Packed Bed Reactor

Introduction

The packed bed reactor is one of the most common reactors in the chemical industry, for use in heterogeneous catalytic processes. In essence, the reactor consists of a container filled with catalyst particles. These particles can be contained within a supporting structure, like tubes or channels, or they can be packed in one single compartment in the reactor.

The structure that is formatted by the packed catalyst particles makes the modeling of mass and energy transport in the reactor a challenging task. The difficulty lies in the description of the porous structure, which gives transport of different orders of magnitudes within the particles and between the particles. In most cases, the structure in between particles is described as macroporous and the particle radius can be of the order of magnitude of 1 mm. When a pressure difference is applied across the bed, convection arises in the macropores. The pores inside the catalyst particles form the microstructure of the bed. The pore radii in the particles is often between one and ten micrometer.

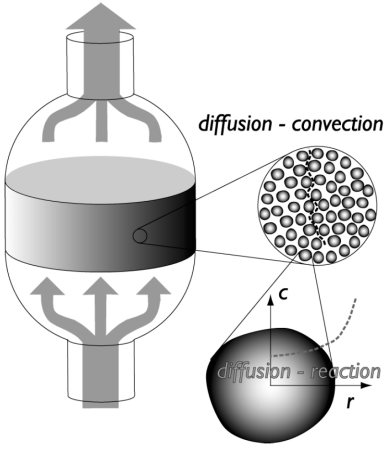

Figure 1: Schematic showing the macro dimension (bed height) and the micro dimension (pellet radial position).

This model presents a simple and fast route to studying microscale and macroscale mass balances in packed beds and other heterogeneous reactors with bimodal pore

distribution. Using a multigeometry approach, the model provides the mass and reaction distributions along the reactor and within each catalyst pellet along the reactor length. This makes it possible to evaluate the utilization of catalyst load, optimal pellet size, or inlet temperature.

In this example, volatile organic compounds (VOC) and CO are oxidized in a catalytic converter. Propylene is used as representative for hydrocarbons present in the feed stream, which could be, for example, exhaust gas from a combustion process.

Model Definition

The following chemical reactions describe the catalytic conversion carbon monoxide and by-product hydrocarbon:

$$\mathrm{CO} + \frac{1}{2}\mathrm{O_2} \rightarrow \mathrm{CO_2} \tag{1}$$

$$\mathrm{C_3H_6} + \frac{9}{2}\mathrm{O_2} \rightarrow 3\mathrm{H_2O} + 3\mathrm{CO_2} \tag{2}$$

For these heterogeneous catalytic reactions the rates (mol/(m^3·s)) are given by (Ref. 1):

$$r_1 = \frac{k_1 c_{\mathrm{CO}}\, c_{\mathrm{O2}}}{(1 + K_{\mathrm{CO}}\, c_{\mathrm{CO}} + K_{\mathrm{C3H6}}\, c_{\mathrm{C3H6}})^2} \tag{3}$$

$$r_2 = \frac{k_2 c_{\mathrm{C3H6}}\, c_{\mathrm{O2}}}{(1 + K_{\mathrm{CO}}\, c_{\mathrm{CO}} + K_{\mathrm{C3H6}}\, c_{\mathrm{C3H6}})^2} \tag{4}$$

The rate and adsorption constants are given by Arrhenius expressions:

$$k = A \exp\left(-\frac{E}{R_g T}\right) \tag{5}$$

The values of the frequency factors and activation energies (J/mol) are taken from the literature (Ref. 2) and presented in Table 1,

TABLE 1: ARRHENIUS PARAMETERS

RATE/ADSORPTION CONSTANT	FREQUENCY FACTOR (JOULE/MOL)	ACTIVATION ENERGY (JOULE/MOL)
k_1	$7.07 \cdot 10^{13}$	$1.09 \cdot 10^{5}$
k_2	$1.47 \cdot 10^{15}$	$1.26 \cdot 10^{5}$

TABLE 1: ARRHENIUS PARAMETERS

RATE/ADSORPTION CONSTANT	FREQUENCY FACTOR (JOULE/MOL)	ACTIVATION ENERGY (JOULE/MOL)
K_{CO}	8.1	-3400
K_{C3H6}	257.9	1588

The chemical reactions given in Equation 1 and Equation 2 describe a process that is limited by the second-order rate expression at high temperatures when the surface coverage is low. At low temperatures the adsorption reactions will be slower and limit the reaction rate due to a shortage of free catalytic sites.

