Created in COMSOL Multiphysics 6.0

# A Multiscale 3D Packed Bed Reactor

## *Introduction*

The packed bed reactor is used in heterogeneous catalytic processes and is one of the most common reactors in the chemical industry. Its basic design is a column filled with porous catalyst particles, and in some cases the reactor also has a specially designed bottom plate through which the reaction mixture enters. The catalyst particles can be contained within a supporting structure, such as tubes or channels, or they can be packed in one single compartment in the reactor.

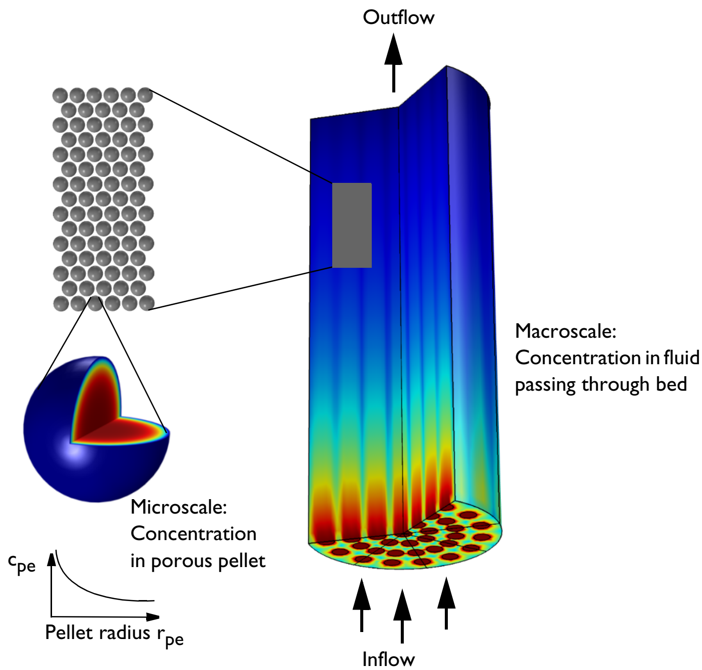


*Figure 1: An example of the macroscale (bed volume with entry holes) and the microscale (pellet) of a packed bed reactor.*

The bed with the packed catalyst particles makes the modeling of mass transport and reactions in the reactor a challenge. The challenge is that species transport and reaction occur in dimensions of different orders of magnitude:

- In the macropores between the dumped pellets, and
- inside the catalyst pellets in micropores.

As such, the problem is regarded as a *multiscale* problem. The Reactive Pellet Bed feature, available with the Transport of Diluted Species interface, is dedicated to these multiscale problems.

The structure between particles in the bed is described as a *macroporous* material of meter dimensions. The particle radii are often in the order of 1 mm. The pores inside the catalyst particles form the microscale structure of the bed. The pore radii in the particles are often between 1 and 10 microns. There are two porosities that are important: bed porosity (macroscale) and pellet porosity (microscale). Sometimes such models are called *double-porosity models*.

When a pressure drop is applied across the bed, flow and convection of the fluid is initiated in the bed. The transport of chemicals inside the pellets are dominated by diffusion.

This model is an extension to the 1D example, Packed Bed Reactor, which contains more complex reactions.

## Model Definition

A model geometry made up of one eighth of the reactor in Figure 1 can be used due to symmetry. The geometry is shown in Figure 2.

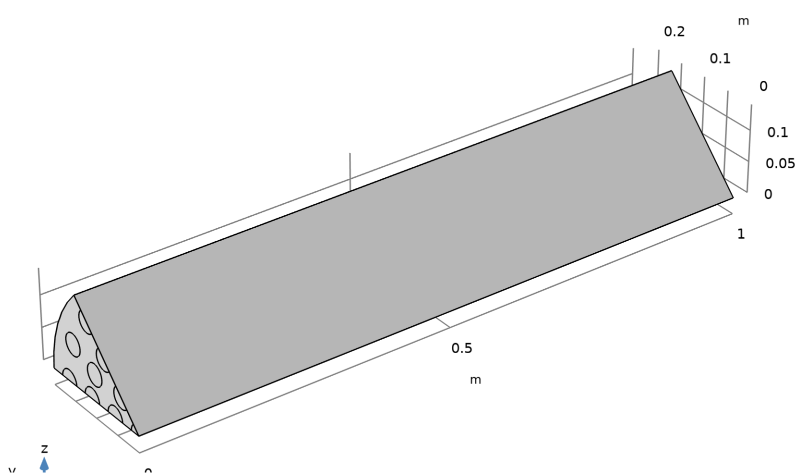


*Figure 2: The packed bed reactor simulation geometry. Symmetry observations enables modeling of 1/8 of the true geometry. The results will be expanded to the true geometry with aid of a sector data set.*

The reversible catalytic chemical reaction occurs inside a pellet. The reactant species $A$ and $B$ forms a product $C$:

$$A + B \leftrightarrow 2C$$

The reaction kinetics are assumed to be equimolecular and are set up with the Chemistry interface. The automatic reaction rate can thus be used and has the following form:

$$r = k^f c_A c_B - k^r c_C^2$$

where $k$ is the rate factor (SI unit: $m^3/(mol \cdot s)$) with the superscripts $f$ and $r$ denoting the forward and reverse reaction, respectively. $c_i$ is the concentration (SI unit: $mol/m^3$) of species $i$. The forward reaction constant is defined with the inbuilt Arrhenius expression and the reverse is computed with the equilibrium constant of the reaction.

The mass transport of the reacting species in the reactor is modeled with the Transport of Diluted Species interface, which accounts for diffusion, convection, and reaction in diluted solutions. The species are assumed to be diluted in water.

