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.

![Diagram of a packed bed reactor](image)

**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.](image)

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·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 \( r = \frac{r_{\text{dim}}}{r_{\text{pe}}} \) 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 \( i \):

\[
4\pi N \left\{ r^2 r_{\text{pe}}^2 c_{\text{pe},i} \frac{\partial c_{\text{pe},i}}{\partial t} + \frac{\partial}{\partial r} \left( -r^2 D_{\text{pe},i} \frac{\partial c_{\text{pe},i}}{\partial r} \right) = r^2 r_{\text{pe}}^2 R_{\text{pe},i} \right\}
\]

Here, \( r \) is a dimensionless radial coordinate that goes from 0 (center) to 1 (pellet surface), \( r_{\text{pe}} \) 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.

\( D_{\text{pe}} \) is an effective diffusion coefficient (SI unit: m\(^2\)/s) and \( R_{\text{pe},i} \) is the reaction source term (SI unit: mol/(m\(^3\)·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, \( h_{D,i} \), such that:

\[
N_{i,\text{inward}} = h_{D,i} (c_i - c_{\text{pe},i}),
\]
where \( N_{i, \text{inward}} \) is the molar flux from the free fluid into a pellet and has the unit moles/\((m^2 \cdot s)\). The mass transfer coefficient is 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**

<table>
<thead>
<tr>
<th>PROPERTY</th>
<th>VALUE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H_r )</td>
<td>1 [m]</td>
<td>Height of the packed bed reactor</td>
</tr>
<tr>
<td>( R_r )</td>
<td>0.2 [m]</td>
<td>Radius of packed bed reactor</td>
</tr>
<tr>
<td>( \rho_b )</td>
<td>0.51 [g/cm³]</td>
<td>Density of packed bed</td>
</tr>
<tr>
<td>( \rho_{pe} )</td>
<td>0.68 [g/cm³]</td>
<td>Density individual pellet</td>
</tr>
<tr>
<td>( \varepsilon_b )</td>
<td>(1 - \frac{\rho_b}{\rho_{pe}})</td>
<td>Macroscale porosity (of bed)</td>
</tr>
<tr>
<td>( \varepsilon_{pe} )</td>
<td>0.70 (-)</td>
<td>Microscale porosity (of pellet)</td>
</tr>
<tr>
<td>( r_{pe} )</td>
<td>0.5 [mm]</td>
<td>Pellet radius (spherical shape)</td>
</tr>
<tr>
<td>( D_{pe,A} )</td>
<td>1.5e-9 [m²/s]</td>
<td>Diffusion coefficient of A in pellet</td>
</tr>
<tr>
<td>( D_{pe,B} )</td>
<td>2e-9 [m²/s]</td>
<td>Diffusion coefficient of B in pellet</td>
</tr>
<tr>
<td>( D_{pe,C} )</td>
<td>0.5e-9 [m²/s]</td>
<td>Diffusion coefficient of C in pellet</td>
</tr>
<tr>
<td>( A )</td>
<td>2e12 [m³/(mol s)]</td>
<td>Frequency factor reaction</td>
</tr>
<tr>
<td>( E )</td>
<td>75000[J/mol]</td>
<td>Activation energy reaction</td>
</tr>
<tr>
<td>( K_{eq0} )</td>
<td>1000</td>
<td>Equilibrium reaction constant</td>
</tr>
<tr>
<td>( \kappa )</td>
<td>1.88e-10 [m²]</td>
<td>Permeability of Bed</td>
</tr>
<tr>
<td>( C_{A,\text{in}} )</td>
<td>1 [mol/m³]</td>
<td>Inlet concentration A</td>
</tr>
<tr>
<td>( C_{B,\text{in}} )</td>
<td>1 [mol/m³]</td>
<td>Inlet concentration B</td>
</tr>
<tr>
<td>( C_{C,\text{in}} )</td>
<td>0 [mol/m³]</td>
<td>Inlet concentration C</td>
</tr>
<tr>
<td>( D_A )</td>
<td>1e-8 [m²/s]</td>
<td>Diffusion coefficient of A in bed</td>
</tr>
<tr>
<td>( D_B )</td>
<td>1.5e-8 [m²/s]</td>
<td>Diffusion coefficient of B in bed</td>
</tr>
<tr>
<td>( D_C )</td>
<td>0.5e-8 [m²/s]</td>
<td>Diffusion coefficient of C in bed</td>
</tr>
<tr>
<td>( p_{\text{Darcy}} )</td>
<td>0.4 [atm]</td>
<td>Inlet pressure offset</td>
</tr>
</tbody>
</table>
Results and Discussion

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

![Velocity Distribution](image)

**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.

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

**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 (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
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. You can read the instructions for building
the geometry in the appendix.