The pressure drop in the reactor is described by the Ergun equation

$$\frac{dP}{dx} = \left(-\frac{\rho u}{\rho g_c D_p}\right)\frac{(1-\Phi)}{\Phi^3}\left[\frac{150(1-\Phi)\eta}{D_p} + 1.75\rho u\right] \tag{6}$$

where P is the pressure (Pa), Φ the porosity, D_p the particle diameter (m), η denotes the gas viscosity (Pa·s)), ρ the gas density (kg/m^3), and x the reactor length (m). u is the reactor flow velocity (m/s) that depends on the pressure drop according to

$$u = u_{\text{feed}} \cdot \frac{c}{c_{\text{feed}}} \cdot \frac{P_{\text{feed}}}{P} \tag{7}$$

where u_{feed} is the inlet velocity and c the total concentration (mol/m^3).

The mass transport in the reactor is given by the convection and diffusion equation

$$\nabla \cdot (-D\nabla c) = R - u \cdot \nabla c \tag{8}$$

where D is the diffusion coefficient (m^2/s) and R is a source term (mol/(m^3·s)). Equation 8 needs to be solved for all species participating in Equation 1 and Equation 2. Each equation also needs proper boundary conditions.

At the inlet the reactant concentration is known:

$$c_{CO} = c_{COin} \tag{9}$$

$$c_{C3H6} = c_{C3H6in} \tag{10}$$

$$c_{O2} = c_{O2in} \tag{11}$$

$$c_{CO2} = 0 \tag{12}$$

$$c_{H2O} = 0 \tag{13}$$

At the outlet, the Outflow condition states that convective mass transport will dominate the species transport across the boundary:

$$\mathbf{n} \cdot (-D\nabla c) = 0 \tag{14}$$

At first glance, these equations appear straight forward, especially if the velocity vector is given by an analytical expression, which is the case for plug flow in a packed bed reactor. However, the source term, R, depends on the transport inside the catalyst particles. The molar flux at the outer surface of the particles multiplied by the available outer surface area of the particles per unit volume gives the proper source term:

$$R = (1 - \varepsilon_b)A_p(\mathbf{N} \cdot \mathbf{n}) \text{ at } r = r_p \tag{15}$$

In this equation, ε_b is the bed porosity, $\mathbf{N}$ denotes the flux vector inside the porous particle (mol/(m^2·s)) and $\mathbf{n}$ is the outward unit vector normal to the particle surface. Equation 15 is only valid at the particle surface, where the independent radius variable r (introduced below) equals the particle radius, r_p. Furthermore, A_p denotes the pellet surface to volume ratio (m^2/m^3). This property is related to the pellet radius as

$$A_p = \frac{3}{r_p} \tag{16}$$

To properly calculate R, a mass balance is required for the catalyst pellet interior. Such a mass balance can be expressed as

$$\nabla \cdot (-D_{pc}\nabla c_p) + R_p = 0 \text{ for } x^2 + y^2 < r_p^2 \tag{17}$$

Here, D_{pc} is the effective diffusion coefficient in the particle, c_p is the species concentration in the particle, and R_p is the reaction rate for the heterogeneous reaction in the particle. In the catalyst pores, transport takes palace by diffusion only.