The reaction inside the pellets is added to the mass balances in the Transport of Diluted Species interface with the Reactive Pellet Bed feature. This feature has a predefined extra dimension (1D) on the normalized radius ($r = r_{\mathrm{dim}}/r_{\mathrm{pe}}$) of the pellet particle. The mesh on the extra dimension has a default of 10 elements with a cubic root sequence distribution. If spherical pellets are selected, the following spherical diffusion/reaction equation is set up and solved along the pellet radius for each species $i$:

$$4\pi N\left\{r^2 {r_{\mathrm{pe}}}^2 \varepsilon_{\mathrm{pe}} \frac{\partial c_{\mathrm{pe},i}}{\partial t} + \frac{\partial}{\partial r}\left(-r^2 D_{\mathrm{pe},i} \frac{\partial c_{\mathrm{pe},i}}{\partial r}\right) = r^2 {r_{\mathrm{pe}}}^2 R_{\mathrm{pe},i}\right\} \quad (1)$$

Here, $r$ is a dimensionless radial coordinate that goes from 0 (center) to 1 (pellet surface), $r_{\mathrm{pe}}$ is the pellet radius, and $N$ the number of pellets per unit volume of bed. The advantage of formulating Equation 1 on a dimensionless 1D geometry is that the pellet radius can be changed without changing the geometry limits.

$D_{\mathrm{pe}}$ is an effective diffusion coefficient (SI unit: $m^2/s$) and $R_{\mathrm{pe},\,i}$ is the reaction source term (SI unit: $mol/(m^3 \cdot s)$). Note that the latter term is taken per unit volume of porous pellet material.

At the pellet-fluid interface, a film condition assumption is made. The flux of mass across the pellet-fluid interface into the pellet is possibly rate determined by the resistance to mass transfer on the bulk fluid side. The resistance is expressed in terms of a film mass transfer coefficient, $h_{D\mathrm{i}}$, such that:

$$N_{i,\mathrm{inward}} = h_{D,\,i}(c_i - c_{\mathrm{pe},\,i}), \quad (2)$$

where $N_{i,\text{ inward}}$ is the molar flux from the free fluid into a pellet and has the unit moles/ $(\text{m}^2\cdot\text{s})$. The mass transfer coefficient to calculated automatically as described in the section *Theory for the Reactive Pellet Bed* in the *Chemical Reaction Engineering Module User's Guide*.

The pressure drop in the reactor is also accounted for and is modeled with the Darcy's Law interface.

In Table 1 the model parameters are tabulated.

TABLE 1: SUMMARY OF INPUT DATA.

| PROPERTY | VALUE | DESCRIPTION |
|---|---|---|
| $H_r$ | 1 [m] | Height of the packed bed reactor |
| $R_r$ | 0.2 [m] | Radius of packed bed reactor |
| $\rho_b$ | 0.51 [g/cm$^3$] | Density of packed bed |
| $\rho_{pe}$ | 0.68 [g/cm$^3$] | Density individual pellet |
| $\varepsilon_b$ | 1-$\rho_b/\rho_{pe}$ | Macroscale porosity (of bed) |
| $\varepsilon_{pe}$ | 0.70 (-) | Microscale porosity (of pellet) |
| $r_{pe}$ | 0.5 [mm] | Pellet radius (spherical shape) |
| $D_{pe,A}$ | 1.5e-9 [m$^2$/s] | Diffusion coefficient of A in pellet |
| $D_{pe,B}$ | 2e-9 [m$^2$/s] | Diffusion coefficient of B in pellet |
| $D_{pe,C}$ | 0.5e-9 [m$^2$/s] | Diffusion coefficient of C in pellet |
| $A$ | 2e12 [m$^3$/(mol s)] | Frequency factor reaction |
| $E$ | 75000[J/mol] | Activation energy reaction |
| $K_{eq0}$ | 1000 | Equilibrium reaction constant |
| kappa | 1.88e-10[m$^2$] | Permeability of Bed |
| $C_{A,in}$ | 1[mol/m$^3$] | Inlet concentration A |
| $C_{B,in}$ | 1[mol/m$^3$] | inlet concentration B |
| $C_{C,in}$ | 0[mol/m$^3$] | inlet concentration C |
| $D_A$ | 1e-8 [m$^2$/s] | Diffusion coefficient of A in bed |
| $D_B$ | 1.5e-8 [m$^2$/s] | Diffusion coefficient of B in bed |
| $D_C$ | 0.5e-8 [m$^2$/s] | Diffusion coefficient of C in bed |
| $p_{Darcy}$ | 0.4 [atm] | Inlet pressure offset |

## *Results and Discussion*

The following figures display the results at 180 s. Figure 3 shows the velocity distribution in the fluid between the pellets.

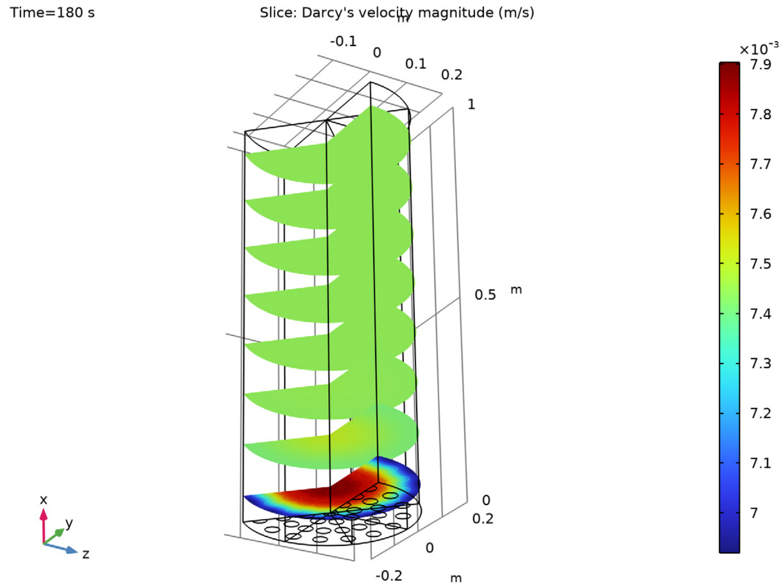


*Figure 3: Velocity distribution on the macroscale.*

Figure 4 shows the macroscale concentration of the reactant $A$ in the bed column fluid. The species is consumed due to the catalytic chemical reaction in the pellets.