1 In the Geometry toolbar, click Insert Sequence.

2 Browse to the model’s Application Libraries folder and double-click the file
   packed_bed_reactor_3d_geom_sequence.mph.

3 In the Geometry toolbar, click Build All.
Specify the material properties. 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 Component** in the window toolbar.
5. In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

**CHEMISTRY (CHEM)**
Start with the **Chemistry** interface and create the needed reaction kinetics expressions by typing in the reaction formulas.

1. In the **Settings** window for **Chemistry**, click to expand the **Mixture Properties** section.
2. 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 \( A+B\leftrightarrow2C \).
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 \( A \) text field, type \( A \).
8. In the \( E \) text field, type \( E \).
9. Locate the **Equilibrium Settings** section. From the **Equilibrium constant** list, choose **User defined**.
10. In the \( K_{eq0} \) text field, type \( K_{eq0} \).

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, under Component 1 (comp1)->Chemistry (chem) 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, under Component 1 (comp1)->Chemistry (chem) 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, under Component 1 (comp1)->Chemistry (chem) 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 Species name text field, type H2O.
4 Locate the Species Type section. From the Species type list, choose Solvent.
5 Locate the General Parameters section. In the M text field, type Mn_solvent.

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.

6 In the Model Builder window, click Chemistry (chem).
7 In the Settings window for Chemistry, locate the Species Matching section.
In the table, enter the following settings:

<table>
<thead>
<tr>
<th>Species</th>
<th>Species type</th>
<th>Molar concentration</th>
<th>Reaction rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Variable, from Reaction</td>
<td>tds.rpb1.cpe_cA</td>
<td>chem.R_A</td>
</tr>
<tr>
<td>B</td>
<td>Variable, from Reaction</td>
<td>tds.rpb1.cpe_cB</td>
<td>chem.R_B</td>
</tr>
<tr>
<td>C</td>
<td>Variable, from Reaction</td>
<td>tds.rpb1.cpe_cC</td>
<td>chem.R_C</td>
</tr>
<tr>
<td>H2O</td>
<td>Constant, solvent</td>
<td>C_solvent</td>
<td>solvent</td>
</tr>
</tbody>
</table>

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.

Click to expand the **Extra Dimension** section. Select the **Define variables in extra dimension** check box.

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

**TRANSPORT OF DILUTED SPECIES (TDS)**

In the **Physics** toolbar, click **Chemistry (chem)** and choose **Transport of Diluted Species (tds)**.

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Diluted Species (tds)**.
2. In the **Settings** window for **Transport of Diluted Species**, locate the **Transport Mechanisms** section.
3. Select the **Mass transfer in porous media** check box.

Transport Properties 1

1. In the **Model Builder** window, under **Component 1 (comp1)>>Transport of Diluted Species (tds)** click **Transport Properties 1**.
2. In the **Settings** window for **Transport Properties**, locate the **Convection** section.
3. From the **u** list, choose **Darcy’s velocity field (dl)**.
4. Locate the **Diffusion** section. In the **DcA** text field, type **DA**.
5. In the **DcB** text field, type **DB**.
6. In the **DcC** text field, type **DC**.

Add the **Reactive Pellet Bed** feature. A predefined extra dimension 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 10 elements with a cubic root sequence distribution.

7. In the **Model Builder** window, click **Transport of Diluted Species (tds)**.
Reactive Pellet Bed 1

1 In the Physics toolbar, click Domains and choose Reactive Pellet Bed.
2 In the Settings window for Reactive Pellet Bed, locate the Domain Selection section.
3 From the Selection list, choose All domains.
4 Locate the Bed Parameters section. In the $\rho_b$ text field, type $\rho_b$.
5 In the $\rho_{pe}$ text field, type $\rho_{pe}$.

