Porous Reactor with Injection Needle

Introduction

This example treats the flow field and species distribution in an experimental reactor for studies of heterogeneous catalysis. The application gives an example of the coupling of free and porous media flow in fixed bed reactors. The model was inspired by numerical experiments performed by Professor Finlayson's graduate students in chemical engineering at the University of Washington in Seattle.

Model Definition

The reactor consists of a tubular structure with an injection tube whose main axis is perpendicular to the reactor axis. 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 Reacting Flow in Porous Media interface. This physics interface supports both free-flow domains and porous-media domains.

Because of symmetry, only one half of the reactor is modeled; see Figure 1.

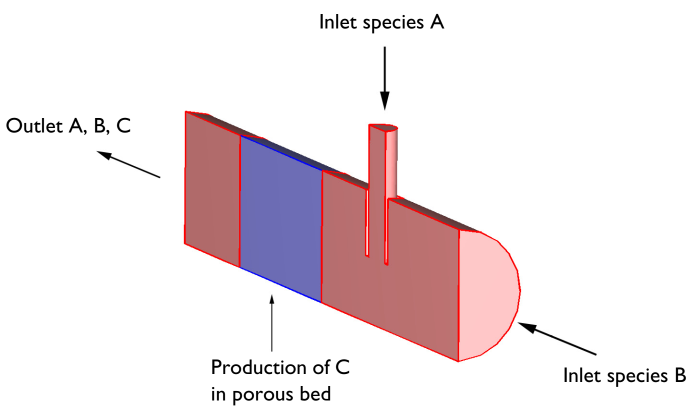


Figure 1: The species A and B enter the reactor from the main and injection tubes, respectively, and react in a fixed porous catalyst bed to produce C.

In the porous bed, a reaction takes place that consumes species A and B and produces C: $A + B \rightarrow C$.

GOVERNING EQUATIONS

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

A Fickian approach for the diffusion term in the mass transport can be utilized by assuming that the modeled species are present in low concentrations compared to the solvent gas. The mass transport for the three species A, B, and C can therefore be modeled with the convection-diffusion equation

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

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·s)). Because the reaction takes place in the porous bed only, the reaction term is zero in the free-flow regions. The reaction is a second order irreversible reaction and the rates are given by

$$\begin{aligned} R_\mathrm{A} &= -k_\mathrm{f} \cdot c_\mathrm{A} \cdot c_\mathrm{B} \\ R_\mathrm{B} &= -k_\mathrm{f} \cdot c_\mathrm{A} \cdot c_\mathrm{B} \\ R_\mathrm{C} &= k_\mathrm{f} \cdot c_\mathrm{A} \cdot c_\mathrm{B} \end{aligned}$$

where k_f is the reaction rate constant, which in turn is temperature dependent according to the Arrhenius law:

$$k_\mathrm{f} = A_\mathrm{f} \cdot \exp\left(\frac{-E_a}{RT}\right)$$

Where A_f is the frequency factor (SI unit: m^3/(mol·s)), E_a is the activation energy (SI unit: J/mol), R the universal gas constant (SI unit: J/(mol·K)), and T the local temperature (SI unit: K). The following data are used for the reaction:

TABLE 1: DATA.

QUANTITY	VALUE
A_f	$1 \cdot 10^6$ m^3/(mol·s)
E_a	$30 \cdot 10^3$ J/mol
R	`R_const` (built in constant)

BOUNDARY CONDITIONS

A constant velocity profile is assumed at the inlet boundaries

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

For the outlet, a pressure condition is applied.

