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.

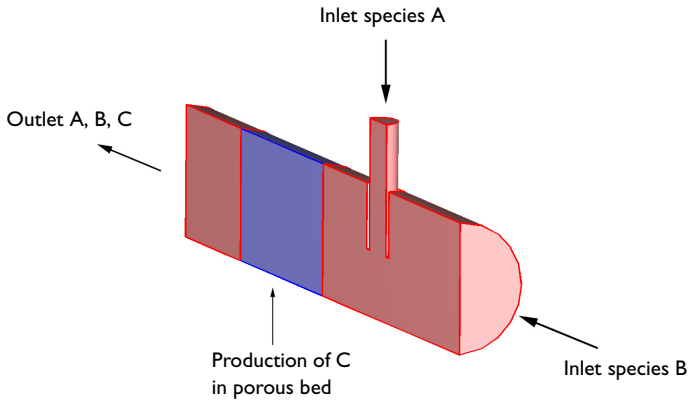


Figure 1: The species A and B enter the reactor from the main and injection tubes, respectively, and react in a fixed porous catalyst bed to produce C.

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

$$R_\mathrm{A} = -k_\mathrm{f} \cdot c_\mathrm{A} \cdot c_\mathrm{B}$$
$$R_\mathrm{B} = -k_\mathrm{f} \cdot c_\mathrm{A} \cdot c_\mathrm{B}$$
$$R_\mathrm{C} = k_\mathrm{f} \cdot c_\mathrm{A} \cdot c_\mathrm{B}$$

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 contant)

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

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

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.

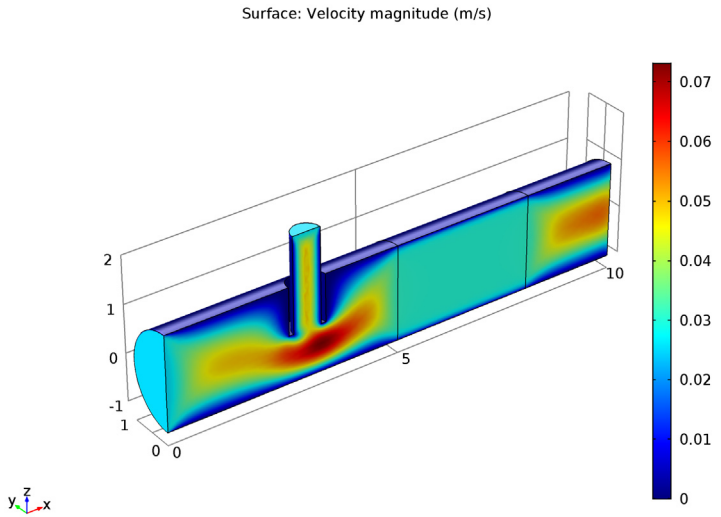


Figure 2: Magnitude of the velocity field in the free and porous reactor domains.

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

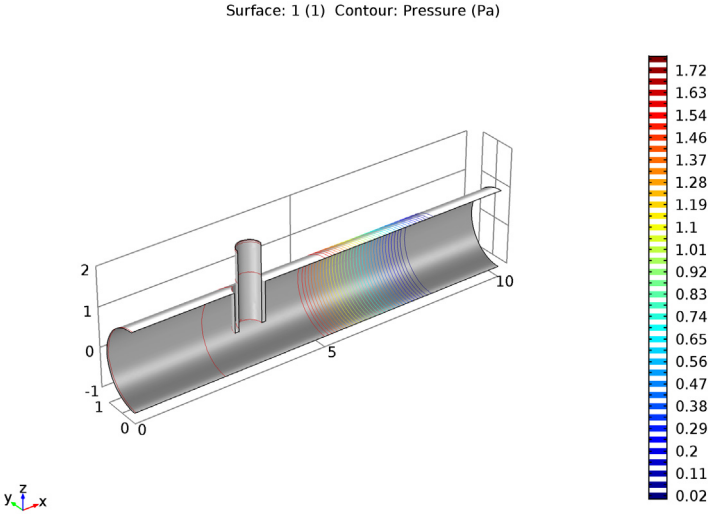


Figure 3: The pressure drop across the reactor.