Equation 17 gives mass balance for each species for the catalyst pellet. Since the pellets are spherical, it is convenient to express these mass balances in spherical coordinates. Equation 17 then becomes

$$\nabla \cdot (-r^2 D_{pc}\nabla c_p) + r^2 R_p = 0 \text{ for } 0 < r < r_p \tag{18}$$

where r (m) is the independent variable for the position along the radius of the particle. The equation is scaled with the particle radius to get a geometry with a lower aspect ratio. This gives the final formulation

$$\nabla \cdot \left(-\left(\frac{r}{r_p}\right)^2 D_{cp} \nabla c_p\right) + \left(\frac{r}{r_p}\right)^2 R_p = 0 \text{ for } 0 < r < 1 \tag{19}$$

The diffusion-reaction equation, combined with the boundary conditions for the particle, give the concentration distribution in the particle. The boundary conditions are

$$-D_{pc} \nabla c_p \cdot \mathbf{n} = 0 \text{ at } r = 0 \tag{20}$$

and

$$c_p = \varepsilon c \text{ at } r = 1 \tag{21}$$

where ε denotes the porosity of the particle, and c and c_p represent the species concentrations in the bulk and in the particle, respectively. The concentration at the surface of the particle is equal to the concentration outside the particle compensated to account for the part of the particle volume that is occupied by solid catalyst support.

The concentration distribution in the particle gives the molar flux at every point in the particles. This implies that the source term for the catalyst bed is given by the solution of the microscale mass balance:

$$R = (1 - por_b) A_p (-D_{pc} \nabla c_p \cdot \mathbf{n}) \tag{22}$$

A complication in solving the derived system of equations is that the macroscale and microscale balances are defined in different coordinate systems. This problem is general for many chemical reaction engineering applications and is often solved by using an analytical approximation of the solution to the microscale balance. However, such an approach cannot be used for complicated reaction mechanisms involving several reaction species. The approach exemplified here is general and can be used for very complex reaction mechanisms involving a large number of species.

Results and Discussion

Figure 2 shows the concentration of reacting species as function of position in the reactor. The levels of carbon monoxide and propylene are significantly reduced.

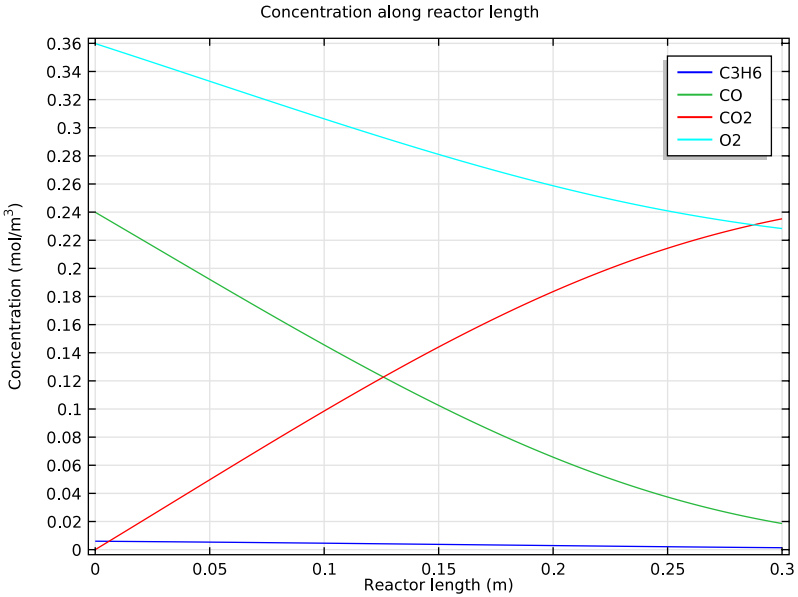

Figure 2: The concentration of reactants and products along the reactor length. The pellet radius r_p is 2.5 mm.

The concentration can also be evaluated within each pellet, revealing whether or not the catalyst comes to efficient use. Figure 3 shows an example of this.