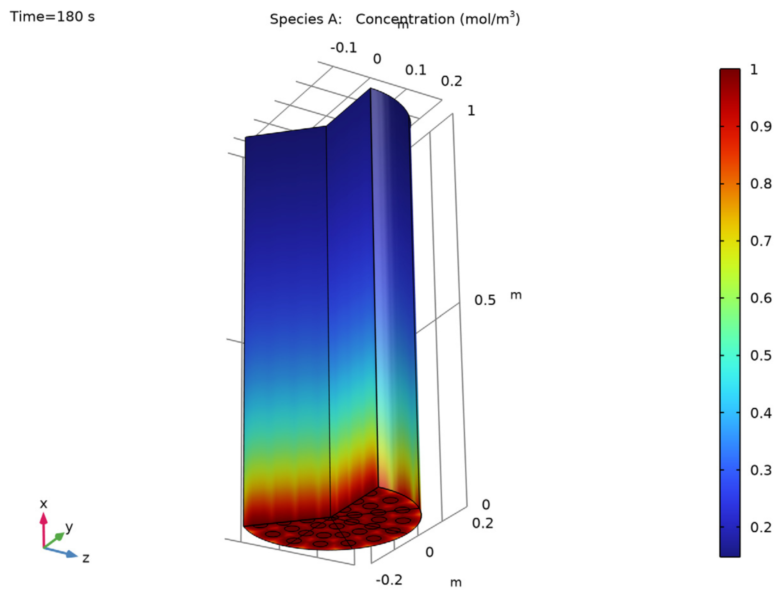


*Figure 4: Concentration of reactant A.*

Streamline plots can be useful to get an understanding of the flow pattern. It can be seen from Figure 5 that no recirculation occurs at the entry holes. The fluid is evenly spread out in the bed chamber as it enters the holes in the bottom place.

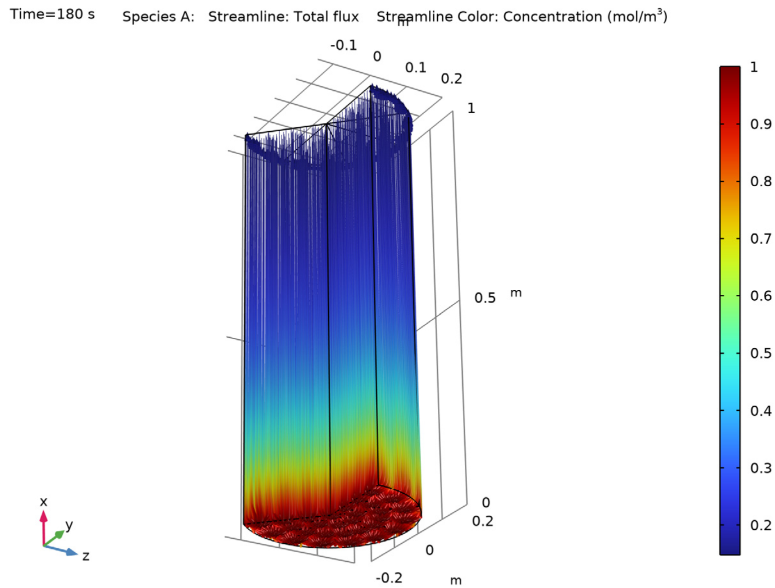


*Figure 5: The streamlines show how the fluid enters the holes and then spread out in the bed volume as it. The colors of the lines represent the reactant concentration in moles/m$^3$.*

A line plot of the concentration in a pellet at a certain position in the bed is interesting in order to understand the local reaction. Figure 6 shows the position at which the pellet line plot is sampled: ($x = 0.5, z = 0, y = 0$), and Figure 7 is the line plot of both the reactant and the product inside a pellet in the same position.

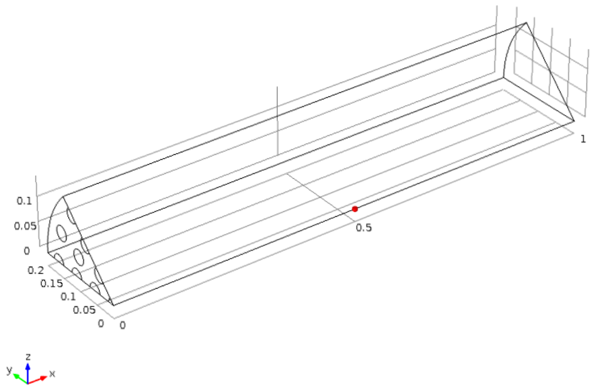


*Figure 6: Coordinate at which the pellet plot is sampled: Centerline of reactor and at 0.5 m height.*

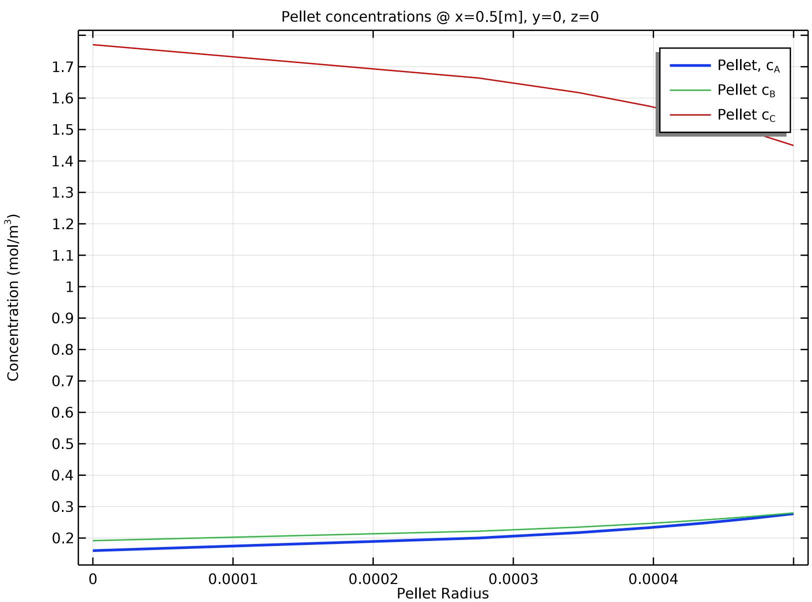


*Figure 7: Concentration of species A, B and C within the pellet at 0.5 m bed height.*

In Figure 8, the concentrations of the species are shown along the reactor height in the center of the geometry. Both the concentrations in the bed and averaged in the pellets are shown and illustrates the local reaction in detail. The species C concentration profiles portray a reaction intense zone within the reactor. A closer look at this zone shows it expanding toward the outlet with time.