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

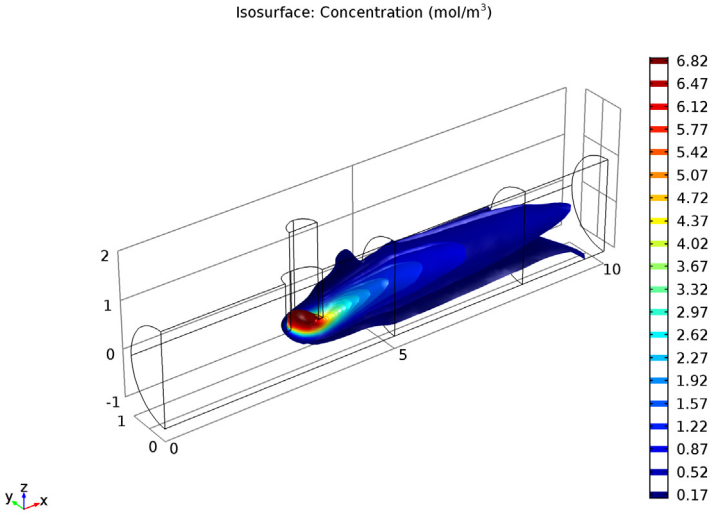


Figure 4: Isoconcentration surfaces for species A.

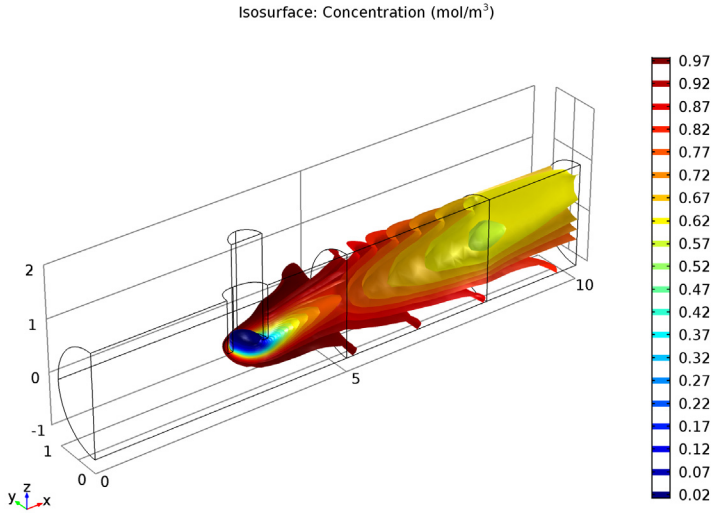


Figure 5: Isoconcentration surfaces for species B.

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

1 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 (rfds)**.

3 Click **Add**.

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

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

c_A
c_B
c_C

6 Click **Study**.

7 In the **Select study** tree, select **Preset Studies>Stationary**.

8 Click **Done**.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

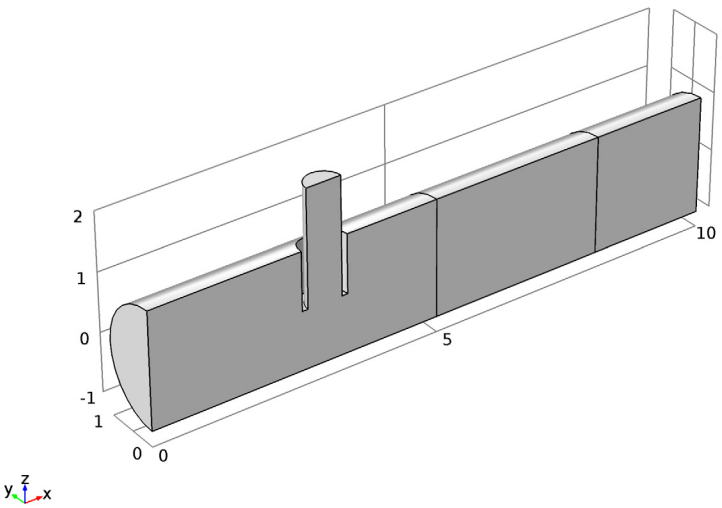
2 In the **Settings** window for Parameters, locate the **Parameters** section.