In the mass transport, the concentrations at the inlet are fixed

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

At the outlet, 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, insulating conditions apply

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

Results and Discussion

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

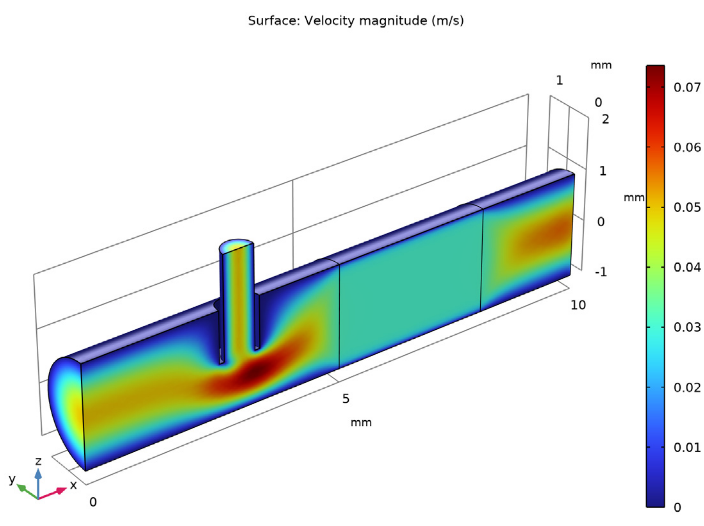


Figure 2: Magnitude of the velocity field in the free and porous reactor domains.

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

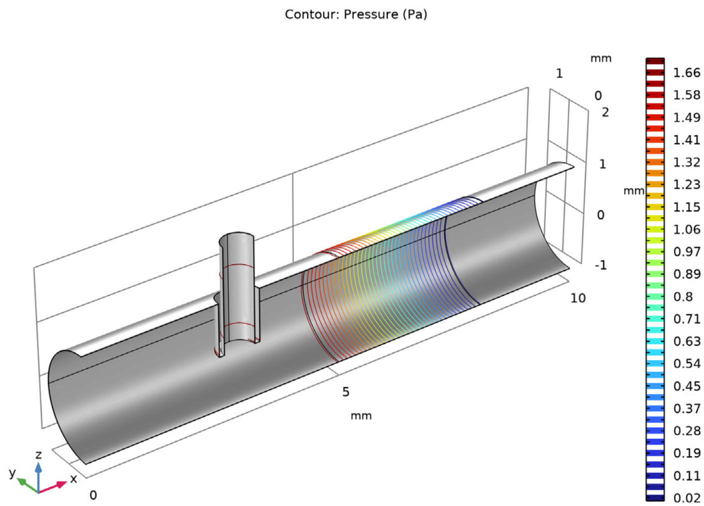


Figure 3: The pressure drop across the reactor.

Figure 4 and Figure 5 show the concentrations of species A and B, respectively.

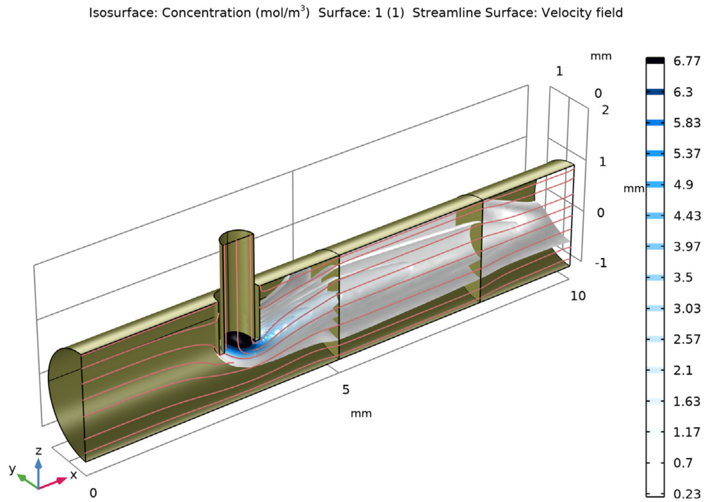


Figure 4: Isoconcentration surfaces for species A.