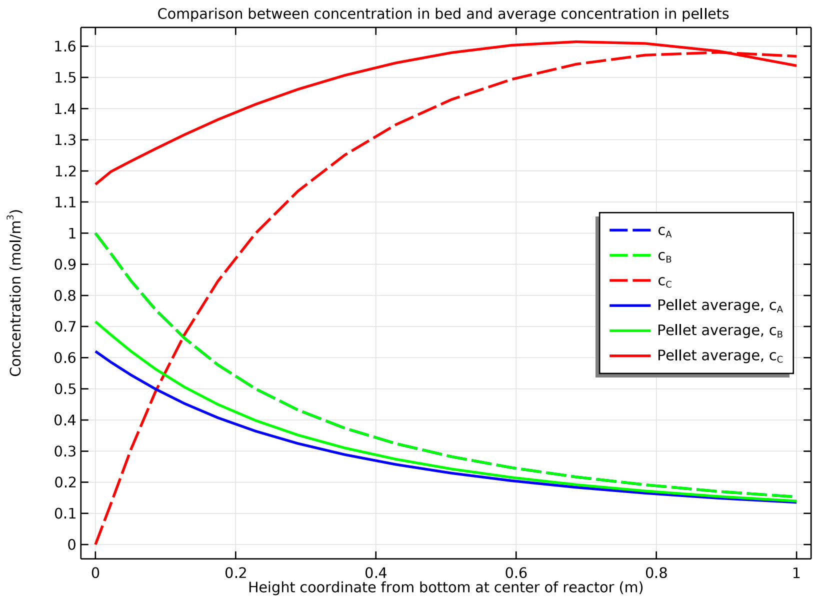


*Figure 8: Concentration of the species in reactor bed and averaged within the pellets along the reactor height.*

Figure 9 shows a 3D concentration plot of the product C within the pellet at the sampled coordinate. It can be seen that the concentration is higher closer to the center of the pellet, where products build up and from where these diffuse into the bulk gas.

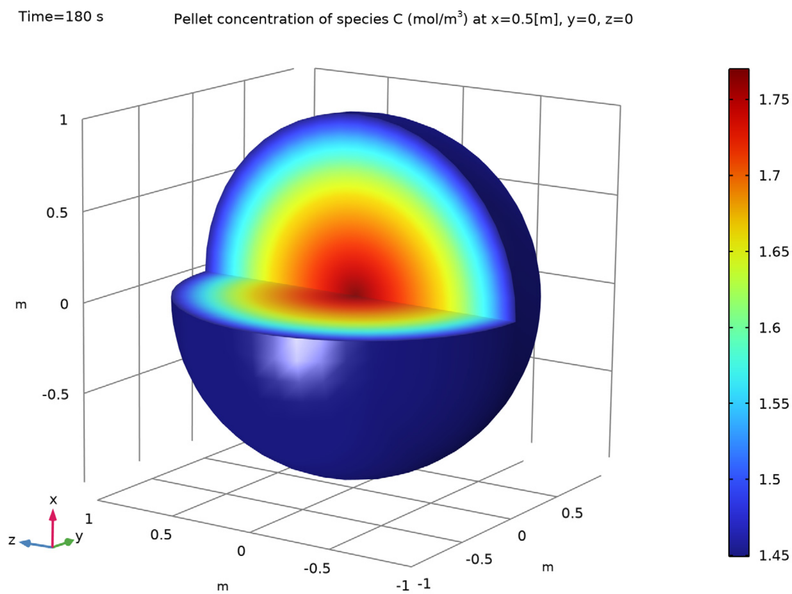


*Figure 9: Concentration of species C at 0.5 m bed height.*

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**Application Library path:** `Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/packed_bed_reactor_3d`

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## *Modeling Instructions*

Start by adding the necessary physics interfaces for a 3D model.

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>Chemistry (chem)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Chemical Species Transport>Transport of Diluted Species in Porous Media (tds)**.

5 Click **Add**.

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

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

| |
|---|
| cA |
| cB |
| cC |

8 In the **Select Physics** tree, select **Fluid Flow>Porous Media and Subsurface Flow>Darcy's Law (dl)**.

9 Click **Add**.

10 Click **Study**.

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

12 Click **Done**.

## GEOMETRY 1

Add the model parameters from a text file.

## 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 `packed_bed_reactor_3d_parameters.txt`.

## GEOMETRY 1

Now create the geometry. You can simplify this by inserting a prepared geometry sequence from a file with prepared geometry selections.

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

2 Right-click **Component 1 (comp1)>Geometry 1** and choose **Insert Sequence**.

**3** Browse to the model's Application Libraries folder and double-click the file `packed_bed_reactor_3d_geom_sequence.mph`.

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

Create a global material. Some properties can be found in the COMSOL built-in materials, other are manually entered.

Assume the reaction mixture has mainly aqueous properties.

### 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 **Built-in>Water, liquid**.

**4** Click **Add to Global Materials** in the window toolbar.

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

Define a porous material for the **Reactive Pellet Bed** feature.

### MATERIALS

#### *Porous Material 1 (pmat1)*

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **More Materials>Porous Material**.

#### *Pellet 1 (pmat1.pellet1)*

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

Enter the properties of the reactive pellet bed.