3 Click **Load from File**.

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

GEOMETRY 1

Create the geometry. To simplify this step, insert a prepared geometry sequence. On the Geometry toolbar, click Insert Sequence. Browse to the model's Model Library folder and double-click the file porous_reactor.mph. The click Build all on the Geometry toolbar.



DEFINITIONS

Explicit 1

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

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

Explicit 2

1 On 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.

Explicit 3

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

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

Explicit 4

1 On 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.

Explicit 5

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

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

Variables 1

1 In the **Model Builder** window, 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 application's Application Library folder and double-click the file `porous_reactor_variables.txt`.

ADD MATERIAL

1 On 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 On the **Home** toolbar, click **Add Material** to close the **Add Material** window.

REACTING FLOW IN POROUS MEDIA (RFDS)

Transport Properties 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Reacting Flow in Porous Media (rfds)** node, then click **Transport Properties 1**.

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

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

4 Locate the **Diffusion** section. 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]`.

Porous Matrix Properties 1

1 On the **Physics** toolbar, click **Domains** and choose **Porous Matrix Properties**.

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

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

4 Locate the **Porous Matrix Properties** section. From the ε_p list, choose **User defined**. In the associated text field, type `0.3`.

5 From the κ list, choose **User defined**. In the associated text field, type `1e-9[m^2]`.

6 From the **Effective mass transport parameters** list, choose **Bruggeman**.

Reactions 1

1 On 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 **Reactions** 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`.

Inlet 1

1 On 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 B**.

4 Locate the **Velocity** section. In the U_0 text field, type `2.5[cm/s]`.

Inlet 2

1 On 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 **Velocity** section. In the U_0 text field, type `2.5[cm/s]`.

Outlet 1

1 On 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 On 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 On 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 On 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 2

1 On 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**.

Symmetry 2

1 On 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

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Build All**.

STUDY 1

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

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

RESULTS

Velocity (rfds)

1 In the **Model Builder** window, expand the **Velocity (rfds)** node.

2 Right-click **Slice 1** and choose **Disable**.

3 Right-click **Velocity (rfds)** and choose **Surface**.

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

5 On the **Velocity (rfds)** toolbar, click **Plot**.

Pressure (rfds)

1 Click the **Zoom Extents** button on the **Graphics** toolbar.

2 In the **Model Builder** window, under **Results** click **Pressure (rfds)**.

3 On the **Pressure (rfds)** toolbar, click **Plot**.

Concentration (rfds)

1 In the **Model Builder** window, under **Results** right-click **Concentration (rfds)** and choose **Rename**.

2 In the **Rename 3D Plot Group** dialog box, type `Concentration species A` in the **New label** text field.

3 Click **OK**.

Concentration species A

1 In the **Model Builder** window, expand the **Results>Concentration species A** node.

2 Right-click **Surface 1** and choose **Disable**.

3 Right-click **Concentration species A** and choose **Isosurface**.

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

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

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

7 On the **Concentration species A** toolbar, click **Plot**.

Concentration species A 1

1 Right-click **Concentration species A** and choose **Duplicate**.

2 In the **Model Builder** window, under **Results** right-click **Concentration species A 1** and choose **Rename**.

3 In the **Rename 3D Plot Group** dialog box, type `Concentration species B` in the **New label** text field.

4 Click **OK**.

Concentration species B

1 In the **Model Builder** window, expand the **Results>Concentration species B** node, then click **Isosurface 1**.

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>Reacting Flow in Porous Media (Transport of Diluted Species)>Species c_B>c_B - Concentration**.

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

4 On the **Concentration species B** toolbar, click **Plot**.