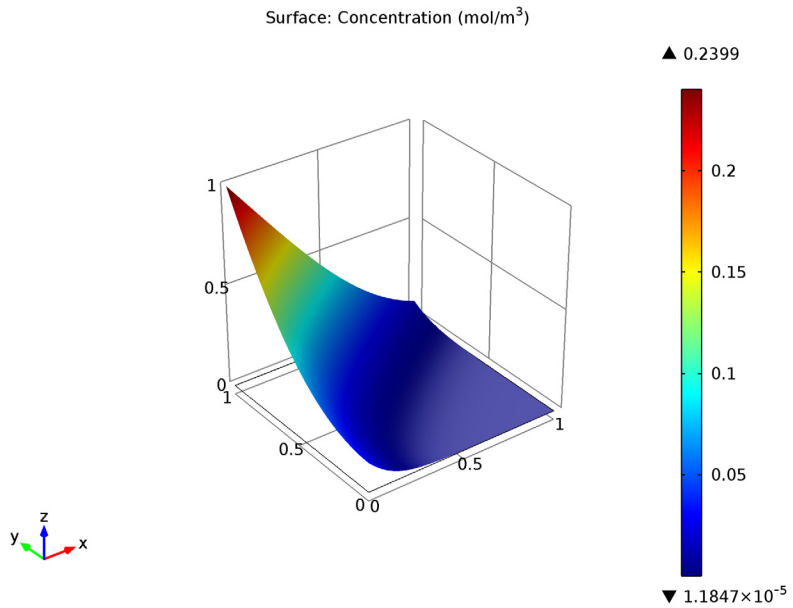

Figure 3: The concentration of in-pellet CO as function of reactor position. The scaled pellet radius is given on the y-axis and the reactor position along the x-axis.

From Figure 3 it is clear that the CO concentration is low at the center of the pellet at all reactor positions. This means that reactor performance is limited by diffusion within the pellets and that active catalyst material in the center of the pellet will never come to use. Reducing the pellet diameter could potentially remedy this situation, and simulation results shown in Figure 4 confirm this notion.

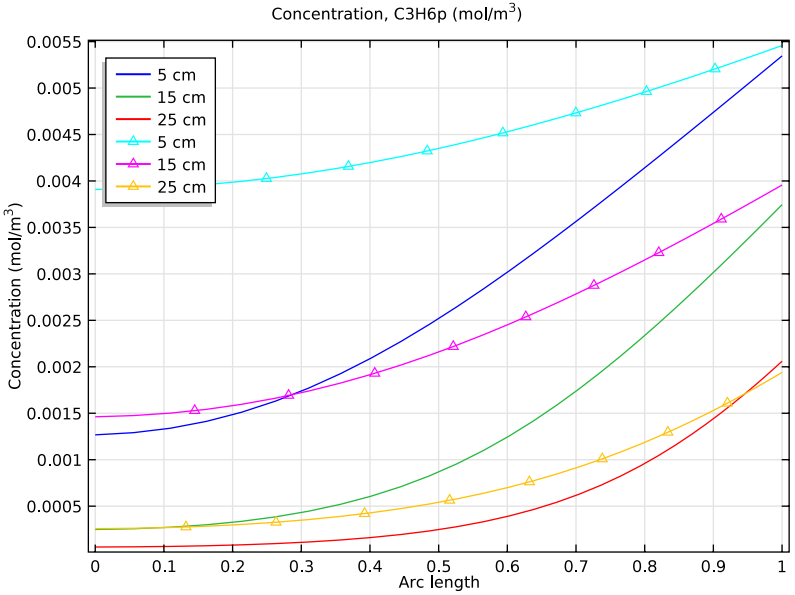

Figure 4: The concentration of in-pellet C_3H_6 at three different reactor positions (5, 15, and 25 cm). Solid lines represents a pellet radius of 2.5 mm and lines with triangular markers represents a pellet radius of 1.8 mm.

With a pellet radius of 2.5 mm, the reactor is limited by the in-pellet diffusion, as is indicated by the slope of the solid lines. The effect of this is that the active sites in the interior of the pellets are not used to their full potential. If the pellet size is reduced (represented by the lines with a triangular marker), the lines level out faster, suggesting larger reaction limited regions. The effect on C_3H_6 conversion in the simulated case is an improvement from 94 % to 97 %.

References

1. S.H. Oh, J.C. Cavendish, and L.L. Hegedus. "Mathematical modeling of catalytic converter lightoff: Single-pellet studies," *AIChE Journal*, vol. 26, no. 6, pp. 935–943, 1980.

2. J.B. Rawlings and J.G. Ekerdt, *Chemical Reactor Analysis and Design Fundamentals*, Nob Hill Publishing, Madison, 2002.

Model Library path: `Chemical_Reaction_Engineering_Module/Packed_Bed_Reactors/packed_bed_reactor`

Modeling Instructions

Start by selecting physics user interfaces for the reactor mass transport and pressure equations.

