

In the Transport of Diluted Species in Porous Catalysts interface, the concentrations at the inflows are fixed:

$$c_i = c_{i0,\text{ inlet}}$$

At the outflow, the convection is assumed to dominate the mass transport:

$$\mathbf{n} \cdot (-D_i \nabla c_i) = 0$$

This implies that the gradient of c_i in the direction perpendicular to the outlet boundary is negligible. This is a common assumption for tubular reactors with a high degree of transport by convection in the direction of the main reactor axis. The condition eliminates the need for specifying a concentration or a fixed value for the flux at the outlet boundary. At all other boundaries, no flux conditions apply:

$$\mathbf{n} \cdot (-D_i \nabla c_i + c_i \mathbf{u}) = 0$$

Figure 2 shows the velocity magnitude. The flow is almost homogeneous in the porous part of the reactor.

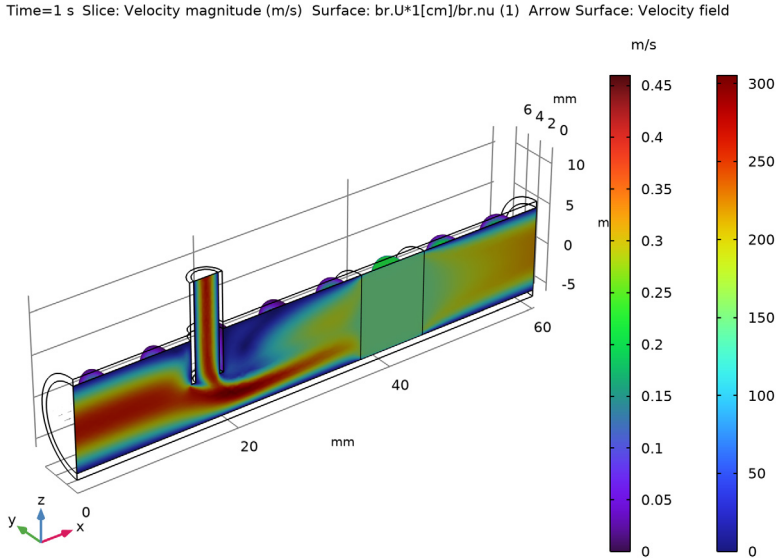

Figure 2: Magnitude of the velocity field in the free and porous reactor domains.

Figure 3 shows the pressure drop, which occurs mainly across the porous bed.

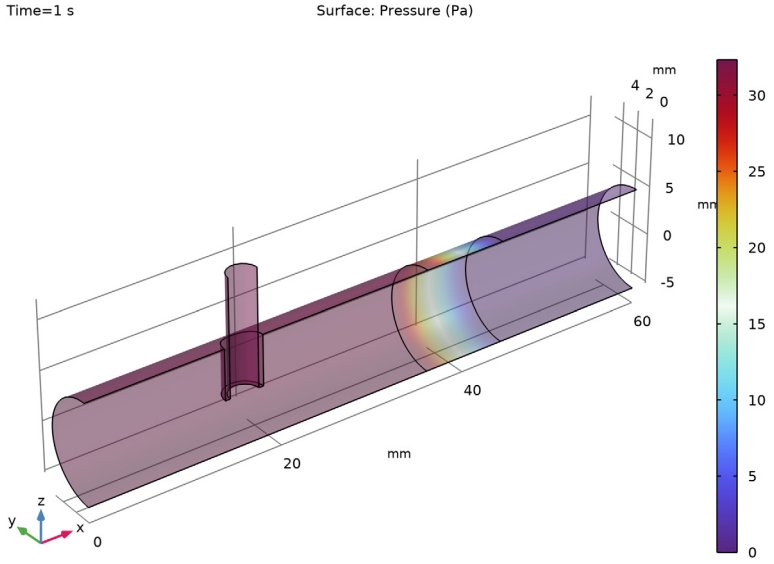

Figure 3: The pressure drop across the reactor.

Figure 4 and Figure 5 show the concentrations of species H_2 and O_2, respectively.

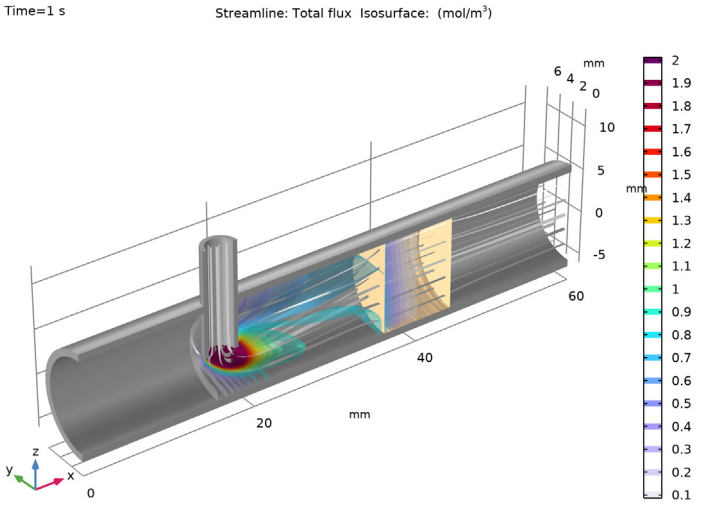

Figure 4: Isoconcentration surfaces for species H_2.

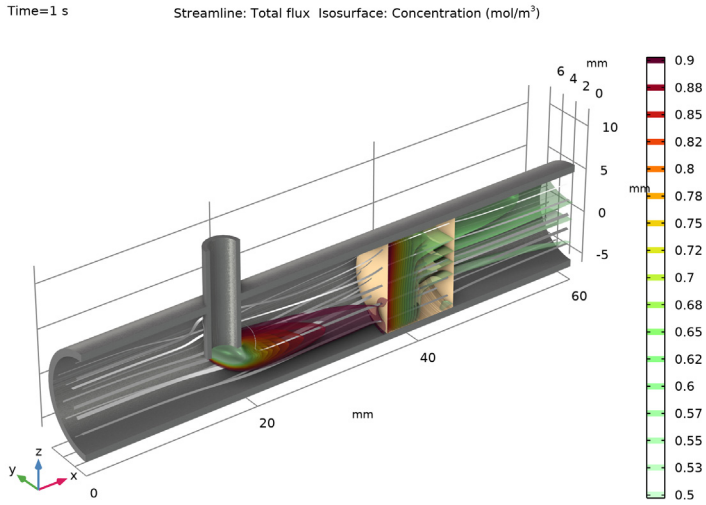

Figure 5: Isoconcentration surfaces for species O_2.