The densities for pellet and bed are used to calculate the bed porosity.
6 Locate the Pellet Shape and Size section. In the $r_{pe}$ text field, type $r_{pe}$.
7 Locate the Pellet Parameters section. In the $\epsilon_{pe}$ text field, type $\epsilon_{pe}$.
8 From the Diffusion model list, choose User defined.
9 In the $D_{peff, cA}$ text field, type $D_{A\text{p}}$.
10 In the $D_{peff, cB}$ text field, type $D_{B\text{p}}$.
11 In the $D_{peff, cC}$ text field, type $D_{C\text{p}}$.

Use a film theory condition to account for any film resistance to mass transfer between the bulk fluid and the pellet. Use spherical pellets.
12 Locate the Pellet-Fluid Surface section. From the Coupling type list, choose Film resistance (mass flux).
13 Locate the Pellet Discretization section. In the $N_{\text{elem}}$ text field, type 6.

Use the reaction rates calculated in the Chemistry interface.

Reactions 1

1 In the Model Builder window, expand the Reactive Pellet Bed 1 node, then click Reactions 1.
2 In the Settings window for Reactions, locate the Reaction Rates section.
3 From the $R_{cA}$ list, choose Rate expression for species A (chem).
4 From the $R_{cB}$ list, choose Rate expression for species B (chem).
5 From the $R_{cC}$ list, choose Rate expression for species C (chem).

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 $c_{0,cA}$ text field, type $C_{A\text{in}}$.
5 In the $c_{0,cB}$ text field, type $C_{B\text{in}}$. 
In the $c_{0,cO}$ 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)**
Last, enter the model specifications for the **Darcy’s Law** interface to compute the convective flow in the reactor.

**Fluid and Matrix Properties 1**
Take the porosity directly from the **Reactive Pellet Bed** feature.

1. In the **Model Builder** window, under **Component 1 (comp1)>Darcy’s Law (dl)** click **Fluid and Matrix Properties 1**.
2. In the **Settings** window for **Fluid and Matrix Properties**, locate the **Matrix Properties** section.
3. From the $\varepsilon_p$ list, choose **User defined**. In the associated text field, type $tds.rpb1.epsilon_b$.
4. From the $\kappa$ list, choose **User defined**. In the associated text field, type $kappa$.
5. In the **Model Builder** window, click **Darcy’s Law (dl)**.

**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 Model Builder window, under Component 1 (comp1) right-click Mesh 1 and choose More Operations>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 Component 1 (comp1)>Mesh 1>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.

Distribution 1
1 In the Model Builder window, right-click Mesh 1 and choose Swept.
2 Right-click Swept 1 and choose Distribution.
3 In the Settings window for Distribution, locate the Distribution section.
4 From the Distribution type list, choose Predefined.
5 In the Number of elements text field, type 15.
6 In the Element ratio text field, type 5.
7 Click Build All.

Since this is a one-way coupled 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 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).

Step 2: 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 box for **Chemistry (chem)** and **Transport of Diluted Species (tds)**.

4 Right-click **Study 1>Step 2: Stationary** and choose **Move Up**.

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

**ROOT**

1 In the **Model Builder** window’s toolbar, click the **Show** button and select **Advanced Results Options** in the menu.

Create views for plotting different angles of the geometry.

**RESULTS**

*View 3D 5*

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.

*View 3D 6*

1 Right-click **Views** and choose **View 3D**.

2 In the **Settings** window for **View 3D**, type **Pellet view** in the **Label** text field.

**Data Sets**

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

*Sector 3D 1*

1 In the **Results** toolbar, click **More Data Sets** 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. Optionally, the 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.

**Pressure (dl)**

1 In the **Model Builder** window, under **Results** click **Pressure (dl)**.
In the Settings window for 3D Plot Group, type Velocity in the Label text field.

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

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

Slice

In the Model Builder window, expand the Results>Velocity node, then click Slice.

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

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

In the Velocity toolbar, click Plot.

Click the Zoom Extents button in the Graphics toolbar.

To create the first xy plot, a new data set is required. Also, the special syntax comp1.atxd3 is needed to plot variables within the pellet.

Concentration (tds) 1

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

In the Settings window for 3D Plot Group, type Concentration, surface in the Label text field.