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

**3** From the **Material** list, choose **Locally defined**.

**4** In the $d_{\mathrm{pe}}$ text field, type `r_pe*2`.

**5** In the $\varepsilon_{\mathrm{pe}}$ text field, type `epsilon_pe`.

**6** Locate the **Pellet Bed Properties** section. In the $\varepsilon p$ text field, type `epsilon_b`.

#### *Fluid 1 (pmat1.fluid1)*

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

## TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

*Packed Bed 1*

Add the **Packed Bed** feature. A extra dimension from porous material is attached to this feature. The extra dimension is 1D on the radial coordinate of the pellet particle of which the radius is normalized to 1. The mesh for the extra dimension has a default of 6 elements with a cubic root sequence distribution.

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Transport of Diluted Species in Porous Media (tds)** and choose **Packed Bed**.
2. In the **Settings** window for **Packed Bed**, locate the **Domain Selection** section.
3. From the **Selection** list, choose **All domains**.

## CHEMISTRY (CHEM)

Go to the **Chemistry** interface and create the needed reaction kinetics expressions by typing in the reaction formulas.

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Chemistry (chem)**.
2. In the **Settings** window for **Chemistry**, locate the **Mixture Properties** section.
3. From the **Phase** list, choose **Liquid**.

*Reaction 1*

1. In the **Physics** toolbar, click **Domains** and choose **Reaction**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `A+B<=>2C`.
4. Click **Apply**.
5. Locate the **Rate Constants** section. Select the **Specify equilibrium constant** check box.
6. Select the **Use Arrhenius expressions** check box.
7. In the $A^{\mathrm{f}}$ text field, type `A`.
8. In the $E^{\mathrm{f}}$ text field, type `E`.
9. Locate the **Equilibrium Settings** section. From the **Equilibrium constant** list, choose **User defined**.
10. In the $K_{\mathrm{eq0}}$ text field, type `Keq0`.

The molar masses for the reacting species can be entered for possible future use. For example, if the mass-based Concentrations feature is used in the **Transport of Diluted Species** interface, it can pick up the molar mass values from the **Chemistry** node automatically.

### *Species: A*

1. In the **Model Builder** window, click **Species: A**.
2. In the **Settings** window for **Species**, locate the **General Parameters** section.
3. In the $M$ text field, type `Mn_A`.

### *Species: B*

1. In the **Model Builder** window, click **Species: B**.
2. In the **Settings** window for **Species**, locate the **General Parameters** section.
3. In the $M$ text field, type `Mn_B`.

### *Species: C*

1. In the **Model Builder** window, click **Species: C**.
2. In the **Settings** window for **Species**, locate the **General Parameters** section.
3. In the $M$ text field, type `Mn_C`.

The reactive species are diluted in water. For completeness, add the solvent H2O, which does not partake in the reactions. It can be used later if the model is extended.

### *Species 1*

1. In the **Physics** toolbar, click **Domains** and choose **Species**.
2. In the **Settings** window for **Species**, locate the **Species Name** section.
3. In the text field, type `H2O`.
4. Locate the **Species Type** section. From the list, choose **Solvent**.
5. Locate the **General Parameters** section. In the $M$ text field, type `Mn_solvent`.
6. In the **Model Builder** window, collapse the **Chemistry (chem)** node.

   Select the **Define variables in extra dimension** check box because the **Chemistry** is coupled to the **Reactive Pellet Bed** feature which is defined in extra dimension.
7. In the **Model Builder** window, click **Chemistry (chem)**.
8. In the **Settings** window for **Chemistry**, click to expand the **Pellet Chemistry** section.
9. Select the **Define variables for porous pellets** check box.

   Now tell the **Chemistry** interface which concentrations to use as input for the rate expressions. Select the pellet concentrations. The entries will at this stage appear yellow since the **Reactive Pellet Bed** feature is not yet created.
10. Locate the **Species Matching** section. From the **Species solved for** list, choose **Transport of Diluted Species in Porous Media**.

**11** Find the **Bulk species** subsection. In the table, enter the following settings:

| Species | Type | Molar concentration | Value (mol/m^3) |
|---|---|---|---|
| A | Variable | tds.cpe_cA | Solved for |
| B | Variable | tds.cpe_cB | Solved for |
| C | Variable | tds.cpe_cC | Solved for |
| H2O | Solvent | User defined | `C_solvent` |

Continue with the **Transport of Diluted Species in Porous Media** interface to set up the mass transport model.

The newly added **Packed Bed** feature overwrites the **Porous Media** feature on the domain. So we can skip setting parameters for the overwritten feature.

## TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

### *Fluid 1*

1. In the **Model Builder** window, expand the **Component 1 (comp1)> Transport of Diluted Species in Porous Media (tds)>Packed Bed 1** node, then click **Fluid 1**.
2. In the **Settings** window for **Fluid**, locate the **Convection** section.
3. From the $\mathbf{u}$ list, choose **Darcy's velocity field (dl/porous1)**.
4. Locate the **Diffusion** section. In the $D_{\mathrm{F,cA}}$ text field, type `DA`.
5. In the $D_{\mathrm{F,cB}}$ text field, type `DB`.
6. In the $D_{\mathrm{F,cC}}$ text field, type `DC`.
7. From the **Effective diffusivity model** list, choose **No correction**.

### *Pellets 1*

Enter the user-defined diffusion coefficients.

### *Diffusion 1*

1. In the **Model Builder** window, expand the **Component 1 (comp1)> Transport of Diluted Species in Porous Media (tds)>Packed Bed 1>Pellets 1** node, then click **Diffusion 1**.
2. In the **Settings** window for **Diffusion**, locate the **Diffusion** section.
3. From the **Diffusion model** list, choose **User defined**.
4. In the $D_{\mathrm{peff,cA}}$ text field, type `DAp`.
5. In the $D_{\mathrm{peff,cB}}$ text field, type `DBp`.
6. In the $D_{\mathrm{peff,cC}}$ text field, type `DCp`.

Use the reaction rates calculated in the **Chemistry** interface.

