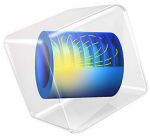

A Multiscale 3D Packed Bed Reactor

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.

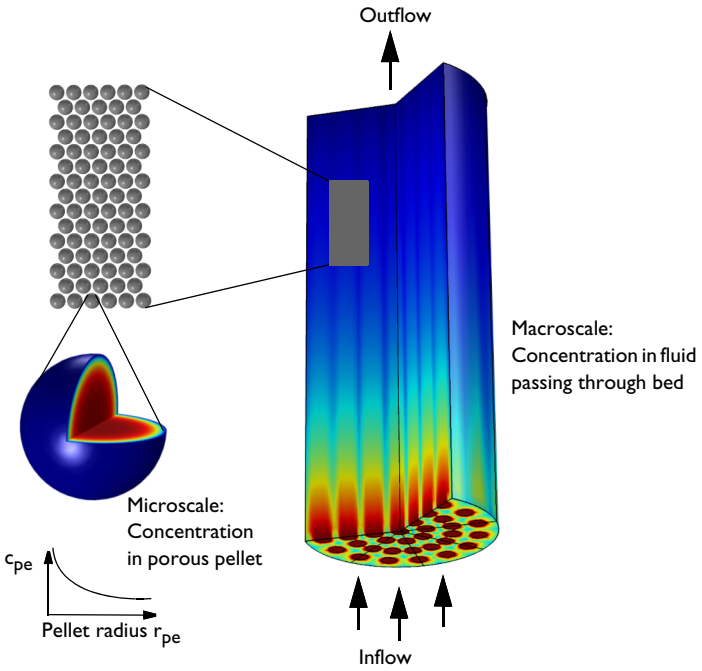

Figure 1: An example of the macroscale (bed volume with entry holes) and the microscale (pellet) of a packed bed reactor.

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.

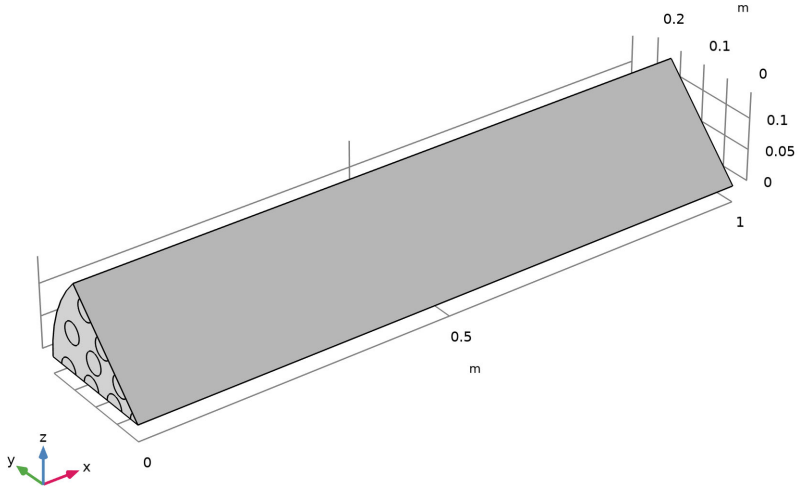

Figure 2: The packed bed reactor simulation geometry. Due to symmetry an 1/8 of the true geometry is modeled. The results will be expanded to the true geometry with aid of a sector data set.

The pressure drop in the reactor is modeled using the Darcy's Law interface.