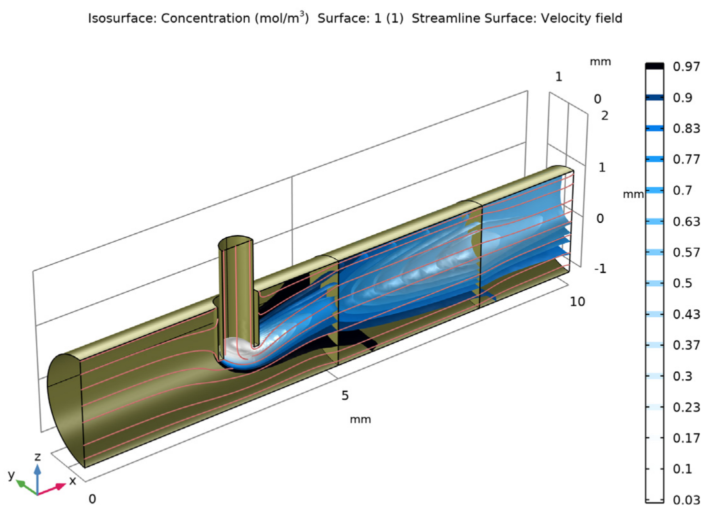


Figure 5: Isoconcentration surfaces for species B.

Figure 4 shows that the concentration of the injected species A decays very rapidly with the distance from the injection point. This implies that the porous bed is not optimally used. Figure 5 shows the isoconcentration surfaces of species B, which is introduced in the main channel of the reactor. The reaction is not uniformly distributed in the catalytic bed and has its maximum close to the radial position of the injection pipe. The low concentration of B at the injection point is due to dilution by the solvent that carries species A.

In summary, the model shows that the injection point is far too close to the porous bed. The reactants are not well mixed and only a fraction of the bed is utilized. A proper design should include a small static mixer after the injection point or a positioning of the injection point further upstream in order to obtain mixing through diffusion.

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 **3D**.

2 In the **Select Physics** tree, select **Chemical Species Transport>Reacting Flow in Porous Media>Transport of Diluted Species**.

3 Click **Add**.

4 In the **Added physics interfaces** tree, select **Transport of Diluted Species in Porous Media (tds)**.

5 In the **Number of species** text field, type 3.

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

c_A
c_B
c_C

7 Click **Study**.

8 In the **Select Study** tree, select **General Studies>Stationary**.

9 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

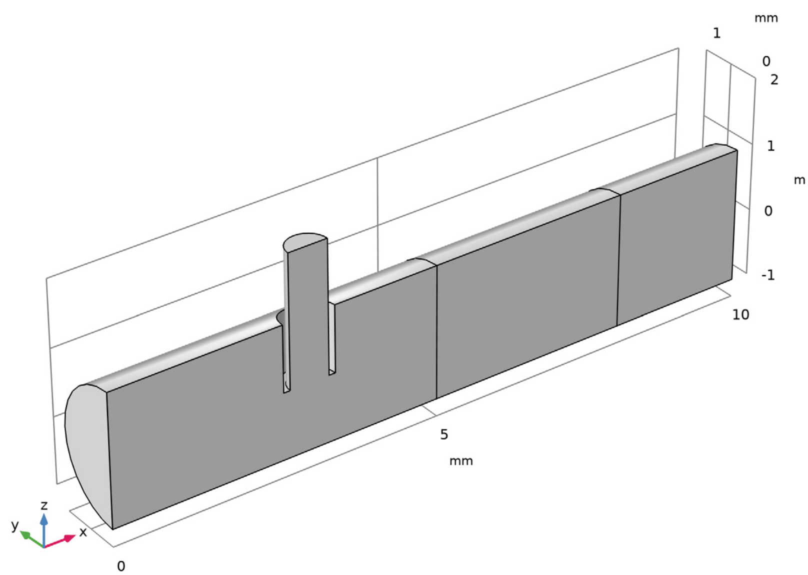
1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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

3 Click **Load from File**.

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

Create the geometry. To simplify this step, insert a prepared geometry sequence. In the **Geometry** toolbar, click **Insert Sequence**. Browse to the model's Application Libraries folder and double-click the file `porous_reactor.mph`. Then click **Build All** In the **Geometry** toolbar.



DEFINITIONS (COMP1)

Catalyst bed

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

2 Right-click **Explicit 1** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Catalyst bed` in the **New label** text field.