### *Reactions 1*

1. In the **Model Builder** window, click **Reactions 1**.
2. In the **Settings** window for **Reactions**, locate the **Reaction Rates** section.
3. From the $R_{\mathrm{pe,cA}}$ list, choose **Reaction rate for species A (chem)**.
4. From the $R_{\mathrm{pe,cB}}$ list, choose **Reaction rate for species B (chem)**.
5. From the $R_{\mathrm{pe,cC}}$ list, choose **Reaction rate for species C (chem)**.
6. Click to expand the **Reacting Volume** section. From the list, choose **Total volume**.

### *Pellet-Fluid Interface 1*

Use a film theory condition (default) to account for any film resistance to mass transfer between the bulk fluid and the pellet. Use spherical pellets.

### *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**.
4. Locate the **Concentration** section. In the $c_{0,\mathrm{cA}}$ text field, type `CA_in`.
5. In the $c_{0,\mathrm{cB}}$ text field, type `CB_in`.
6. In the $c_{0,\mathrm{cC}}$ text field, type `CC_in`.

### *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**.

## DARCY'S LAW (DL)

Lastly, enter the model specifications for the **Darcy's Law** interface to compute the convective flow in the reactor.

### *Porous Matrix 1*

1. In the **Model Builder** window, under **Component 1 (comp1)>Darcy's Law (dl)>Porous Medium 1** click **Porous Matrix 1**.
2. In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.
3. From the κ list, choose **User defined**. In the associated text field, type `kappa`.

*Pressure 1*

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

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

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

*Pressure 2*

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

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

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

4 Locate the **Pressure** section. In the $p_0$ text field, type `p_Darcy`.

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

First create a free triangular mesh at the reactor inlet and sweep that mesh along the $x$ direction (the height) of the reactor.

## MESH 1

*Free Triangular 1*

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

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

3 From the **Selection** list, choose **Bottom plate**.

*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 **Predefined** list, choose **Fine**.

*Swept 1*

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

*Distribution 1*

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

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

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

4 In the **Number of elements** text field, type `15`.

5 In the **Element ratio** text field, type `5`.

**6** Click **Build All**.

Since this is a one-way problem, it can be solved in two steps in order to consume less memory: First solve the **Darcy's law** interface for the velocity, which is a stationary problem. Then solve the **Transport of Diluted Species** interface with a time dependent study step.

## 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(0,10,180)`.
4. Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Darcy's Law (dl)**.

### *Stationary*

1. In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.
2. In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
3. In the table, clear the **Solve for** check boxes for **Chemistry (chem)** and **Transport of Diluted Species in Porous Media (tds)**.
4. Right-click **Study 1>Step 2: Stationary** and choose **Move Up**.
5. In the **Study** toolbar, click **Compute**.

## RESULTS

1. Click the **Show More Options** button in the **Model Builder** toolbar.
2. In the **Show More Options** dialog box, select **Results>Views** in the tree.
3. In the tree, select the check box for the node **Results>Views**.
4. Click **OK**.

   Create views for plotting different angles of the geometry.

### *Column view*

1. In the **Model Builder** window, under **Results** right-click **Views** and choose **View 3D**.
2. In the **Settings** window for **View 3D**, type `Column view` in the **Label** text field.

### *Pellet view*

1. Right-click **Views** and choose **View 3D**.
2. In the **Settings** window for **View 3D**, type `Pellet view` in the **Label** text field.

### *Sector 3D 1*

Create a dataset that can be used to plot the column with a sector cut-out for better view.

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

2 In the **Settings** window for **Sector 3D**, locate the **Axis Data** section.

3 In row **Point 2**, set **X** to 1 and **z** to 0.

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

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

6 In the **Number of sectors to include** text field, type 5.

Adjust the view angle of the plot with the mouse, then go to the **Views** -> **Column view** under **Results** and select the **Lock camera** check-box to save the view.

First create Figure 3 showing the velocity distribution in the reactor.

### *Velocity*

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

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

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

4 Locate the **Plot Settings** section. From the **View** list, choose **Column view**.

### *Slice 1*

1 Right-click **Velocity** and choose **Slice**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Darcy's Law> Velocity and pressure>dl.U - Darcy's velocity magnitude - m/s**.

3 Locate the **Plane Data** section. In the **Planes** text field, type 8.

4 In the **Velocity** toolbar, click **Plot**.

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

Continue with Figure 4 illustrating the concentration of species A in the reactor.

### *Concentration, A, Surface (tds)*

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

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

3 From the **Dataset** list, choose **Sector 3D 1**.

4 Locate the **Plot Settings** section. From the **View** list, choose **Column view**.

5 In the **Concentration, A, Surface (tds)** toolbar, click **Plot**.

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

Continue with the xy plot inside pellet.

### *Pellet x-y plot*

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

2 In the **Settings** window for **1D Plot Group**, type `Pellet x-y plot` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Click to expand the **Title** section. In the **Title** text area, type `Pellet concentrations @ x=0.5[m], y=0, z=0`.

### *A*

1 In the **Model Builder** window, expand the **Pellet x-y plot** node, then click **Species A**.

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

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `atxd3(0.5, 0, 0, tds.cpe_cA)`.

The syntax `atxd3(0.5,0,0,comp1.tds.cpe_cA)` means that you visualize the internal pellet concentration 0.5 m from the inlet, and in the center of the column.

4 In the **Description** text field, type `pellet (tds.cpe_cA) @ x=0.5[m], y=0, z=0`.

5 Click to expand the **Coloring and Style** section. In the **Width** text field, type `2`.

6 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

| Legends |
|---|
| Pellet, c<sub>A</sub> |

### *B*

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

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

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `atxd3(0.5, 0, 0, tds.cpe_cB)`.

4 In the **Description** text field, type `pellet (tds.cpe_cB) @ x=0.5[m], y=0, z=0`.

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

| Legends |
|---|
| Pellet c<sub>B</sub> |

### *C*

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

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

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `atxd3(0.5, 0, 0, tds.cpe_cC)`.