Figure 4 shows that the concentration of the injected species H_2 decreases very rapidly with distance from the injection point due to quick mixing with the main flow. It also

shows that hydrogen is consumed in the porous catalyst domain. The rate of hydrogen oxidation is significantly lower after about half the bed length, meaning that half the bed is poorly utilized. This indicates an opportunity for optimizing the reactor design by, for example, using a thinner catalyst bed. Figure 5 shows the isoconcentration surfaces of species O_2, which is introduced in the main channel of the reactor. Similar to the species H_2, its concentration also decreases across the porous domain. The injection of H_2 results in a reduction in O_2 concentration at the injection point.

Figure 6 and Figure 7 show the surface concentration distributions along the centerline of the porous catalyst bed for adsorbed, and for surface species, respectively. There is a surplus of oxygen in the gas phase. The surface-gas equilibrium, as expressed by the Langmuir isotherm, limits the conversion of hydrogen to water, so that the concentration of hydrogen in the gas phase does not reach zero. As the hydrogen concentration in the gas phase outside the porous catalyst decreases, the adsorption rate of hydrogen decreases, and thus also the hydrogen adatom concentration on the surface. With less hydrogen present on the surface, the rate of oxygen removal (water formation) from the surface decreases. The net effect is that, after about half the bed length, the empty Rh surface sites are successively covered by oxygen adatoms. At the end of the bed, the majority of surface sites are covered by oxygen atoms.

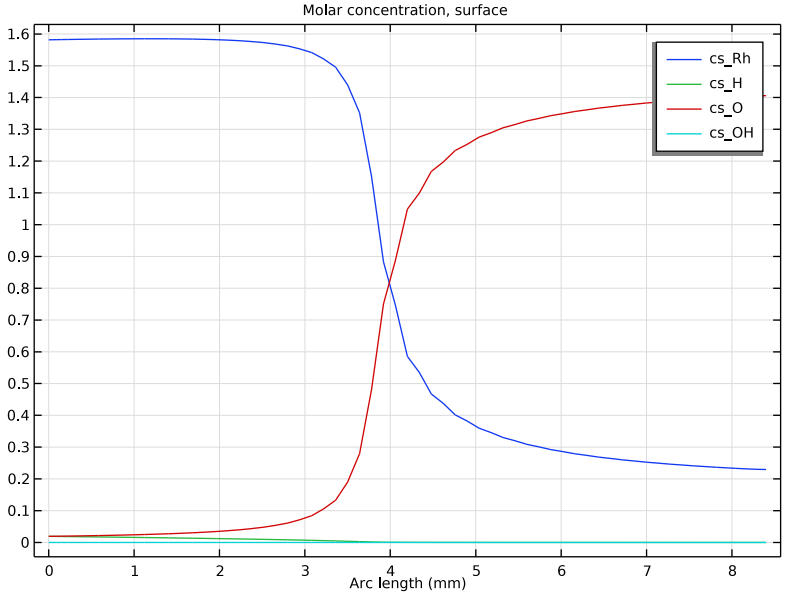

Figure 6: Concentration distribution along the centerline of catalyst for surface species.

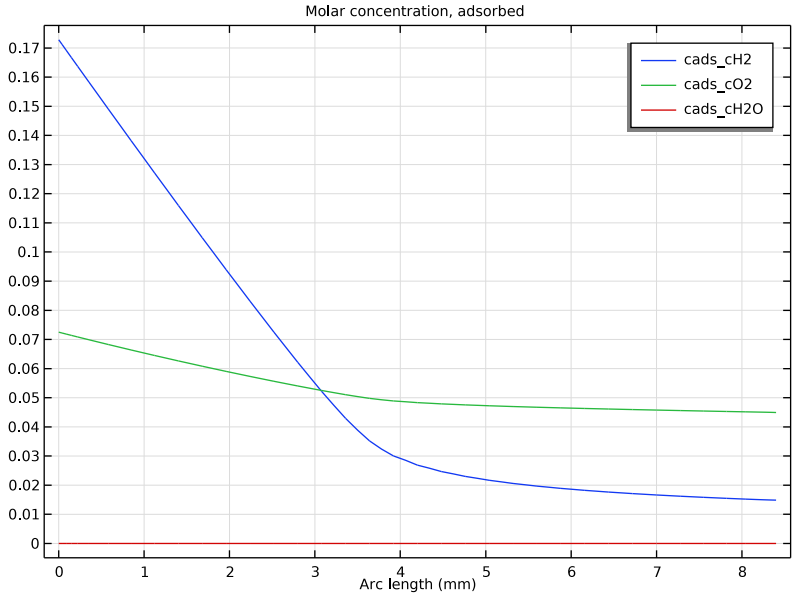

Figure 7: Concentration distribution along the centerline of catalyst for adsorbed species.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/porous_reactor`

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

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

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

6 Click **Done**.

Load reaction parameters (general) from a text file.

GLOBAL DEFINITIONS

Parameters 1, reaction

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

2 In the **Settings** window for **Parameters**, type `Parameters 1, reaction` in the **Label** text field.

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

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

REACTION ENGINEERING (RE)

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

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

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

Create the `H2+O2` reaction system over the `Rh/Al2O3` catalyst.

Reaction 1

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

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

3 In the **Formula** text field, type `H2+2Rh(ads)<=>2H(ads)`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. In the k^{f} text field, type `kf1`.

6 In the k^{r} text field, type `kr1`.

Reaction 2

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

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

3 In the **Formula** text field, type `O2+2Rh(ads)<=>2O(ads)`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. In the k^{f} text field, type `kf2`.

6 In the k^{r} text field, type `kr2`.

Reaction 3

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

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

3 In the **Formula** text field, type `H2O+Rh(ads)<=>H2O(ads)`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. In the k^{f} text field, type `kf3`.

6 In the k^{r} text field, type `kr3`.

Reaction 4

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

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

3 In the **Formula** text field, type `O(ads)+H(ads)<=>OH(ads)+Rh(ads)`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. In the k^{f} text field, type `kf4`.

6 In the k^{r} text field, type `kr4`.

Reaction 5

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

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

3 In the **Formula** text field, type `OH(ads)+H(ads)<=>H2O(ads)+Rh(ads)`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. In the k^{f} text field, type `kf5`.

6 In the k^{r} text field, type `kr5`.

Reaction 6

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

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

3 In the **Formula** text field, type `OH(ads)+OH(ads)<=>O(ads)+H2O(ads)`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. In the k^{f} text field, type `kf6`.

6 In the k^{r} text field, type `kr6`.

Species 1

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

Add a solvent (`N2`). It is not involved in any reaction but it will later be exported to a space-dependent model.

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

3 In the text field, type `N2`.

4 Locate the **Type** section. From the list, choose **Solvent**.

Enter the reactive specific surface for the surface reactions.