From the **File** menu, choose **New**.

NEW

1 In the **New** window, click the **Model Wizard** button.

MODEL WIZARD

1 In the **Model Wizard** window, click the **1D** button.

2 In the **Select physics** tree, select **Chemical Species Transport>Transport of Diluted Species (chds)**.

3 Click the **Add** button.

4 In the **Number of species** edit field, type `5`.

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

C3H6
CO
CO2
H2O
O2

6 In the **Select physics** tree, select **Mathematics>PDE Interfaces>Coefficient Form PDE (c)**.

7 Click the **Add** button.

8 In the **Field name** edit field, type `P`.

9 In the **Dependent variables** table, enter the following settings:

P

10 Click the **Study** button.

11 In the tree, select **Preset Studies for Selected Physics>Stationary**.

12 Click the **Done** button.

GEOMETRY 1

Interval 1

1 In the **Model Builder** window, under **Component 1** right-click **Geometry 1** and choose **Interval**.

2 In the **Interval** settings window, locate the **Interval** section.

3 In the **Right endpoint** edit field, type `0.3`.

4 Click the **Build Selected** button.

GLOBAL DEFINITIONS

Parameters

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

2 In the **Parameters** settings window, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Model Library folder and double-click the file `packed_bed_reactor_parameters.txt`.

Variables 1

1 In the **Model Builder** window, right-click **Global Definitions** and choose **Variables**.

2 In the **Variables** settings window, locate the **Variables** section.

3 Click **Load from File**.

4 Browse to the model's Model Library folder and double-click the file `packed_bed_reactor_variables_global.txt`.

TRANSPORT OF DILUTED SPECIES

Follow these steps to set up mass transport equations for the packed bed.

Convection and Diffusion 1

1 In the **Model Builder** window, expand the **Component 1>Transport of Diluted Species** node, then click **Convection and Diffusion 1**.

2 In the **Convection and Diffusion** settings window, locate the **Model Inputs** section.

3 Specify the **u** vector as

u	x

4 Locate the **Diffusion** section. In the D_{C3H6} edit field, type `D_C3H6`.

5 In the D_{CO} edit field, type `D_CO`.

6 In the D_{CO2} edit field, type `D_CO2`.

7 In the D_{H2O} edit field, type `D_H2O`.

8 In the D_{O2} edit field, type `D_O2`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1>Transport of Diluted Species** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the *C3H6* edit field, type `1e-6`.

4 In the *CO* edit field, type `1e-6`.

5 In the *CO2* edit field, type `1e-6`.

6 In the *H2O* edit field, type `1e-6`.

7 In the *O2* edit field, type `1e-6`.

Reactions 1

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

2 Select Domain 1 only.

3 In the **Reactions** settings window, locate the **Reactions** section.

4 In the R_{C3H6} edit field, type `-Ap*C3H6flux*(1-por_b)`.

5 In the R_{CO} edit field, type `-Ap*COflux*(1-por_b)`.

6 In the R_{CO2} edit field, type `-Ap*CO2flux*(1-por_b)`.

7 In the R_{H2O} edit field, type `-Ap*H2Oflux*(1-por_b)`.

8 In the R_{O2} edit field, type `-Ap*O2flux*(1-por_b)`.

You will define the flux variables later on, after having set up the pellet model. Note that the volume fraction of the catalytic particles in reactor is (1-por_b).

Inflow 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundary 1 only.

3 In the **Inflow** settings window, locate the **Concentration** section.

4 In the $c_{0,C3H6}$ edit field, type `x_C3H6_feed*Ctot_feed`.

5 In the $c_{0,CO}$ edit field, type `x_CO_feed*Ctot_feed`.

6 In the $c_{0,O2}$ edit field, type `x_O2_feed*Ctot_feed`.

Outflow 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 2 only.

COEFFICIENT FORM PDE

Follow the steps below to specify the Ergun equation for the pressure drop in the reactor.