A reversible catalytic chemical reaction occurs inside the pellets. 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 ($r = r_{dim}/r_{pe}$) 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:

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

Here, r is a dimensionless radial coordinate that goes from 0 (center) to 1 (pellet surface), r_{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_{pe} is an effective diffusion coefficient (SI unit: m^2/s) and $R_{pe,\,i}$ 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_{Di}, such that:

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

where $N_{i,\text{ inward}}$ is the molar flux from the free fluid into a pellet and has the SI unit moles/(m^2·s). The mass transfer coefficient is defined in terms of the Sherwood number

$$\text{Sh} = \frac{h_\text{D}}{(D_\text{pe}/r_\text{pe})} \tag{3}$$

In this model the Frössling correlation is used

$$\text{Sh} = 0.2 + 0.552\text{Re}^{1/2}\text{Sc}^{1/3} \tag{4}$$

It is applicable for mass transfer from spherical particles and relates the Sherwood number to the pellet Reynolds number and the Schmidt number

$$\text{Re} = \frac{r_\text{pe}U}{\nu}, \ \text{Sc} = \frac{\nu}{D_\text{pe}}, \tag{5}$$

Here U is fluid velocity in the bed and ν is the kinematic viscosity of the fluid.

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
ρ_b	0.51 [g/cm^3]	Density of packed bed
ρ_pe	0.68 [g/cm^3]	Density individual pellet
ε_b	1-$\rho_\text{b}/\rho_\text{pe}$	Macroscale porosity (of bed)
ε_pe	0.70 (-)	Microscale porosity (of pellet)
r_pe	0.5 [mm]	Pellet radius (spherical shape)
$D_\text{pe,A}$	1.5e-9 [m^2/s]	Diffusion coefficient of A in pellet
$D_\text{pe,B}$	2e-9 [m^2/s]	Diffusion coefficient of B in pellet
$D_\text{pe,C}$	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
$C_\text{A,in}$	1[mol/m^3]	Inlet concentration A

TABLE 1: SUMMARY OF INPUT DATA.

PROPERTY	VALUE	DESCRIPTION
$C_{B,in}$	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.

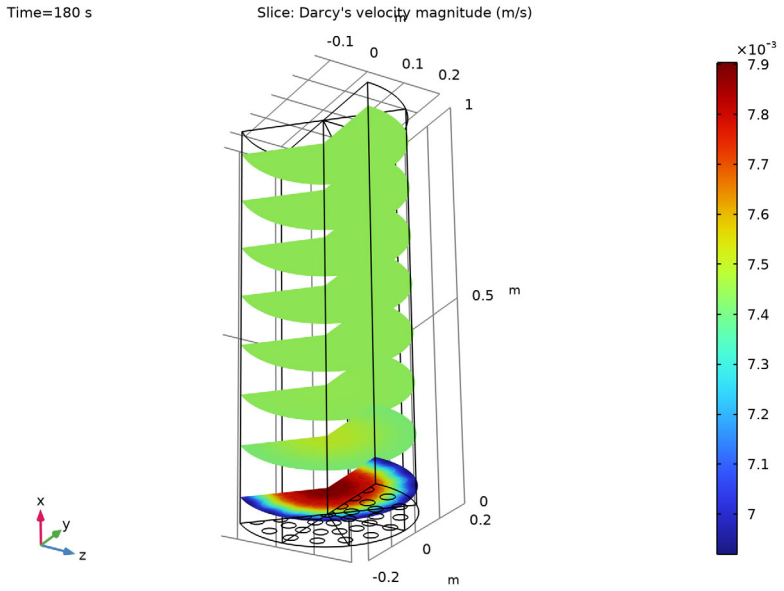

Figure 3: Velocity distribution on the macroscale.

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.