5 In the **Model Builder** window, click **Reaction Engineering (re)**.

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

7 Find the **Surface reaction area** subsection. Click the **Surface area to volume ratio** button.

8 In the a_s text field, type `cat_area`.

Initial Values 1

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

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

3 In the table, enter the following settings:

Species	Concentration (mol/m^3)
H2	`c0H2_inflow`
N2	`c0N2`
O2	`c0O2_inflow`

4 Locate the **Surface Species Initial Values** section. In the Γ_s text field, type `2.72E-5`.

5 In the table, enter the following settings:

Species	Surface concentration (mol/m^2)	Site occupancy number (1)
H(ads)	`c0H_surf`	1
H2O(ads)	`c0H2O_surf`	1
O(ads)	`c0O_surf`	1
OH(ads)	`c0OH_surf`	1
Rh(ads)	`c0Rh_surf`	1

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

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

3 In the **Output times** text field, type `range(0,0.01,0.2)`.

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

RESULTS

Concentration (re), bulk species

1 Right-click **Results>Concentration (re)** and choose **Rename**.

2 In the **Rename 1D Plot Group** dialog box, type `Concentration (re), bulk species` in the **New label** text field.

3 Click **OK**.

Plot the bulk species concentrations.

Global 1

1 In the **Model Builder** window, expand the **Concentration (re), bulk species** node, then click **Global 1**.

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

3 Click **Clear Table**.

4 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.c_H2 - Concentration - mol/m³**.

5 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.c_H2O - Concentration - mol/m³**.

6 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.c_O2 - Concentration - mol/m³**.

7 In the **Concentration (re), bulk species** toolbar, click **Plot**.

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

Create a figure for surface species concentrations.

Concentration (re), surface species

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

2 In the **Settings** window for **1D Plot Group**, type `Concentration (re), surface species` in the **Label** text field.

Global 1

1 Right-click **Concentration (re), surface species** and choose **Global**.

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

3 Click **Clear Table**.

4 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.csurf_H_surf - Surface concentration - mol/m²**.

5 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.csurf_O_surf - Surface concentration - mol/m²**.

6 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.csurf_OH_surf - Surface concentration - mol/m²**.

7 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.csurf_H2O_surf - Surface concentration - mol/m²**.

8 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.csurf_Rh_surf - Surface concentration - mol/m²**.

9 Click the **x-Axis Log Scale** button in the **Graphics** toolbar.

10 Click the **y-Axis Log Scale** button in the **Graphics** toolbar.

11 In the **Concentration (re), surface species** toolbar, click **Plot**.

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

Export catalytic oxidation of hydrogen over `Rh/Al2O3` to a space-dependent model.

REACTION ENGINEERING (RE)

Generate Space-Dependent Model 1

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

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

3 Find the **Chemical species transport** subsection. From the list, choose **Transport of Diluted Species in Porous Catalysts: New**.

4 Locate the **Study Type** section. From the **Study type** list, choose **Time dependent**.

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

Load catalyst parameters from a text file.

GLOBAL DEFINITIONS

Parameters 2, catalyst

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Parameters 2, catalyst` in the **Label** text field.

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

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

COMPONENT 2 (COMP2)

Build the geometry for the catalytic reactor.

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

GEOMETRY 1(3D)

1 In the **Model Builder** window, expand the **Component 2 (comp2)>Geometry 1(3D)** node, then click **Geometry 1(3D)**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **mm**.

Cylinder 1 (cyl1)

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

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

3 In the **Radius** text field, type `do_reac/2`.

4 In the **Height** text field, type `5*do_reac`.

5 Locate the **Axis** section. From the **Axis type** list, choose **Cartesian**.

6 In the **x** text field, type `1`.

7 In the **z** text field, type `0`.

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

Layer name	Thickness (mm)
`Layer 1`	`wt_reac`

Cylinder 2 (cyl2)

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

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

3 In the **Radius** text field, type `do_reac/2-wt_reac`.

4 In the **Height** text field, type `0.7*do_reac`.

5 Locate the **Position** section. In the **x** text field, type `3*do_reac`.

6 Locate the **Axis** section. From the **Axis type** list, choose **Cartesian**.

7 In the **x** text field, type `1`.

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

Cylinder 3 (cyl3)

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

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

3 In the **Radius** text field, type `do_needle/2`.

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

5 Locate the **Position** section. In the **x** text field, type `2.7*do_reac/2`.

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

Layer name	Thickness (mm)
`Layer 1`	`wt_needle`

Difference 1 (dif1)

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

2 Select the object **cyl1** only.

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

4 Click to select the **Activate Selection** toggle button for **Objects to subtract**.

5 Select the object **cyl3** only.

6 Select the **Keep objects to subtract** check box.

Union 1 (uni1)

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

2 Select the objects **cyl3** and **dif1** only.

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

4 Click the **Paste Selection** button for **Input objects**.

5 In the **Paste Selection** dialog box, type `cyl2` in the **Selection** text field.

6 Click **OK**.

Block 1 (blk1)

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

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

3 In the **Width** text field, type `5*do_reac`.

4 In the **Depth** text field, type `2*do_reac`.

5 In the **Height** text field, type `3*do_reac`.

6 Locate the **Position** section. In the **y** text field, type `-2*do_reac`.

7 In the **z** text field, type `-1.5*do_reac`.

Difference 2 (dif2)

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

2 Select the object **uni1** only.

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

4 Click to select the **Activate Selection** toggle button for **Objects to subtract**.

5 Select the object **blk1** only.

Form Union (fin)

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

Add a **Mesh Control Faces** feature to control the mesh in the vertical injection needle.

Mesh Control Faces 1 (mcf1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Mesh Control Faces**.

Select the faces corresponding to the symmetry plane and the outlet into the reactor.

2 On the object **fin**, select Boundaries 19 and 20 only.

Ignore Faces 1 (igf1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Ignore Faces**.

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

3 Click the **Paste Selection** button for **Faces to ignore**.

4 In the **Paste Selection** dialog box, type `11,20` in the **Selection** text field.

5 Click **OK**.

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

DEFINITIONS (COMP2)

Create a geometry selection list for model entities.