1 In the **Model Builder** window, under **Component 1** click **Coefficient Form PDE**.

2 In the **Coefficient Form PDE** settings window, locate the **Units** section.

3 Find the **Source term quantity** subsection. From the list, choose **Pressure (Pa)**.

4 In the **Unit** edit field, type `N/m^3`.

Coefficient Form PDE 1

1 In the **Model Builder** window, expand the **Coefficient Form PDE** node, then click **Coefficient Form PDE 1**.

2 In the **Coefficient Form PDE** settings window, locate the **Diffusion Coefficient** section.

3 In the *c* edit field, type `0`.

4 Locate the **Source Term** section. In the *f* edit field, type `Px+beta*(F/F0)*(P_feed/P)`.

5 Locate the **Damping or Mass Coefficient** section. In the d_a edit field, type `0`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1>Coefficient Form PDE** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the P edit field, type `P_feed`.

Dirichlet Boundary Condition 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Dirichlet Boundary Condition**.

2 Select Boundary 1 only.

3 In the **Dirichlet Boundary Condition** settings window, locate the **Dirichlet Boundary Condition** section.

4 In the *r* edit field, type `P_feed`.

ROOT

The source terms in the reactor mass balances depend on the surface fluxes from the catalyst pellets. Therefore, set up a separate model calculating the mass transport and reaction in the pellets.

On the **Home** toolbar, click **Add Component** and choose **2D**.

COMPONENT 2

On the **Home** toolbar, click **Add Physics**.

ADD PHYSICS

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

2 In the **Add physics** tree, select **Chemical Species Transport>Transport of Diluted Species (chds)**.

3 Click to expand the **Dependent variables** section. Locate the **Dependent Variables** section. In the **Number of species** edit field, type `5`.

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

C3H6p
COp
CO2p
H2Op
O2p

5 In the **Add physics** window, click **Add to Component**.

GEOMETRY 2

Square 1

1 In the **Model Builder** window, under **Component 2** right-click **Geometry 2** and choose **Square**.

2 Right-click **Square 1** and choose **Build Selected**.

TRANSPORT OF DILUTED SPECIES 2

Convection and Diffusion 1

Use the full diffusivity matrix to specify that diffusion occurs only in the radial pellet direction, corresponding to the direction of the y-axis in the 2D geometry.

1 In the **Model Builder** window, expand the **Component 2>Transport of Diluted Species 2** node, then click **Convection and Diffusion 1**.

2 In the **Convection and Diffusion** settings window, locate the **Diffusion** section.

3 From the symmetry property list, choose **Anisotropic**.

4 In the D_{C3H6p} table, enter the following settings:

0	0
0	(D_C3H6/rp^2)*y^2

5 From the symmetry property list, choose **Anisotropic**.

6 In the D_{COp} table, enter the following settings:

0	0
0	(D_CO/rp^2)*y^2

7 From the symmetry property list, choose **Anisotropic**.

8 In the D_{CO2p} table, enter the following settings:

0	0
0	(D_CO2/rp^2)*y^2

9 From the symmetry property list, choose **Anisotropic**.

10 In the D_{H2Op} table, enter the following settings:

0	0
0	(D_H2O/rp^2)*y^2

11 From the symmetry property list, choose **Anisotropic**.

12 In the D_{O2p} table, enter the following settings:

0	0
0	(D_O2/rp^2)*y^2

Initial Values 1

1 In the **Model Builder** window, under **Component 2>Transport of Diluted Species 2** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the *C3H6p* edit field, type `1e-6`.

4 In the *COp* edit field, type `1e-6`.

5 In the *CO2p* edit field, type `1e-6`.

6 In the *H2Op* edit field, type `1e-6`.

7 In the *O2p* edit field, type `1e-6`.

Reactions 1

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

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

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

4 Locate the **Reactions** section. In the R_{C3H6p} edit field, type `-y^2*R2`.

5 In the R_{COp} edit field, type `-y^2*R1`.

6 In the R_{CO2p} edit field, type `y^2*(R1+3*R2)`.

7 In the R_{H2Op} edit field, type `y^2*3*R2`.

8 In the R_{O2p} edit field, type `-y^2*(0.5*R1+4.5*R2)`.

Concentration 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Concentration**.

Species concentrations calculated by the reactor model serve as boundary conditions for the pellet model. You define the variables in a later step.