4 In the **Description** text field, type `pellet (comp1.tds.cpe_cC) @ x=0.5[m], y=0, z=0`.

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

| Legends |
| --- |
| Pellet c<sub>C</sub> |

7 In the **Pellet x-y plot** toolbar, click **Plot**.

### *Pellet x-y plot*

1 In the **Model Builder** window, click **Pellet x-y plot**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box.

4 In the associated text field, type `Pellet Radius`.

5 Select the **y-axis label** check box.

6 In the associated text field, type `Concentration (mol/m<sup>3</sup>)`.

7 In the **Pellet x-y plot** toolbar, click **Plot**.

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

Next plot is created to visualize the difference in species' average concentrations in the pellets and the reactor bed in the same plot. The figure requires a new dataset.

### *Cut Line 3D 1*

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

### *Concentration comparison*

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

2 In the **Settings** window for **1D Plot Group**, type `Concentration comparison` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 From the **Dataset** list, choose **Cut Line 3D 1**.

5 Locate the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Comparison between concentration in bed and average concentration in pellets`.

7 Locate the **Plot Settings** section. Select the **x-axis label** check box.

8 In the associated text field, type `Height coordinate from bottom at center of reactor (m)`.

9 Select the **y-axis label** check box.

10 In the associated text field, type `Concentration (mol/m<sup>3</sup>)`.

11 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

*A, bed*

1 Right-click **Concentration comparison** and choose **Line Graph**.

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

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

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

5 In the **Width** text field, type `2`.

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

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

8 In the table, enter the following settings:

| Legends |
| --- |
| c<sub>A</sub> |

*B, bed*

1 Right-click **A, bed** and choose **Duplicate**.

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

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

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

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

| Legends |
| --- |
| c<sub>B</sub> |

*C, bed*

1 Right-click **B, bed** and choose **Duplicate**.

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

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

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

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

| **Legends** |
| --- |
| c<sub>C</sub> |

*A, pellet*

1 Right-click **C, bed** and choose **Duplicate**.

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

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `tds.pb1.pts1.avecpe_cA`.

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

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

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

| **Legends** |
| --- |
| Pellet average, c<sub>A</sub> |

*B, pellet*

1 Right-click **A, pellet** and choose **Duplicate**.

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

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `tds.pb1.pts1.avecpe_cB`.

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

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

| **Legends** |
| --- |
| Pellet average, c<sub>B</sub> |

*C, pellet*

1 Right-click **B, pellet** and choose **Duplicate**.

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

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `tds.pb1.pts1.avecpe_cC`.

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

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

| Legends |
| --- |
| Pellet average, c<sub>C</sub> |

6 In the **Concentration comparison** toolbar, click **Plot**.

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

Lastly, create the figure showing the concentration of species C in a pellet. The pellet is located at (0.5,0,0) and is visualized with a new dataset.

### *Cut Point 3D 1*

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

The next step is to create the image showing the coordinates of the visualized pellet.

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

3 In the **X** text field, type `0.5`.

4 In the **Y** text field, type `0`.

5 In the **Z** text field, type `0`.

6 Click **Plot**.

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

### *Revolution 1D 1*

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

2 In the **Settings** window for **Revolution 1D**, click to expand the **Revolution Layers** section.

3 In the **Start angle** text field, type `-90`.

4 In the **Revolution angle** text field, type `180`.

### *Revolution 2D 2*

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

2 In the **Settings** window for **Revolution 2D**, click to expand the **Revolution Layers** section.

3 In the **Revolution angle** text field, type `270`.

### *Pellet 3D plot*

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Revolution 2D 2**.

4 Locate the **Plot Settings** section. From the **View** list, choose **Pellet view**.

5 Clear the **Plot dataset edges** check box.

*Surface 1*

1 Right-click **Pellet 3D plot** and choose **Surface**.

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

3 In the **Expression** text field, type comp1.atxd3(0.5,0,0,comp1.tds.cpe_cC).

4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type Pellet concentration of species C (mol/m<sup>3</sup>) at x=0.5[m], y=0, z=0.

Adjust the view angle of the plot with the mouse, then go to the **Views - Pellet** under **Results** and select the **Lock camera** check-box to change the view.

6 In the **Pellet 3D plot** toolbar, click **Plot**.

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

8 In the **Pellet 3D plot** toolbar, click **Plot**.

*Concentration, A, Streamline (tds)*

Modify the default streamline plot. For high plot performance it is good to make them start on a cut plane above the bottom.

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

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

3 From the **Dataset** list, choose **Sector 3D 1**.

4 Locate the **Plot Settings** section. From the **View** list, choose **Column view**.

*Cut Plane 1*

1 In the **Model Builder** window, expand the **Concentration, A, Streamline (tds)** node.

2 Right-click **Results>Datasets** and choose **Cut Plane**.

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

4 From the **Dataset** list, choose **Sector 3D 1**.

5 Locate the **Plane Data** section. In the **X-coordinate** text field, type 0.005.

*Streamline 1*

1 In the **Model Builder** window, under **Results>Concentration, A, Streamline (tds)** click **Streamline 1**.

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

3 In the **Points** text field, type 1000.

4 From the **Along curve or surface** list, choose **Cut Plane 1**.

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

6 In the **Tube radius expression** text field, type `cA[m^4/mol]`.

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

8 In the associated text field, type `.004`.

You can zoom in by pressing down the middle mouse button and moving the mouse forward. Hold down the **Ctrl**-button to dolly in the camera position.

9 In the **Concentration, A, Streamline (tds)** toolbar, click **Plot**.

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

## *Appendix — Geometry 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 Click **Done**.

### GEOMETRY 1

#### *Work Plane 1 (wp1)*

1 In the **Geometry** toolbar, click **Work Plane**.

2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.

3 From the **Plane** list, choose **yz-plane**.

4 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. Click **New**.