Catalyst Bed

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

2 Right-click **Component 2 (comp2)>Definitions** and choose **Selections>Explicit**.

3 In the **Settings** window for **Explicit**, type `Catalyst Bed` in the **Label** text field.

4 Select Domain 4 only.

Symmetry plane

1 In the **Definitions** toolbar, click  **Explicit**.

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

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

4 Select Boundaries 5, 19, and 22 only.

Inlet species O2

1 In the **Definitions** toolbar, click  **Explicit**.

2 In the **Settings** window for **Explicit**, type `Inlet species O2` in the **Label** text field.

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

4 Select Boundary 4 only.

Inlet species H2

1 In the **Definitions** toolbar, click  **Explicit**.

2 In the **Settings** window for **Explicit**, type `Inlet species H2` in the **Label** text field.

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

4 Select Boundary 15 only.

Outlet

1 In the **Definitions** toolbar, click  **Explicit**.

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

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

4 Select Boundary 25 only.

First Free-Porous Interface

1 In the **Definitions** toolbar, click  **Cylinder**.

2 In the **Settings** window for **Cylinder**, type `First Free-Porous Interface` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Size and Shape** section. In the **Top distance** text field, type `0.5*do_reac`.

5 In the **Bottom distance** text field, type `0`.

6 Locate the **Position** section. In the **x** text field, type `2.5*do_reac`.

7 In the **y** text field, type `0.25*do_reac`.

8 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

Free Flow Domains

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domains 2 and 5 only.

Free and Porous Media Domains

1 In the **Definitions** toolbar, click **Union**.

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

3 Locate the **Input Entities** section. Under **Selections to add**, click **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Catalyst Bed** and **Free Flow Domains**.

5 Click **OK**.

Solid Domains

1 In the **Definitions** toolbar, click **Adjacent**.

2 In the **Settings** window for **Adjacent**, type `Solid Domains` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Input selections**, click **Add**.

4 In the **Add** dialog box, select **Free and Porous Media Domains** in the **Input selections** list.

5 Click **OK**.

6 In the **Settings** window for **Adjacent**, locate the **Output Entities** section.

7 From the **Geometric entity level** list, choose **Adjacent domains**.

Solid Bnds

1 In the **Definitions** toolbar, click **Adjacent**.

2 In the **Settings** window for **Adjacent**, type `Solid Bnds` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Input selections**, click **Add**.

4 In the **Add** dialog box, select **Solid Domains** in the **Input selections** list.

5 Click **OK**.

Porous Bed Bnds

1 In the **Definitions** toolbar, click **Adjacent**.

2 In the **Settings** window for **Adjacent**, type `Porous Bed Bnds` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Input selections**, click **Add**.

4 In the **Add** dialog box, select **Catalyst Bed** in the **Input selections** list.

5 Click **OK**.

Outer Bnds

1 In the **Definitions** toolbar, click **Difference**.

2 In the **Settings** window for **Difference**, type `Outer Bnds` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Under **Selections to add**, click **Add**.

5 In the **Add** dialog box, select **Solid Bnds** in the **Selections to add** list.

6 Click **OK**.

7 In the **Settings** window for **Difference**, locate the **Input Entities** section.

8 Under **Selections to subtract**, click **Add**.

9 In the **Add** dialog box, select **Porous Bed Bnds** in the **Selections to subtract** list.

10 Click **OK**.

Bed Bnds

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `18,20,21` in the **Selection** text field.

6 Click **OK**.

COMPONENT 2 (COMP2)

Add a **Brinkman Equations** interface to the newly generated component.

ADD PHYSICS

1 In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Fluid Flow>Porous Media and Subsurface Flow>Brinkman Equations (br)**.

4 Click **Add to Component 2** in the window toolbar.

5 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

MATERIALS

Add a Material node for nitrogen.

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

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

3 In the tree, select **Liquids and Gases>Gases>Nitrogen**.

4 Click **Add to Component** in the window toolbar.

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

Add a porous material for the **Porous Catalyst** feature.

MATERIALS

Porous Material 1 (pmat1)

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

2 Select Domain 4 only.

Fluid 1 (pmat1.fluid1)

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

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

3 From the **Material** list, choose **Nitrogen (mat1)**.

Solid 1 (pmat1.solid1)

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

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

3 In the θ_s text field, type `0.7`.

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

Property	Variable	Value	Unit	Property group
Density	rho	2800	kg/m³	Basic

Porous Material 1 (pmat1)

1 In the **Model Builder** window, click **Porous Material 1 (pmat1)**.

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

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Permeability	kappa_iso ; kappaii = kappa_iso, kappaij = 0	1e-9	m^2	Basic

MULTIPHYSICS

Reacting Flow, Diluted Species 1 (rfd1)

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

TRANSPORT OF DILUTED SPECIES IN POROUS CATALYSTS (TDS)

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

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

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

Set all parameters for the **Porous Catalyst** feature and its subfeatures.

Porous Catalyst 1

Assume that all the bulk species (from the **Transport of Diluted Species** interface) are adsorbed into the catalyst. Enter the initial concentrations for the these species.

1 In the **Model Builder** window, expand the **Transport of Diluted Species in Porous Catalysts (tds)** node, then click **Porous Catalyst 1**.

2 In the **Settings** window for **Porous Catalyst**, locate the **Adsorbed Species** section.

3 In the $\Gamma_{0,cH2ads}$ text field, type 0.

4 In the $\Gamma_{0,cH2Oads}$ text field, type 0.

5 In the $\Gamma_{0,cO2ads}$ text field, type 0.

The surface species H2O is assumed to be an adsorbed species. Remove it from the **Surface Species** table.

6 Locate the **Surface Species** section. Click to select row number 2 in the table.

7 Click **Delete**.

Enter the initial molar concentrations for the other surface species.

8 In the table, enter the following settings:

Surface species	Initial values (mol/m^2)
H	c0H_surf
O	c0O_surf
OH	c0OH_surf
Rh	c0Rh_surf

Fluid 1

Select the diffusion coefficients from **Chemistry**.

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

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

3 From the D_{cH2} list, choose **Diffusion coefficient , H2 in N2 (solvent) (chem)**.

4 From the D_{cH2O} list, choose **Diffusion coefficient , H2O in N2 (solvent) (chem)**.

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

6 From the **Effective diffusivity model** list, choose **Bruggeman model**.

Adsorption 1

Enter the model parameters for the **Langmuir** adsorption isotherm model.

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

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

3 Select the **Species cH2** check box.

4 In the $K_{\mathrm{L,cH2}}$ text field, type `klH2_ads`.

5 In the $c_{\mathrm{P,max,cH2}}$ text field, type `cplH2_ads`.

6 In the $h_{\mathrm{LDF,cH2}}$ text field, type `kfH2_ads`.

7 Select the **Species cH2O** check box.

8 In the $K_{\mathrm{L,cH2O}}$ text field, type `klH2O_ads`.

9 In the $c_{\mathrm{P,max,cH2O}}$ text field, type `cplH2O_ads`.

10 In the $h_{\mathrm{LDF,cH2O}}$ text field, type `kfH2O_ads`.

11 Select the **Species cO2** check box.

12 In the $K_{\mathrm{L,cO2}}$ text field, type `klO2_ads`.

13 In the $c_{\mathrm{P,max,cO2}}$ text field, type `cpl02_ads`.

14 In the $h_{\mathrm{LDF,cO2}}$ text field, type `kf02_ads`.

Surface Reaction 1

The adsorbed species `H20` also takes part in the surface reactions. Couple its reaction rate to the surface species `H20` in **Chemistry**.