4 Click **OK**.

5 Select Domain 2 only.

Symmetry plane

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

2 In the **Model Builder** window, right-click **Explicit 2** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Symmetry plane` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

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

7 Select Boundaries 2, 12, and 16 only.

Inlet species B

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

2 Right-click **Explicit 3** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Inlet species B` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

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

7 Select Boundary 1 only.

Inlet species A

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

2 In the **Model Builder** window, right-click **Explicit 4** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Inlet species A` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

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

7 Select Boundary 8 only.

Outlet

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

2 Right-click **Explicit 5** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Outlet` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

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

7 Select Boundary 19 only.

Ball 1

1 In the **Model Builder** window, right-click **Selections** and choose **Ball**.

2 In the **Settings** window for **Ball**, locate the **Geometric Entity Level** section.

3 From the **Level** list, choose **Boundary**.

4 Locate the **Ball Radius** section. In the **Radius** text field, type `15`.

5 Click the **Zoom to Selection** button in the **Graphics** toolbar.

Walls and free-porous media interfaces

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

2 In the **Settings** window for **Difference**, type `Walls and free-porous media interfaces` 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 **Ball 1** 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, in the **Selections to subtract** list, choose **Symmetry plane**, **Inlet species B**, **Inlet species A**, and **Outlet**.

10 Click **OK**.

Variables 1

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

2 In the **Settings** window for **Variables**, 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 **Variables** section. Click **Load from File**.

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

MATERIALS

Note that a **Porous Material** node has been created automatically when adding an entry from the **Reacting Flow in Porous Media** branch. Now add Nitrogen from the **Material Library** to define the fluid properties in the model.

Add Material

From the **Home** menu, choose **Add Material**.

ADD MATERIAL

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

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

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

4 From the **Home** menu, choose **Add Material**.

MATERIALS

Nitrogen (mat1)

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

2 From the **Selection** list, choose **All domains**.

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

4 Right-click **Component 1 (comp1)>Materials>Nitrogen (mat1)** and choose **Move Up**.

Porous Material 1 (pmat1)

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

2 Select Domain 2 only.

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

4 In the table, enter the following settings:

Property	**Variable**	**Value**	**Unit**	**Property group**
Permeability	kappa_iso ; kappaii = kappa_iso, kappaij = 0	1e-9	m²	Basic

Fluid (pmat1.fluid)

1 In the **Model Builder** window, expand the **Porous Material 1 (pmat1)** node, then click **Fluid (pmat1.fluid)**.

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

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

Solid (pmat1.solid)

1 In the **Model Builder** window, click **Solid (pmat1.solid)**.

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

3 In the θ_s text field, type `0.7`.

GLOBAL DEFINITIONS

Default Model Inputs

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

2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.

3 In the tree, select **General>Temperature (K) - minput.T**.

4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type `T_iso`.

BRINKMAN EQUATIONS (BR)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Brinkman Equations (br)**.

2 In the **Settings** window for **Brinkman Equations**, locate the **Physical Model** section.

3 Clear the **Neglect inertial term (Stokes flow)** check box.

Fluid Properties 1

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

2 Select Domains 1 and 3 only.

Inlet 1

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

2 Select Boundary 1 only.

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

4 From the **Selection** list, choose **Inlet species B**.

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

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

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 A**.

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

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

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 Select Boundaries 2, 12, and 16 only.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Diluted Species in Porous Media (tds)>Porous Medium 1** click **Fluid 1**.

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

3 In the $D_{F,cA}$ text field, type `1e-6[m^2/s]`.

4 In the $D_{F,cB}$ text field, type `1e-6[m^2/s]`.

5 In the $D_{F,cC}$ text field, type `1e-6[m^2/s]`.

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

Transport Properties 1

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

2 Select Domains 1 and 3 only.

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

4 In the D_{cA} text field, type `1e-6[m^2/s]`.

5 In the D_{cB} text field, type `1e-6[m^2/s]`.

6 In the D_{cC} text field, type `1e-6[m^2/s]`.

Reactions 1

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

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

3 From the **Selection** list, choose **Catalyst bed**.

4 Locate the **Reaction Rates** section. In the R_{cA} text field, type `-k_f*c_A*c_B`.

5 In the R_{cB} text field, type `-k_f*c_A*c_B`.

6 In the R_{cC} text field, type `k_f*c_A*c_B`.

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 B**.