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

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

In the Concentration, surface toolbar, click Plot.

Click the Zoom Extents button in the Graphics toolbar.

To create the first xy plot, a new data set is required. Also, the special syntax comp1.atxd3 is needed to plot variables within the pellet.

Study 1/Solution 1 (3) (sol1)

In the Model Builder window, under Results right-click Study 1/Solution 1 (sol1) and choose Duplicate.

In the Settings window for Solution, locate the Solution section.

From the Component list, choose Extra Dimension from Reactive Pellet Bed 1 (tds_rpb1_xdim).

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

1D Plot Group 6

In the Model Builder window, under Results right-click 1D Plot Group 6 and choose Line Graph.
2 In the Settings window for 1D Plot Group, type Pellet x-y plot in the Label text field.
3 Click to expand the Title section. From the Title type list, choose Manual.
4 In the Title text area, type Pellet concentrations @ x=0.5[m], y=0, z=0.
5 Locate the Data section. From the Data set list, choose Study 1/Solution 1 (3) (sol1).

**Line Graph 1**

1 In the Model Builder window, under Results>Pellet x-y plot click Line Graph 1.
2 In the Settings window for Line Graph, type A in the Label text field.
3 Locate the Selection section. From the Selection list, choose All domains.
4 Locate the y-Axis Data section. In the Expression text field, type comp1.atxd3(0.5,0,0,comp1.tds.rpb1.cpe_cA).

   The syntax comp1.atxd3(0.5,0,0,comp1.tds.rpb1.cpe_cA) means that you visualize the internal pellet concentration 0.5 m from the inlet, and in the center of the column.
5 Select the Description check box.
6 In the associated text field, type pellet (comp1.tds.rpb1.cpe_cA) @ x=0.5[m], y=0, z=0.
7 Click to expand the Coloring and Style section. In the Width text field, type 2.
8 Click to expand the Legends section. Select the Show legends check box.
9 From the Legends list, choose Manual.
10 In the table, enter the following settings:

<table>
<thead>
<tr>
<th>Legends</th>
<th>Pellet, c&lt;sub&gt;A&lt;/sub&gt;</th>
</tr>
</thead>
</table>

**A 1**

1 Right-click Results>Pellet x-y plot>A and choose Duplicate.
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 comp1.atxd3(0.5,0,0,comp1.tds.rpb1.cpe_cB).
4 In the Description text field, type pellet (comp1.tds.rpb1.cpe_cB) @ x=0.5[m], y=0, z=0.
5 Locate the **Legends** section. In the table, enter the following settings:

<table>
<thead>
<tr>
<th>Legends</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pellet (c_B)</td>
</tr>
<tr>
<td>(B)</td>
</tr>
</tbody>
</table>

1 Right-click **Results>Pellet x-y plot>B** and choose **Duplicate**.

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 \(\text{comp1.atxd3}(0.5,0,0,\text{comp1.tds.rpb1.cpe_cC})\).

4 In the **Description** text field, type \(\text{pellet (comp1.tds.rpb1.cpe_cC)} @ x=0.5[m], y=0, z=0\).

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

<table>
<thead>
<tr>
<th>Legends</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pellet (c_C)</td>
</tr>
</tbody>
</table>

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

**Pellet x-y plot**

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

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

3 From the **Time selection** list, choose **Last**.

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

5 In the associated text field, type **Normalized Pellet Radius \((r/rpe)\)**.

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

7 In the associated text field, type **Concentration \((mol/m^3)\)**.

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

9 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 data set.

**Cut Line 3D**

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

2 Click **1D Plot Group**.
1D Plot Group 7

1 In the Model Builder window, under Results click 1D Plot Group 7.

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 Data set 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/m³).