5 In the **New Cumulative Selection** dialog box, type `Inlet` in the **Name** text field.

6 Click **OK**.

7 In the **Settings** window for **Work Plane**, click **Show Work Plane**.

*Work Plane 1 (wp1)>Circle 1 (c1)*

1 In the **Work Plane** toolbar, click **Circle**.
2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.
3 In the **Radius** text field, type `0.017`.
4 In the **Sector angle** text field, type `45`.
5 Click **Build Selected**.

*Work Plane 1 (wp1)>Circle 2 (c2)*

1 Right-click **Component 1 (comp1)>Geometry 1>Work Plane 1 (wp1)>Plane Geometry>Circle 1 (c1)** and choose **Duplicate**.
2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.
3 In the **Sector angle** text field, type `180`.
4 Locate the **Position** section. In the **xw** text field, type `0.017*2+0.02`.

*Work Plane 1 (wp1)>Circle 3 (c3)*

1 Right-click **Component 1 (comp1)>Geometry 1>Work Plane 1 (wp1)>Plane Geometry>Circle 2 (c2)** and choose **Duplicate**.
2 In the **Settings** window for **Circle**, locate the **Position** section.
3 In the **xw** text field, type `0.017*4+0.02*2`.

*Work Plane 1 (wp1)>Circle 4 (c4)*

1 Right-click **Component 1 (comp1)>Geometry 1>Work Plane 1 (wp1)>Plane Geometry>Circle 3 (c3)** and choose **Duplicate**.
2 In the **Settings** window for **Circle**, locate the **Position** section.
3 In the **xw** text field, type `0.017*6+0.02*3`.

*Work Plane 1 (wp1)>Circle 5 (c5)*

1 Right-click **Component 1 (comp1)>Geometry 1>Work Plane 1 (wp1)>Plane Geometry>Circle 4 (c4)** and choose **Duplicate**.
2 In the **Settings** window for **Circle**, locate the **Position** section.
3 In the **xw** text field, type `0.017*2+0.02`.
4 Locate the **Rotation Angle** section. In the **Rotation** text field, type `180`.

*Work Plane 1 (wp1)>Circle 6 (c6)*

1 Right-click **Component 1 (comp1)>Geometry 1>Work Plane 1 (wp1)>Plane Geometry>Circle 5 (c5)** and choose **Duplicate**.
2 In the **Settings** window for **Circle**, locate the **Position** section.

3 In the **xw** text field, type 0.017*4+0.02*2.

*Work Plane 1 (wp1)>Circle 7 (c7)*

1 Right-click **Component 1 (comp1)>Geometry 1>Work Plane 1 (wp1)>Plane Geometry>Circle 6 (c6)** and choose **Duplicate**.

2 In the **Settings** window for **Circle**, locate the **Position** section.

3 In the **xw** text field, type 0.017*6+0.02*3.

4 In the **Work Plane** toolbar, click **Build All**.

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

*Work Plane 1 (wp1)>Rotate 1 (rot1)*

1 In the **Work Plane** toolbar, click **Transforms** and choose **Rotate**.

2 Select the objects **c5**, **c6**, and **c7** only.

3 In the **Settings** window for **Rotate**, locate the **Rotation** section.

4 In the **Angle** text field, type 45.

5 Click **Build Selected**.

*Work Plane 1 (wp1)>Circle 8 (c8)*

1 In the **Model Builder** window, under **Component 1 (comp1)>Geometry 1>Work Plane 1 (wp1)>Plane Geometry** right-click **Circle 7 (c7)** and choose **Duplicate**.

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

3 In the **Sector angle** text field, type 360.

4 Locate the **Position** section. In the **xw** text field, type 0.017*4+0.02*2.

5 Locate the **Rotation Angle** section. In the **Rotation** text field, type 0.

6 Click **Build Selected**.

*Work Plane 1 (wp1)>Circle 9 (c9)*

1 Right-click **Component 1 (comp1)>Geometry 1>Work Plane 1 (wp1)>Plane Geometry>Circle 8 (c8)** and choose **Duplicate**.

2 In the **Settings** window for **Circle**, locate the **Position** section.

3 In the **xw** text field, type 0.017*6+0.02*3.

4 Click **Build Selected**.

*Work Plane 1 (wp1)>Rotate 2 (rot2)*

1 In the **Work Plane** toolbar, click **Transforms** and choose **Rotate**.

2 Select the objects **c8** and **c9** only.

3 In the **Settings** window for **Rotate**, locate the **Rotation** section.

4 In the **Angle** text field, type `22.5`.

5 Click **Build Selected**.

*Work Plane 2 (wp2)*

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Work Plane**.

2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.

3 From the **Plane** list, choose **yz-plane**.

4 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. Click **New**.

5 In the **New Cumulative Selection** dialog box, type `Bottom plate` in the **Name** text field.

6 Click **OK**.

*Work Plane 2 (wp2)>Plane Geometry*

In the **Model Builder** window, click **Plane Geometry**.

*Work Plane 2 (wp2)>Circle 1 (c1)*

1 In the **Work Plane** toolbar, click **Circle**.

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

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

4 In the **Sector angle** text field, type `45`.

5 Click **Build Selected**.

*Extrude 1 (ext1)*

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Extrude**.

2 In the **Settings** window for **Extrude**, click **Build Selected**.

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

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

Create the last two selections.

5 In the **Model Builder** window, click **Extrude 1 (ext1)**.

6 In the **Settings** window for **Extrude**, click **Build Selected**.

*Symmetry planes*

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

2 In the **Settings** window for **Explicit Selection**, locate the **Entities to Select** section.

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

4 On the object **ext1**, select Boundaries 2 and 3 only.

5 In the **Label** text field, type `Symmetry planes`.

Create the **Outlet** selection.

*Outlet*

1 Right-click **Symmetry planes** and choose **Duplicate**.

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

3 Locate the **Entities to Select** section. Find the **Entities to select** subsection. Click to select the **Activate Selection** toggle button.

4 In the tree, select **ext1>2** and **ext1>3**.

5 Click **Remove from Selection**.

6 On the object **ext1**, select Boundary 5 only.

7 Click **Build All Objects**.