2 Select Boundary 3 only.

3 In the **Concentration** settings window, locate the **Concentration** section.

4 Select the **Species C3H6p** check box.

5 In the $c_{0,C3H6p}$ edit field, type `C3H6bulk`.

6 Select the **Species COp** check box.

7 In the $c_{0,\mathrm{COp}}$ edit field, type `CObulk`.

8 Select the **Species CO2p** check box.

9 In the $c_{0,CO2p}$ edit field, type `CO2bulk`.

10 Select the **Species H2Op** check box.

11 In the $c_{0,H2Op}$ edit field, type `H2Obulk`.

12 Select the **Species O2p** check box.

13 In the $c_{0,O2p}$ edit field, type `O2bulk`.

14 In the **Model Builder** window's toolbar, click the **Show** button and select **Advanced Physics Options** in the menu.

15 Click to expand the **Constraint settings** section. Locate the **Constraint Settings** section. From the **Apply reaction terms on** list, choose **Individual dependent variables**.

DEFINITIONS

Complete the model setup by coupling the reactor and pellet models. First use a general extrusion component coupling to make the reactor species concentrations available in the pellet model.

General Extrusion 1

1 On the **Definitions** toolbar, click **Component Couplings** and choose **General Extrusion**.

2 In the **General Extrusion** settings window, locate the **Source Selection** section.

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

4 Locate the **Destination Map** section. In the **x-expression** edit field, type `x*0.30`.

5 Locate the **Source** section. Select the **Use source map** check box.

General Extrusion 2

Next, set up another general extrusion coupling in the pellet model for use when calculating the species flux at the pellet boundary.

1 On the **Definitions** toolbar, click **Component Couplings** and choose **General Extrusion**.

2 In the **General Extrusion** settings window, locate the **Source Selection** section.

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

4 Select Boundary 3 only.

5 Locate the **Destination Map** section. In the **x-expression** edit field, type `x/0.30`.

6 Clear the **y-expression** edit field.

7 Locate the **Source** section. Select the **Use source map** check box.

8 Clear the **y-expression** edit field.

Variables 2

Read in the variable file that defines the species fluxes at the pellet boundary.

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Variables** settings window, locate the **Variables** section.

3 Click **Load from File**.

4 Browse to the model's Model Library folder and double-click the file `packed_bed_reactor_variables_1d.txt`.

Note that these variables use the extrusion coupling operator that you just defined.

Variables 3

Now, read in the variable file that defines the bulk species concentrations.

1 Right-click **Definitions** and choose **Variables**.
2 In the **Variables** settings window, locate the **Geometric Entity Selection** section.
3 From the **Geometric entity level** list, choose **Boundary**.
4 Select Boundary 3 only.
5 Locate the **Variables** section. Click **Load from File**.
6 Browse to the model's Model Library folder and double-click the file `packed_bed_reactor_variables_2d.txt`.

As you can see, these variables use the extrusion coupling operator you defined in the reactor model.

MESH 1

Size

1 In the **Model Builder** window, under **Component 1** right-click **Mesh 1** and choose **Edge**.
2 In the **Size** settings window, locate the **Element Size** section.
3 Click the **Custom** button.
4 Locate the **Element Size Parameters** section. In the **Maximum element size** edit field, type `0.0025`.
5 Click the **Build All** button.

MESH 2

Mapped 1

In the **Model Builder** window, under **Component 2** right-click **Mesh 2** and choose **Mapped**.

Distribution 1

1 In the **Model Builder** window, under **Component 2>Mesh 2** right-click **Mapped 1** and choose **Distribution**.
2 Select Boundaries 1 and 4 only.
3 In the **Distribution** settings window, locate the **Distribution** section.
4 From the **Distribution properties** list, choose **Predefined distribution type**.
5 In the **Number of elements** edit field, type `30`.
6 In the **Element ratio** edit field, type `0.2`.

Distribution 2

1 Right-click **Mapped 1** and choose **Distribution**.
2 Select Boundary 3 only.

3 In the **Distribution** settings window, locate the **Distribution** section.

4 In the **Number of elements** edit field, type 120.

5 Click the **Build All** button.

STUDY 1

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

RESULTS

Concentration (chds)

Fist adapt the default plot to show the species concentrations in the reactor as functions of the position.