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

2 In the **Settings** window for **Surface Reaction**, locate the **Surface Reaction Rate for Adsorbed Species** section.

3 From the $R_{\mathrm{cadscH2O}}{}^{\mathrm{s}}$ list, choose **Surface reaction rate for surface species H20_surf (chem)**.

CHEMISTRY 1 (CHEM)

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

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

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

Species	Species concentration type	Surface concentration (mol/m^2)
H2O(ads)	Variable	`tds.cads_cH20`

DEFINITIONS (COMP2)

Variables 1, bulk concentration defined from surface concentration

1 In the **Model Builder** window, under **Component 2 (comp2)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables 1, bulk concentration defined from surface concentration` in the **Label** text field.

Load variable definitions from a text file.

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

4 Select Domain 4 only.

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

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

TRANSPORT OF DILUTED SPECIES IN POROUS CATALYSTS (TDS)

Initial Values 1

1 In the **Model Builder** window, under **Component 2 (comp2)> Transport of Diluted Species in Porous Catalysts (tds)** click **Initial Values 1**.

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

3 In the $cH2$ text field, type `0`.

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

Add necessary features to the **Transport of Diluted Species** interface.

Transport Properties 1

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

2 Select Domains 2 and 5 only.

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

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

5 From the D_{cH2} list, choose **Diffusion coefficient , H2 in N2 (solvent) (chem)**.

6 From the D_{cH2O} list, choose **Diffusion coefficient , H2O in N2 (solvent) (chem)**.

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

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 plane**.

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 **Inlet species O2**.

4 Locate the **Concentration** section. In the $c_{0,\mathrm{cO2}}$ text field, type `cO2_inflow`.

Inflow 2

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 **Inlet species H2**.

4 Locate the **Concentration** section. In the $c_{0,\mathrm{cH2}}$ text field, type `cH2_inflow`.

Outflow 1

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

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

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

BRINKMAN EQUATIONS (BR)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Brinkman Equations (br)**.

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

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

4 Locate the **Physical Model** section. Clear the **Neglect inertial term (Stokes flow)** check box.

5 Click to expand the **Discretization** section. From the **Discretization of fluids** list, choose **P1+P1**.

Fluid Properties 1

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

2 Select Domains 2 and 5 only.

Inlet 1

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

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

3 From the **Selection** list, choose **Inlet species O2**.

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

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `v_inlet`.

Inlet 2

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

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

3 From the **Selection** list, choose **Inlet species H2**.

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

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `v_inlet`.

Outlet 1

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

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

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

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 plane**.

MESH 1

Size 1

1 In the **Model Builder** window, under **Component 2 (comp2)** right-click **Mesh 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 Click the **Zoom Extents** button in the **Graphics** toolbar.

5 Select Domain 5 only.

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

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

Size

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

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

3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 From the **Predefined** list, choose **Coarse**.

Size 2

1 In the **Model Builder** window, right-click **Mesh 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 **Boundary**.

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `6,9,10,14,20,23` in the **Selection** text field.

6 Click **OK**.

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

8 From the **Calibrate for** list, choose **Fluid dynamics**.

9 From the **Predefined** list, choose **Fine**.

Free Triangular 1

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

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

3 From the **Selection** list, choose **First Free-Porous Interface**.

Size 1

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

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

3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 From the **Predefined** list, choose **Fine**.

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 Click  **Paste Selection**.

5 In the **Paste Selection** dialog box, type `31,32` in the **Selection** text field.

6 Click **OK**.

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

8 From the **Calibrate for** list, choose **Fluid dynamics**.

9 Click the **Custom** button.

10 Locate the **Element Size Parameters** section.

11 Select the **Maximum element size** check box. In the associated text field, type `0.5`.

Swept 1

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

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

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

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

Distribution 1

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

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

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

4 In the **Number of elements** text field, type `30`.

Corner Refinement 1

1 In the **Mesh** toolbar, click  **More Attributes** and choose **Corner Refinement**.

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

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

4 Select Domains 2 and 4–6 only.

5 Locate the **Boundary Selection** section. Click **Paste Selection**.

6 In the **Paste Selection** dialog box, type `6,9,10,14,20,23` in the **Selection** text field.

7 Click **OK**.

Free Tetrahedral 1

In the **Mesh** toolbar, click **Free Tetrahedral**.

Size 1

1 Right-click **Free Tetrahedral 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 **Boundary**.

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `26` in the **Selection** text field.

6 Click **OK**.

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

8 From the **Calibrate for** list, choose **Fluid dynamics**.

Size 2

1 In the **Model Builder** window, right-click **Free Tetrahedral 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 **Boundary**.

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `2,6` in the **Selection** text field.

6 Click **OK**.

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

8 From the **Calibrate for** list, choose **Fluid dynamics**.

9 Click the **Custom** button.

10 Locate the **Element Size Parameters** section.

11 Select the **Maximum element size** check box. In the associated text field, type `0.9`.

Boundary Layers 1

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

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

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

4 From the **Selection** list, choose **Free Flow Domains**.

5 Click to expand the **Corner Settings** section. From the **Handling of sharp edges** list, choose **Trimming**.

Boundary Layer Properties

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

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `6,9,10,14,18,21,23` in the **Selection** text field.

5 Click **OK**.

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

7 In the **Number of layers** text field, type `2`.

8 In the **Stretching factor** text field, type `1.75`.

9 In the **Thickness adjustment factor** text field, type `4.5`.

Boundary Layers 2

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

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

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

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

5 Locate the **Corner Settings** section. From the **Handling of sharp edges** list, choose **Trimming**.

6 Click to expand the **Transition** section. Clear the **Smooth transition to interior mesh** check box.

Boundary Layer Properties

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

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `18,20,21` in the **Selection** text field.

5 Click **OK**.

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

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

8 In the **Stretching factor** text field, type `1.25`.

9 In the **Thickness adjustment factor** text field, type `2.75`.

10 Click **Build All**.

STUDY 2

Step 2: Stationary

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

There are two study steps in **Study 2**. The first **Stationary** study step solves for the pressure and velocity (from the **Brinkman Equations**) which is supposed to reach stationary state quickly and is insignificantly affected by the concentration field. The second **Time Dependent** study step solves for the molar concentrations (from the **Transport of Diluted Species** interface) with the velocity field from the first study step.