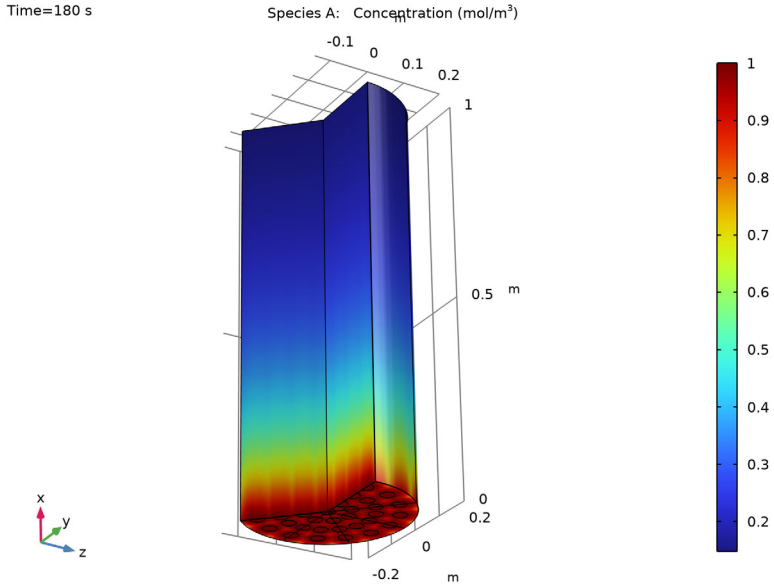

Figure 4: Concentration of reactant A.

Streamline plots can be useful to get an understanding of the flow pattern. It can be seen from Figure 5 that no recirculation occurs downstream from the entry holes. The fluid is evenly spread out in the bed chamber shortly after entering from through the bottom plate.

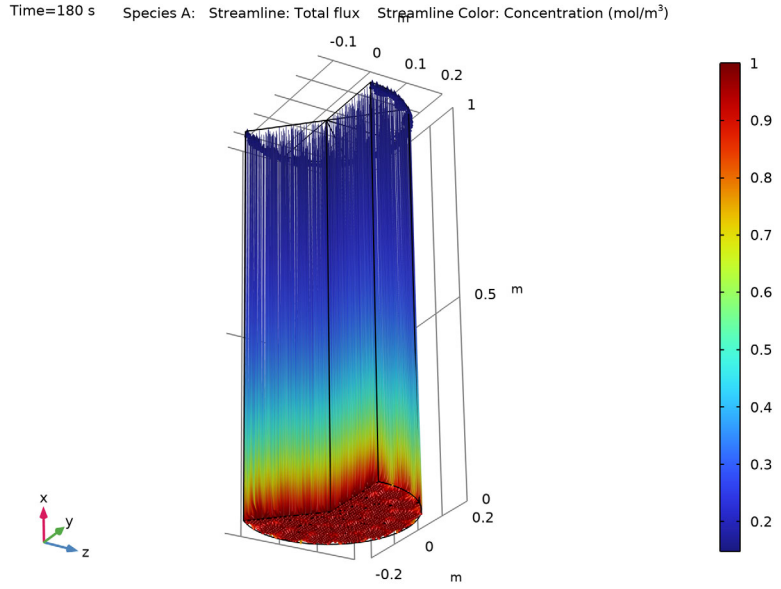

Figure 5: The streamlines show how the fluid enters the holes and then spread out in the bed volume as it. The colors of the lines represent the reactant concentration in moles/m^3.

A line plot of the concentration inside a pellet at a certain position in the bed is useful in order to understand the kinetics at that point. Here a sampling point on the symmetry axis half way through the reactor (at $x = 0.5, z = 0, y = 0$) is used. The point is shown in Figure 6. and. In Figure 7 line plots of the reactants and the product inside a pellet at the sampling point is shown. Species A and B originates in bed pores and diffuses into the

porous pellet, while at the same time forming species C. The diffusion coefficient of B is higher than that of A, leading to a higher concentration of B in the pellet center.

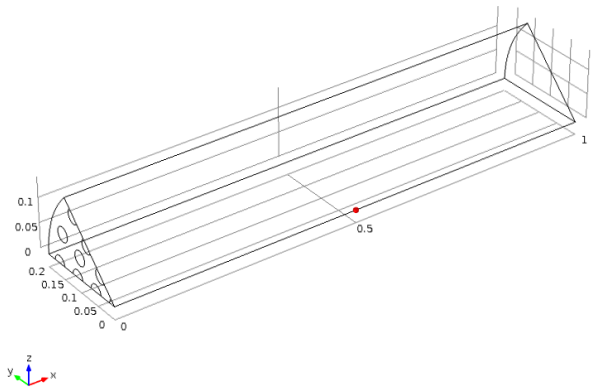

Figure 6: The position where the pellet plot is evaluated: Centerline of reactor at a height of 0.5 m.