1 In the **1D Plot Group** settings window, click to expand the **Title** section.

2 From the **Title type** list, choose **Manual**.

3 In the **Title** text area, type `Concentration along reactor length`.

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

5 In the associated edit field, type `Reactor length (m)`.

6 In the **Model Builder** window, expand the **Concentration (chds)** node, then click **Line Graph 1**.

7 In the **Line Graph** settings window, click to expand the **Legends** section.

8 Select the **Show legends** check box.

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

10 In the table, enter the following settings:

Legends
C3H6

11 On the **1D plot group** toolbar, click **Plot**.

12 Right-click **Results>Concentration (chds)>Line Graph 1** and choose **Duplicate**.

13 In the **Line Graph** settings window, locate the **y-Axis Data** section.

14 In the **Expression** edit field, type C0.

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

Legends
C0

16 Right-click **Results>Concentration (chds)>Line Graph 2** and choose **Duplicate**.

17 In the **Line Graph** settings window, locate the **y-Axis Data** section.

18 In the **Expression** edit field, type `CO2`.

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

Legends
CO2

20 Right-click **Results>Concentration (chds)>Line Graph 3** and choose **Duplicate**.

21 In the **Line Graph** settings window, locate the **y-Axis Data** section.

22 In the **Expression** edit field, type `O2`.

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

Legends
O2

24 On the **1D plot group** toolbar, click **Plot**.

Concentration (chds2)

Now plot the concentration of CO in the pellet of the catalytic bed.

1 In the **Model Builder** window, expand the **Results>Concentration (chds2)** node, then click **Surface 1**.

2 In the **Surface** settings window, locate the **Expression** section.

3 In the **Expression** edit field, type `COp`.

4 Right-click **Results>Concentration (chds2)>Surface 1** and choose **Height Expression**.

STUDY 1

To investigate if better pellet utilization can be achieved, reduce the pellet size. This affects the packing of the catalyst and reduces the diffusive length within the pellets.

Step 1: Stationary

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Stationary**.

2 In the **Stationary** settings window, click to expand the **Study extensions** section.

3 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

4 Click **Add**.

5 In the table, enter the following settings:

Auxiliary parameter	Parameter value list
rp	0.0025 0.0018

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

RESULTS

Data Sets

Create plots of the propene concentration distribution in the pellets, evaluated at reactor positions 5 cm, 15 cm, and 25 cm.

1 On the **Results** toolbar, click **Cut Line 2D**.

2 In the **Cut Line 2D** settings window, locate the **Line Data** section.

3 In row **Point 1**, set **x** to 5/30.

4 In row **Point 2**, set **x** to 5/30.

5 In row **Point 2**, set **y** to 1.

6 Select the **Additional parallel lines** check box.

7 In the **Distances** edit field, type -10/30 -20/30.

8 Click the **Plot** button.

1D Plot Group 4

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

2 On the **1D plot group** toolbar, click **Line Graph**.

3 In the **Line Graph** settings window, locate the **Data** section.

4 From the **Data set** list, choose **Cut Line 2D 1**.

5 From the **Parameter selection (rp)** list, choose **From list**.

6 In the **Parameter values (rp)** list, choose **0.0025** and **0.0018**.

7 Locate the **y-Axis Data** section. In the **Expression** edit field, type C3H6p.

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
5 cm

Legends
15 cm
25 cm

11 Right-click **Results>1D Plot Group 4>Line Graph 1** and choose **Duplicate**.

12 In the **Line Graph** settings window, locate the **Data** section.

13 In the **Parameter values (rp)** list, select **0.0018**.

14 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Marker** list, choose **Triangle**.

15 In the **Model Builder** window, click **1D Plot Group 4**.

16 In the **1D Plot Group** settings window, click to expand the **Legend** section.

17 From the **Position** list, choose **Upper left**.

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

19 In the **Title** text area, type `Concentration, C3H6p (mol/m<sup>3</sup>)`.

20 On the **1D plot group** toolbar, click **Plot**.