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

Line Graph 1

1 Right-click Results>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:

<table>
<thead>
<tr>
<th>Legends</th>
<th>c&lt;sub&gt;A&lt;/sub&gt;</th>
</tr>
</thead>
</table>

A, bed 1

1 Right-click Results>Concentration comparison>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:

<table>
<thead>
<tr>
<th>Legends</th>
</tr>
</thead>
<tbody>
<tr>
<td>c&lt;sub&gt;B&lt;/sub&gt;</td>
</tr>
</tbody>
</table>

* B, bed 1

1 Right-click **Results>Concentration comparison>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:

<table>
<thead>
<tr>
<th>Legends</th>
</tr>
</thead>
<tbody>
<tr>
<td>c&lt;sub&gt;C&lt;/sub&gt;</td>
</tr>
</tbody>
</table>

* C, bed 1

1 Right-click **Results>Concentration comparison>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.rpb1.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:

<table>
<thead>
<tr>
<th>Legends</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pellet average, c&lt;sub&gt;A&lt;/sub&gt;</td>
</tr>
</tbody>
</table>

* A, pellet 1

1 Right-click **Results>Concentration comparison>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.rpb1.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:

<table>
<thead>
<tr>
<th>Legends</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pellet average, c&lt;sub&gt;B&lt;/sub&gt;</td>
</tr>
</tbody>
</table>
B, pellet 1

1 Right-click Results>Concentration comparison>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.rpb1.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:

<table>
<thead>
<tr>
<th>Legends</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pellet average, $c_\text{C}$</td>
</tr>
</tbody>
</table>

6 In the Concentration comparison toolbar, click Plot.

7 Click the Zoom Extents button in the Graphics toolbar.

Last, 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 data set.

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 Data Sets 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 Data Sets 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.

4 In the Results toolbar, click 3D Plot Group.
3D Plot Group 8

1. In the Model Builder window, under Results click 3D Plot Group 8.
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 Data set list, choose Revolution 2D.
4. Locate the Plot Settings section. From the View list, choose Pellet view.
5. Clear the Plot data set edges check box.

Surface 1

1. Right-click Results>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.rpb1.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. Optionally, the go to the Views - Pellet under Results and select the Lock camera check-box to save the view.

6. In the Pellet 3D plot toolbar, click Plot.
7. Click the Zoom Extents button in the Graphics toolbar.

3D Plot Group 1

1. In the Model Builder window, under Results click 3D Plot Group 1.
2. In the Settings window for 3D Plot Group, type Concentration, isosurface in the Label text field.
3. Locate the Data section. From the Data set list, choose Sector 3D.
4. Locate the Plot Settings section. From the View list, choose Column view.

Slice 1

1. In the Model Builder window, expand the Results>Concentration, isosurface node.
2. Right-click Slice 1 and choose Disable.

Isosurface 1

1. In the Model Builder window, under Results right-click Concentration, isosurface and choose Isosurface.
2. In the Settings window for Isosurface, locate the Levels section.
3. In the Total levels text field, type 10.
4. Click the Zoom Extents button in the Graphics toolbar.
In the Concentration, isosurface toolbar, click Plot.

Concentration (tds)
1 In the Model Builder window, under Results click Concentration (tds).
2 In the Settings window for 3D Plot Group, type Concentration, slice in the Label text field.
3 Locate the Data section. From the Data set list, choose Sector 3D 1.
4 Locate the Plot Settings section. From the View list, choose Column view.
5 In the Concentration, slice toolbar, click Plot.

Pressure (dl) 1
1 In the Model Builder window, under Results click Pressure (dl) 1.
2 In the Settings window for 3D Plot Group, locate the Plot Settings section.
3 From the View list, choose Column view.
4 Locate the Data section. From the Data set list, choose Sector 3D 1.
5 In the Pressure (dl) 1 toolbar, click Plot.

Concentration, surface
Create a streamline plot. For high plot performance it is good to make them start on a cut plane above the bottom.

Concentration, surface 1
1 In the Model Builder window, under Results right-click Concentration, surface and choose Duplicate.
2 In the Settings window for 3D Plot Group, type Streamlines in the Label text field.

Surface
1 In the Model Builder window, expand the Results>Streamlines node.
2 Right-click Surface and choose Disable.

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 Data set list, choose Sector 3D 1.
4 Locate the Plane Data section. In the X-coordinate text field, type 0.005.

Streamline 1
1 In the Model Builder window, under Results right-click Streamlines and choose Streamline.
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.

Color Expression 1

1 Right-click Results>Streamlines>Streamline 1 and choose Color Expression.

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.

2 In the Streamlines toolbar, click Plot.

3 Click the Zoom Extents button in the Graphics toolbar.