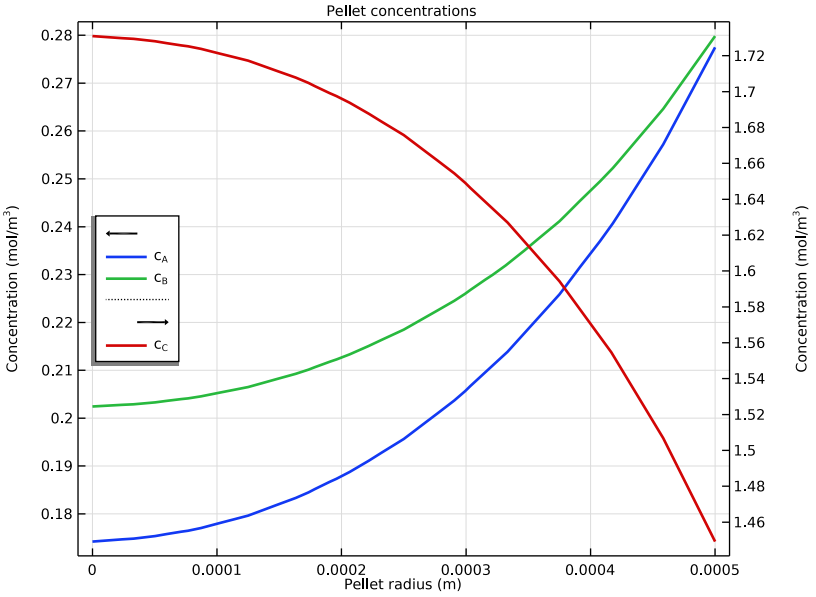

Figure 7: Species concentration within the pellet, in the at the end of the simulation (t = 180 s).

It is also valuable to simultaneously compare the development in the micro scale and the macro scale. This is done in Figure 8 where the pellet concentration of species A is visualized using on spherical pellets in a regular grid pattern. For comparison, the bed concentration of the same species is also plotted on a cut plane through the reactor.

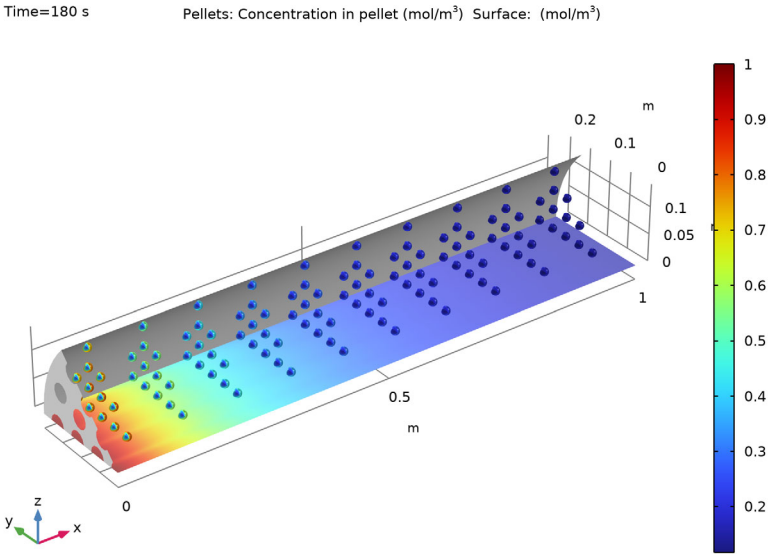

Figure 8: Concentration of species A in the reactor. The spheres show the pellet concentration in the corresponding positions. The development in the pellets can be compared to the bed concentration plotted on a cut plane.