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

3 In the table, enter the following settings:

Physics interface	Solve for	Equation form
Reaction Engineering (re)		Automatic (Time dependent)
Chemistry 1 (chem)	√	Automatic (Stationary)
Transport of Diluted Species in Porous Catalysts (tds)		Automatic (Time dependent)
Brinkman Equations (br)	√	Automatic (Stationary)

4 In the table, enter the following settings:

Multiphysics couplings	Solve for	Equation form
Reacting Flow, Diluted Species 1 (rfd1)		Automatic (Time dependent)

5 Right-click **Step 2: Stationary** and choose **Move Up**.

Step 2: Time Dependent

1 In the **Model Builder** window, click **Step 2: Time Dependent**.

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

3 In the **Output times** text field, type `range(0,0.05,1)`.

4 Locate the **Physics and Variables Selection** section. In the table, enter the following settings:

Physics interface	Solve for	Equation form
Reaction Engineering (re)		Automatic (Time dependent)
Chemistry 1 (chem)	√	Automatic (Time dependent)
Transport of Diluted Species in Porous Catalysts (tds)	√	Automatic (Time dependent)
Brinkman Equations (br)		Automatic (Stationary)

Solution 2 (sol2)

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

Step 2: Time Dependent

1 In the **Model Builder** window, under **Study 2** click **Step 2: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, click to expand the **Values of Dependent Variables** section.

3 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

Solution 2 (sol2)

1 In the **Model Builder** window, expand the **Solution 2 (sol2)** node.

Set the scaling factor to 1 for the bulk species dependent variables.

2 In the **Model Builder** window, expand the **Study 2>Solver Configurations> Solution 2 (sol2)>Dependent Variables 2** node, then click **Concentration (comp2.cH2)**.

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

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

5 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 2** click **Concentration (comp2.cH2O)**.

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

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

8 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 2** click **Concentration (comp2.cO2)**.

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

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

Set the scaling factor to **Initial value based** for the adsorbed species dependent variables.

11 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 2** click **Adsorbed concentration (comp2.tds.cads_cH2)**.

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

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

14 In the **Scale** text field, type `cH2_ads_scale`.

15 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 2** click **Adsorbed concentration (comp2.tds.cads_cH2O)**.

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

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

18 In the **Scale** text field, type `cH2O_ads_scale`.

19 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 2** click **Adsorbed concentration (comp2.tds.cads_cO2)**.

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

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

22 In the **Scale** text field, type `cO2_ads_scale`.

Set the scaling factors for all surface species dependent variables.

23 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 2** click **Surface concentration (comp2.tds.csurf_H)**.

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

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

26 In the **Scale** text field, type `cH_surf_scale`.

27 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 2** click **Surface concentration (comp2.tds.csurf_O)**.

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

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

30 In the **Scale** text field, type `cO_surf_scale`.

31 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 2** click **Surface concentration (comp2.tds.csurf_OH)**.

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

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

34 In the **Scale** text field, type `cOH_surf_scale`.

35 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 2** click **Surface concentration (comp2.tds.csurf_Rh)**.

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

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

38 In the **Scale** text field, type `cRh_surf_scale`.

39 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)** click **Time-Dependent Solver 1**.

40 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Absolute Tolerance** section.

41 In the **Tolerance factor** text field, type `0.05`.

42 Click to expand the **Time Stepping** section. Find the **Algebraic variable settings** subsection. From the **Error estimation** list, choose **Exclude algebraic**.

43 Right-click **Study 2>Solver Configurations>Solution 2 (sol2)>Time-Dependent Solver 1** and choose **Segregated**.

44 In the **Model Builder** window, expand the **Study 2>Solver Configurations>Solution 2 (sol2)>Time-Dependent Solver 1** node, then click **Segregated 1**.

45 In the **Settings** window for **Segregated**, locate the **General** section.

46 From the **Stabilization and acceleration** list, choose **Anderson acceleration**.

47 In the **Dimension of iteration space** text field, type `5`.

48 In the **Mixing parameter** text field, type `0.9`.

49 In the **Iteration delay** text field, type `1`.

50 Right-click **Study 2>Solver Configurations>Solution 2 (sol2)>Time-Dependent Solver 1>Segregated 1** and choose **Segregated Step**.

51 In the **Settings** window for **Segregated Step**, type `Concentrations` in the **Label** text field.

52 Locate the **General** section. Under **Variables**, click + **Add**.

53 In the **Add** dialog box, in the **Variables** list, choose **Concentration (comp2.cH2)**, **Concentration (comp2.cH2O)**, and **Concentration (comp2.cO2)**.

54 Click **OK**.

55 In the **Settings** window for **Segregated Step**, click to expand the **Method and Termination** section.

56 From the **Jacobian update** list, choose **Once per time step**.

57 Right-click **Segregated 1** and choose **Segregated Step**.

58 In the **Settings** window for **Segregated Step**, type `Surface concentrations` in the **Label** text field.

59 Locate the **General** section. Under **Variables**, click + **Add**.

60 In the **Add** dialog box, in the **Variables** list, choose **Adsorbed concentration (comp2.tds.cads_cH2)**, **Adsorbed concentration (comp2.tds.cads_cH2O)**, **Adsorbed concentration (comp2.tds.cads_cO2)**, **Surface concentration (comp2.tds.csurf_H)**, **Surface concentration (comp2.tds.csurf_O)**, **Surface concentration (comp2.tds.csurf_OH)**, and **Surface concentration (comp2.tds.csurf_Rh)**.

61 Click **OK**.

62 In the **Settings** window for **Segregated Step**, locate the **Method and Termination** section.

63 From the **Jacobian update** list, choose **Once per time step**.

64 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)>Time-Dependent Solver 1>Segregated 1** right-click **Segregated Step** and choose **Delete**.

Add a **Lower Limit** to the surface species dependent variables.

65 Right-click **Study 2>Solver Configurations>Solution 2 (sol2)>Time-Dependent Solver 1>Segregated 1** and choose **Lower Limit**.

66 In the **Settings** window for **Lower Limit**, locate the **Lower Limit** section.

67 In the **Lower limits (field variables)** text field, type `comp2.tds.csurf_Rh 1e-16 comp2.tds.csurf_H 1e-16 comp2.tds.csurf_O 1e-16 comp2.tds.csurf_OH 1e-16`.

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

RESULTS

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 **Study 2/Solution Store 1 (sol3)**.

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

5 In the **z-coordinate** text field, type `-0.5`.

Cut Line 3D 1

1 In the **Results** toolbar, click **Cut Line 3D**.

2 In the **Settings** window for **Cut Line 3D**, locate the **Line Data** section.

3 In row **Point 1**, set **x** to `3*do_reac`.

4 In row **Point 2**, set **x** to `3.7*do_reac`.

Velocity (br)

1 In the **Model Builder** window, under **Results** click **Velocity (br)**.

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

3 Select the **Show units** check box.

The following steps reproduce, in turn, the plots shown in Figure 2, Figure 3, Figure 4, and Figure 5.