4 Locate the **Concentration** section. In the $c_{0,\mathrm{cB}}$ text field, type `1[mol/m^3]`.

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 A**.

4 Locate the **Concentration** section. In the $c_{0,\mathrm{cA}}$ text field, type `7[mol/m^3]`.

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**.

MESH 1

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

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

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

The **Size 1** node added by default refines the mesh on boundaries corresponding to walls. Duplicate this node and apply the same settings to the boundaries corresponding to the needle symmetry plane and the needle outlet to refine the mesh on these boundaries as well.

Size 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** right-click **Size 1** and choose **Duplicate**.
2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
3 Click **Clear Selection**.
4 Select Boundaries 20 and 21 only.
5 Drag and drop below **Size 1**.
6 Click **Build All**.

STUDY 1

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

RESULTS

Velocity (br)

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

Velocity, Surface

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.
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 **Velocity, Surface** toolbar, click **Plot**.
3 Click the **Zoom Extents** button in the **Graphics** toolbar.

Pressure (br)

1 Click the **Zoom Extents** button in the **Graphics** toolbar.
2 In the **Model Builder** window, under **Results** click **Pressure (br)**.
3 In the **Pressure (br)** toolbar, click **Plot**.

Symmetry surface

1 In the **Model Builder** window, expand the **Results>Datasets** node.
2 Right-click **Results>Datasets** and choose **Surface**.
3 In the **Settings** window for **Surface**, type `Symmetry surface` in the **Label** text field.
4 Locate the **Selection** section. From the **Selection** list, choose **Symmetry plane**.

Concentration, c_A, Isosurface

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

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

Isosurface 1

1 Right-click **Concentration, c_A, Isosurface** and choose **Isosurface**.

2 In the **Settings** window for **Isosurface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Transport of Diluted Species in Porous Media>Species c_A>c_A - Concentration - mol/m³**.

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

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

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

Surface 1

1 In the **Model Builder** window, right-click **Concentration, c_A, Isosurface** and choose **Surface**.

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

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

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

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

6 On Windows, click the colored bar underneath, or — if you are running the cross-platform desktop — the **Color** button.

7 Click **Define custom colors**.

8 Set the RGB values to 128, 128, and 64, respectively.

9 Click **Add to custom colors**.

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

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 **Walls and free-porous media interfaces**.

4 In the **Concentration, c_A, Isosurface** toolbar, click **Plot**.

Concentration, c_A, Isosurface

In the **Model Builder** window, under **Results** click **Concentration, c_A, Isosurface**.

Streamline Surface 1

1 In the **Concentration, c_A, Isosurface** toolbar, click **More Plots** and choose **Streamline Surface**.

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

3 From the **Dataset** list, choose **Symmetry surface**.

4 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Uniform density**.

5 In the **Separating distance** text field, type `0.027`.

6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Tube**.

7 In the **Tube radius expression** text field, type `0.01`.

8 Select the **Radius scale factor** check box.

9 Find the **Point style** subsection. From the **Color** list, choose **Custom**.

10 On Windows, click the colored bar underneath, or — if you are running the cross-platform desktop — the **Color** button.

11 Click **Define custom colors**.

12 Set the RGB values to 255, 128, and 128, respectively.

13 Click **Add to custom colors**.

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

15 In the **Concentration, c_A, Isosurface** toolbar, click **Plot**.

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

Concentration, c_B, Isosurface

1 Right-click **Concentration, c_A, Isosurface** and choose **Duplicate**.

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

Isosurface 1

1 In the **Model Builder** window, expand the **Concentration, c_B, Isosurface** node, then click **Isosurface 1**.

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

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

4 In the **Concentration, c_B, Isosurface** toolbar, click **Plot**.

Concentration, c_C, Isosurface

1 In the **Model Builder** window, right-click **Concentration, c_B, Isosurface** and choose **Duplicate**.

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

Isosurface 1

1 In the **Model Builder** window, expand the **Concentration, c_C, Isosurface** node, then click **Isosurface 1**.

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

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

4 In the **Concentration, c_C, Isosurface** toolbar, click **Plot**.