In Figure 9 a line plot is used to evaluate the development in the reactor. Here the bed concentrations and the average pellet concentrations are plotted against the reactor height. It can be noted that species A and B exhibit a very similar development though the reactor. The inlet concentration of species C is zero, but inside the pellets significant levels of C is produced already at the inlet.

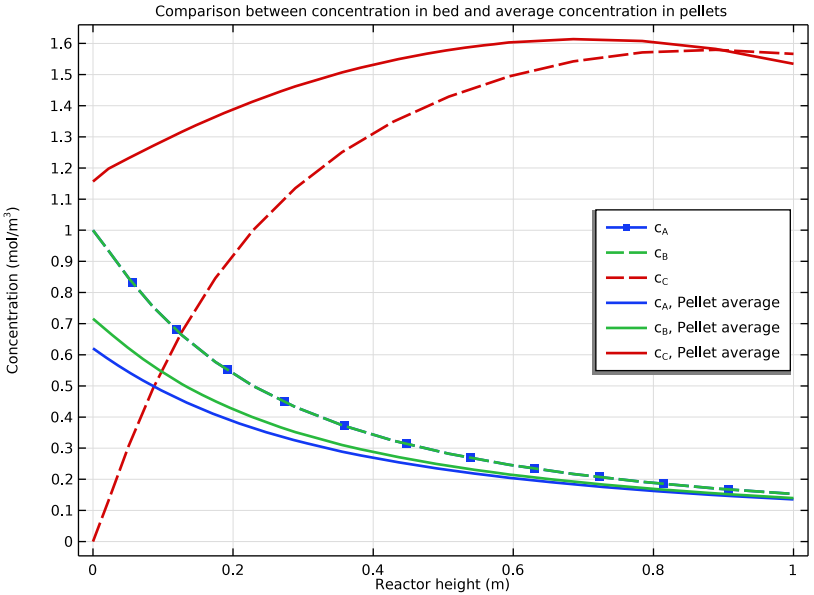

Figure 9: Species concentrations in the reactor bed as well as averaged pellet concentrations, plotted along the reactor height.

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 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**.

GLOBAL DEFINITIONS

Parameters 1

Add the model parameters from a text file.

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_{pe} text field, type `r_pe*2`.

5 In the ε_{pe} text field, type `epsilon_pe`.

6 Locate the **Pellet Bed Properties** section. In the ε_p text field, type `epsilon_b`.

7 Click to expand the **Mesh** section. From the **Distribution** list, choose **Linear**.

8 In the **Number of elements** text field, type `12`.

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^{f} text field, type `A`.

8 In the E^{f} 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 `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 **Chemical Formula** 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 **Chemical Formula** 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 **Chemical Formula** 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 **Name** section.

3 In the text field, type `H2O`.

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

5 Locate the **Chemical Formula** 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, under **Component 1 (comp1)>Transport of Diluted Species in Porous Media (tds)>Packed Bed 1** 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**.

Enter the user-defined diffusion coefficients.

Diffusion 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Transport of Diluted Species in Porous Media (tds)>Packed Bed 1>Pellets 1** 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.

Add a step function which can be used to smoothly ramp up the concentrations at the inlet.

DEFINITIONS (COMP1)

Step 1 (step1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Step**.

2 In the **Settings** window for **Step**, click to expand the **Smoothing** section.

3 In the **Size of transition zone** text field, type `1`.

4 Locate the **Parameters** section. In the **Location** text field, type `0.5[s]`.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

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*step1(t)`.

5 In the $c_{0,\mathrm{cB}}$ text field, type `CB_in*step1(t)`.

6 In the $c_{0,\mathrm{cC}}$ text field, type `CC_in*step1(t)`.

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.

Bed Concentration, A, Surface (tds)

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

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

Continue with concentrations inside pellet at a given point in main geometry.