Slice

1 In the **Model Builder** window, expand the **Velocity (br)** node, then click **Slice**.

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

3 In the **Planes** text field, type `8`.

4 Locate the **Coloring and Style** section. Click  **Change Color Table**.

5 In the **Color Table** dialog box, select **Rainbow>Spectrum** in the tree.

6 Click **OK**.

Velocity, Surface

1 In the **Model Builder** window, under **Results** click **Velocity (br)**.

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

Surface 1

1 Right-click **Velocity, Surface** and choose **Surface**.

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

3 In the **Expression** text field, type `br.U*1[cm]/br.nu`.

Selection 1

1 Right-click **Surface 1** and choose **Selection**.

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

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

Transparency 1

1 In the **Model Builder** window, right-click **Surface 1** and choose **Transparency**.

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

3 Set the **Transparency** value to **0**.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Velocity, Surface** 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 Locate the **Expression** section. In the **x-component** text field, type `u`.

5 In the **y-component** text field, type `v`.

6 In the **z-component** text field, type `w`.

7 Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type `300`.

8 Locate the **Coloring and Style** section. From the **Color** list, choose **Gray**.

9 In the **Velocity, Surface** toolbar, click **Plot**.

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

Pressure (br)

1 In the **Model Builder** window, under **Results** click **Pressure (br)**.

2 In the **Pressure (br)** toolbar, click **Plot**.

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

Concentration, H2, Surface (tds)

1 In the **Model Builder** window, click **Concentration, H2, Surface (tds)**.

2 In the **Settings** window for **3D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **Automatic**.

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

Surface: pipe

1 In the **Model Builder** window, expand the **Concentration, H2, Surface (tds)** node, then click **Surface 1**.

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

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

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

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

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

Selection 1

1 Right-click **Surface: pipe** and choose **Selection**.

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

3 From the **Selection** list, choose **Outer Bnds**.

Surface: Catalyst

1. In the **Model Builder** window, right-click **Concentration, H2, Surface (tds)** and choose **Surface**.
2. In the **Settings** window for **Surface**, type `Surface: Catalyst` in the **Label** text field.
3. Locate the **Expression** section. In the **Expression** text field, type `1`.
4. Locate the **Title** section. From the **Title type** list, choose **None**.
5. Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
6. From the **Color** list, choose **Gray**.

Selection 1

1. Right-click **Surface: Catalyst** and choose **Selection**.
2. In the **Settings** window for **Selection**, locate the **Selection** section.
3. From the **Selection** list, choose **Bed Bnds**.

Material Appearance 1

1. In the **Model Builder** window, right-click **Surface: Catalyst** and choose **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 **Wood**.

Streamline 1

1. In the **Model Builder** window, right-click **Concentration, H2, Surface (tds)** and choose **Streamline**.
2. In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
3. In the **Number** text field, type `10`.
4. Locate the **Selection** section. Click  **Paste Selection**.
5. In the **Paste Selection** dialog box, type `18` in the **Selection** text field.
6. Click **OK**.
7. In the **Settings** window for **Streamline**, locate the **Coloring and Style** section.
8. Find the **Line style** subsection. From the **Type** list, choose **Ribbon**.
9. In the **Width expression** text field, type `br.U*1[s]`.
10. Find the **Point style** subsection. From the **Color** list, choose **White**.

Concentration, cH2, Isosurface

1. Right-click **Concentration, H2, Surface (tds)** and choose **Isosurface**.

2 In the **Settings** window for **Isosurface**, type `Concentration, cH2, Isosurface` in the **Label** text field.

3 Locate the **Levels** section. From the **Entry method** list, choose **Levels**.

4 In the **Levels** text field, type `range(0.1,0.1,2)`.

5 Locate the **Coloring and Style** section. Click **Change Color Table**.

6 In the **Color Table** dialog box, select **Rainbow>Prism** in the tree.

7 Click **OK**.

Transparency 1

1 Right-click **Concentration, cH2, Isosurface** and choose **Transparency**.

2 In the **Concentration, H2, Surface (tds)** toolbar, click **Plot**.

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

Surface 1

1 In the **Model Builder** window, expand the **Results>Concentration, H2O, Surface (tds)** node, then click **Surface 1**.

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

3 Click **Change Color Table**.

4 In the **Color Table** dialog box, select **Rainbow>Prism** in the tree.

5 Click **OK**.

Concentration, O2, Surface (tds)

1 In the **Model Builder** window, under **Results** click **Concentration, O2, Surface (tds)**.

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

3 From the **Title type** list, choose **Automatic**.

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

Surface: Pipe

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

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

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

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

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

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

Selection 1

1 Right-click **Surface: Pipe** and choose **Selection**.

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

3 From the **Selection** list, choose **Outer Bnds**.

Surface: Catalyst

1 In the **Model Builder** window, right-click **Concentration, O2, Surface (tds)** and choose **Surface**.

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

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

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

Selection 1

1 Right-click **Surface: Catalyst** and choose **Selection**.

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

3 From the **Selection** list, choose **Bed Bnds**.

Material Appearance 1

1 In the **Model Builder** window, right-click **Surface: Catalyst** and choose **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 **Wood**.

Streamline 1

1 In the **Model Builder** window, right-click **Concentration, O2, Surface (tds)** and choose **Streamline**.

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

3 In the **x-component** text field, type `tds.tflux_cO2x`.

4 In the **y-component** text field, type `tds.tflux_cO2y`.

5 In the **z-component** text field, type `tds.tflux_cO2z`.

6 Locate the **Streamline Positioning** section. In the **Number** text field, type `10`.

7 Locate the **Selection** section. Click  **Paste Selection**.

8 In the **Paste Selection** dialog box, type `18` in the **Selection** text field.

9 Click **OK**.

10 In the **Settings** window for **Streamline**, locate the **Coloring and Style** section.

11 Find the **Line style** subsection. From the **Type** list, choose **Ribbon**.

12 In the **Width expression** text field, type `br.U*1[s]`.

13 Find the **Point style** subsection. From the **Color** list, choose **White**.

Concentration, cO2, Isosurface

1 Right-click **Concentration, O2, Surface (tds)** and choose **Isosurface**.

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

3 In the **Expression** text field, type `cO2`.

4 In the **Label** text field, type `Concentration, cO2, Isosurface`.

5 Locate the **Levels** section. From the **Entry method** list, choose **Levels**.

6 In the **Levels** text field, type `range(0.5,0.025,0.9)`.

7 Locate the **Coloring and Style** section. Click **Change Color Table**.

8 In the **Color Table** dialog box, select **Traffic>TrafficFlow** in the tree.

9 Click **OK**.

Transparency 1

1 Right-click **Concentration, cO2, Isosurface** and choose **Transparency**.

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

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

Plot the bulk species concentrations (mol/m^3) in the porous domain.