Pellet Concentration at (0.5[m], 0[m], 0[m])

1 In the **Model Builder** window, expand the **Results>Pellet Concentration at (0[m], 0[m], 0[m]) (tds)** node, then click **Pellet Concentration at (0[m], 0[m], 0[m]) (tds)**.

2 In the **Settings** window for **1D Plot Group**, type `Pellet Concentration at (0.5[m], 0[m], 0[m])` 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`.

5 Locate the **Plot Settings** section. Select the **Two y-axes** check box.

6 In the table, select the **Plot on secondary y-axis** check box for **Species C**.

7 Locate the **Legend** section. From the **Position** list, choose **Middle left**.

Species A

1 In the **Model Builder** window, expand the **Pellet Concentration at (0.5[m], 0[m], 0[m])** node, then click **Species A**.

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

3 In the **Expression** text field, type `atxd3(0.5[m], 0[m], 0[m], tds.cpe_cA)`.

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

4 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

5 Click to expand the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `c<sub>A</sub>`.

Species B

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

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

3 In the **Expression** text field, type `atxd3(0.5[m], 0[m], 0[m], tds.cpe_cB)`.

4 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

5 Locate the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `c<sub>B</sub>`.

Species C

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

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

3 In the **Expression** text field, type `atxd3(0.5[m], 0[m], 0[m], tds.cpe_cC)`.

4 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

5 Locate the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `c<sub>C</sub>`.

6 In the **Pellet Concentration at (0.5[m], 0[m], 0[m])** toolbar, click **Plot**.

Pellet concentration, A

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

2 In the **Model Builder** window, under **Results** click **Pellet concentration, A**.

3 In the **Pellet concentration, A** toolbar, click **Plot**.

Pellet concentration, A 1

Right-click **Pellet concentration, A** and choose **Duplicate**.

Pellets 1

1 In the **Model Builder** window, expand the **Pellet concentration, A 1** node, then click **Pellets 1**.

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

3 From the **Solution parameters** list, choose **From parent**.

4 Locate the **Coloring and Style** section.

5 Select the **Radius scale factor** check box. In the associated text field, type `15`.

Pellet and Bed Concentration, A

1 In the **Model Builder** window, under **Results** click **Pellet concentration, A 1**.

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

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

Surface 1

Right-click **Pellet and Bed Concentration, A** and choose **Surface**.

Selection 1

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

2 Select Boundary 3 only.

Surface 1

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

2 In the **Settings** window for **Surface**, click to expand the **Inherit Style** section.

3 From the **Plot** list, choose **Pellets 1**.

Surface: Outer Wall

1 In the **Model Builder** window, right-click **Pellet and Bed Concentration, A** and choose **Surface**.

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

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

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

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

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

Selection 1

1 Right-click **Surface: Outer Wall** and choose **Selection**.

2 Select Boundaries 4 and 12 only.

3 In the **Pellet and Bed Concentration, A** toolbar, click  **Plot**.

Pellet and Bed Concentration, A

1 In the **Model Builder** window, click **Pellet and Bed Concentration, A**.

2 Drag and drop below **Pellet concentration, C**.

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 **Dataset** list, choose **Cut Line 3D 1**.

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

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.

8 Select the **x-axis label** check box. In the associated text field, type `Reactor height (m)`.

9 Select the **y-axis label** check box. In the associated text field, type `Concentration (mol/m<sup>3</sup>)`.

10 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 **Width** list, choose **2**.

5 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.

6 From the **Positioning** list, choose **Interpolated**.

7 In the **Number** text field, type `11`.

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

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

10 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. Find the **Line markers** subsection. From the **Marker** list, choose **None**.

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

Legends
c_B

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

Legends
c_C

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 **Cycle (reset)**.

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

Legends
c_A, Pellet average

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 **Cycle**.

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

Legends
c_B, Pellet average

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

Legends
`c<sub>C</sub>, Pellet average`

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

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

Bed 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 **Bed 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 **Bed 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>Bed 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. 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.

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

9 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**.