Porous domain: bulk species

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

2 In the **Settings** window for **1D Plot Group**, type `Porous domain: bulk species` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 3D 1**.

4 From the **Time selection** list, choose **From list**.

5 In the **Times (s)** list, select **1**.

Line Graph 1

1 Right-click **Porous domain: bulk species** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click to expand the **Title** section.

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Molar concentration, bulk`.

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

6 Find the **Include** subsection. Clear the **Solution** check box.

7 Select the **Expression** check box.

Line Graph 2

1 In the **Model Builder** window, right-click **Porous domain: bulk species** and choose **Line Graph**.

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

3 In the **Expression** text field, type `c02`.

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

5 Locate the **Legends** section. Select the **Show legends** check box.

6 Find the **Include** subsection. Clear the **Solution** check box.

7 Select the **Expression** check box.

Line Graph 3

1 Right-click **Porous domain: bulk species** and choose **Line Graph**.

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

3 In the **Expression** text field, type `cH20`.

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

5 Locate the **Legends** section. Select the **Show legends** check box.

6 Find the **Include** subsection. Clear the **Solution** check box.

7 Select the **Expression** check box.

8 In the **Porous domain: bulk species** toolbar, click **Plot**.

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

Plot the species concentrations (mol/m^3) being converted from surface species in the porous domain.

Porous domain: bulk species

Right-click **Porous domain: bulk species** and choose **Duplicate**.

Porous domain: surface species

1 In the **Model Builder** window, expand the **Results>Porous domain: bulk species 1** node, then click **Porous domain: bulk species 1**.

2 In the **Settings** window for **1D Plot Group**, type `Porous domain: surface species` in the **Label** text field.

Line Graph 1

1 In the **Model Builder** window, click **Line Graph 1**.

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

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

4 Locate the **Title** section. In the **Title** text area, type `Molar concentration, surface`.

Line Graph 2

1 In the **Model Builder** window, click **Line Graph 2**.

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

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

Line Graph 3

1 In the **Model Builder** window, click **Line Graph 3**.

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

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

4 Right-click **Line Graph 3** and choose **Duplicate**.

Line Graph 4

1 In the **Model Builder** window, click **Line Graph 4**.

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

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

4 In the **Porous domain: surface species** toolbar, click **Plot**.

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

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

Plot the species concentrations (mol/m^3) being converted from adsorbed species in the porous domain.

Porous domain: bulk species

In the **Model Builder** window, under **Results** right-click **Porous domain: bulk species** and choose **Duplicate**.

Porous domain: adsorbed species

1 In the **Model Builder** window, expand the **Results>Porous domain: bulk species 1** node, then click **Porous domain: bulk species 1**.

2 In the **Settings** window for **1D Plot Group**, type `Porous domain: adsorbed species` in the **Label** text field.

Line Graph 1

1 In the **Model Builder** window, click **Line Graph 1**.

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

3 In the **Expression** text field, type `cads_cH2`.

4 Locate the **Title** section. In the **Title** text area, type `Molar concentration, adsorbed`.

Line Graph 2

1 In the **Model Builder** window, click **Line Graph 2**.

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

3 In the **Expression** text field, type `cads_cO2`.

Line Graph 3

1 In the **Model Builder** window, click **Line Graph 3**.

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

3 In the **Expression** text field, type `cads_cH2O`.

4 In the **Porous domain: adsorbed species** toolbar, click **Plot**.

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

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

Porous domain: bulk species

In the **Model Builder** window, under **Results** right-click **Porous domain: bulk species** and choose **Duplicate**.

Porous domain: all species

1 In the **Model Builder** window, expand the **Results>Porous domain: bulk species 1** node, then click **Porous domain: bulk species 1**.

2 In the **Settings** window for **1D Plot Group**, type `Porous domain: all species` in the **Label** text field.

Bulk: cH2

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, type `Bulk: cH2` in the **Label** text field.

3 Locate the **Title** section. In the **Title** text area, type `Molar concentration`.

Bulk: cO2

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Line Graph 2**.

2 In the **Settings** window for **Line Graph**, type `Bulk: cO2` in the **Label** text field.

Bulk: cH2O

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Line Graph 3**.

2 In the **Settings** window for **Line Graph**, type `Bulk: cH2O` in the **Label** text field.

Bulk: cH2O, Bulk: cO2

1 In the **Model Builder** window, under **Results>Porous domain: all species**, Ctrl-click to select **Bulk: cO2** and **Bulk: cH2O**.

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

Surface: cs_Rh

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Bulk: cO2.1**.

2 In the **Settings** window for **Line Graph**, type `Surface: cs_Rh` in the **Label** text field.

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

Surface: cs_H

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Bulk: cH2O 1**.

2 In the **Settings** window for **Line Graph**, type `Surface: cs_H` in the **Label** text field.

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

Surface: cs_H, Surface: cs_Rh

1 In the **Model Builder** window, under **Results>Porous domain: all species**, Ctrl-click to select **Surface: cs_Rh** and **Surface: cs_H**.

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

Surface: cs_O

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Surface: cs_Rh 1**.

2 In the **Settings** window for **Line Graph**, type `Surface: cs_O` in the **Label** text field.

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

Surface: cs_OH

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Surface: cs_H 1**.

2 In the **Settings** window for **Line Graph**, type `Surface: cs_OH` in the **Label** text field.

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

4 Right-click **Surface: cs_OH** and choose **Duplicate**.

Adsorbed: cads_cH2

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Surface: cs_OH 1**.

2 In the **Settings** window for **Line Graph**, type `Adsorbed: cads_cH2` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `cads_cH2`.

4 Right-click **Adsorbed: cads_cH2** and choose **Duplicate**.

Adsorbed: cads_cO2

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Adsorbed: cads_cH2.1**.

2 In the **Settings** window for **Line Graph**, type `Adsorbed: cads_cO2` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `cads_cO2`.

4 Right-click **Adsorbed: cads_cO2** and choose **Duplicate**.

Adsorbed: cads_cH2O

1 In the **Model Builder** window, under **Results>Porous domain: all species** click **Adsorbed: cads_cO2.1**.

2 In the **Settings** window for **Line Graph**, type `Adsorbed: cads_cH2O` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `cads_cH2O`.

4 In the **Porous domain: all species** toolbar, click **Plot**.

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