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 arise in the macropores. The pores inside the catalyst particles form the microstructure of the bed. The pore radius in the particles is often between one and ten micrometer.

This model presents a simple and fast alternative for 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:

$$CO + \frac{1}{2}O_2 \rightarrow CO_2 \qquad (8\text{-}143)$$

$$C_3H_2 + \frac{9}{2}O_2 \rightarrow 3H_2O + 3CO_2 \tag{8-144}$$
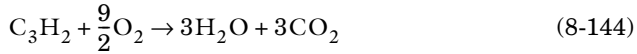
For these heterogeneous catalytic reactions the rates $(mol/(m^3 \cdot s))$ are given by

$$r_1 = \frac{k_1 c_{CO} c_{O2}}{(1 + K_{CO} c_{CO} + K_{C3H6} c_{C3H6})^2} \tag{8-145}$$

$$r_2 = \frac{k_2 c_{C3H6} c_{O2}}{(1 + K_{CO} c_{CO} + K_{C3H6} c_{C3H6})^2} \tag{8-146}$$

The rate and adsorption constants are given by Arrhenius expressions:

$$k = A \exp\left(-\frac{E}{R_g T}\right) \tag{8-147}$$

The values of the frequency factors and activation energies (J/mol) are taken from the literature (Ref 2) and presented in Table 8-3.

TABLE 8-3: 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	$1.47 \cdot 10^{15}$	$1.26 \cdot 10^5$
K_{CO}	8.1	-3400
K_{C3H6}	257.9	1588

The chemical reactions given in Equation 8-143 and Equation 8-144 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 adsorbtion 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

$$\frac{dP}{dx} = \left(-\frac{\rho u}{\rho g_c D_p}\right) \frac{(1-\Phi)}{\Phi^3} \left[\frac{150(1-\Phi)\mu}{D_p} + 1.75\rho u\right] \tag{8-148}$$

where P is the pressure (kPa), Φ the porosity, D_p the particle diameter (m), μ denotes the gas viscosity $(kg/(m \cdot s))$, 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

$$u = u_{\text{feed}} \cdot \frac{C}{C_{\text{feed}}} \cdot \frac{P_{\text{feed}}}{P} \qquad (8\text{-}149)$$

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

$$\nabla \cdot (-D\nabla c) = R - u \cdot \nabla c \qquad (8\text{-}150)$$

where D is the diffusion coefficient (m^2/s) and R is a source term (mol/(m^3·s)). Equation 8-150 needs to be solved for all species participating in Equation 8-143 and Equation 8-144. Each equation also needs proper boundary conditions.

At the inlet the reactant concentration is known:

$$c_{\text{CO}} = c_{\text{COin}} \qquad (8\text{-}151)$$

$$c_{\text{C3H6}} = c_{\text{C3H6in}} \qquad (8\text{-}152)$$

$$c_{\text{O2}} = c_{\text{O2in}} \qquad (8\text{-}153)$$

$$c_{\text{CO2}} = 0 \qquad (8\text{-}154)$$

$$c_{\text{H2O}} = 0 \qquad (8\text{-}155)$$

At the outlet, the convective flux condition will let the product and reactants leave with the flow.

$$\mathbf{n} \cdot (-D\nabla c) = 0 \qquad (8\text{-}156)$$

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:

$$R = A_{\text{p}}(\mathbf{N} \cdot \mathbf{n}) \qquad \text{at } r = r_{\text{p}} \qquad (8\text{-}157)$$

In this equation, $\mathbf{N}$ denotes the flux inside the porous particle (mol/(m^2·s)) and $\mathbf{n}$ is the outward unit vector normal to the particle surface. Equation 8-157 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

$$A_p = \frac{r_p}{3} \tag{8-158}$$

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

$$\nabla \cdot (-D_{pc}\nabla c_p) + R_p = 0 \qquad \text{for } x^2 + y^2 < r_p^2 \tag{8-159}$$

Here, D_{pc} is the effective diffusion coefficient in the particle, c_p is the 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 8-159 gives mass balance for each species for the catalyst pellet. Because the pellets are spherical, it is convenient to express these mass balances in spherical coordinates. Equation 8-159 then becomes

$$\nabla \cdot (-r^2 D_{pc}\nabla c_p) + r^2 R_p = 0 \qquad \text{for } 0 < r < r_p \tag{8-160}$$

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:

$$\nabla \cdot \left(-\frac{r^2}{r_p^2} D_{pc}\nabla c_p\right) + r^2 R_p = 0 \qquad \text{for } 0 < r < 1 \tag{8-161}$$

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

$$-D_{pc}\nabla c_p \cdot \mathbf{n} = 0 \qquad \text{at } r = 0 \tag{8-162}$$

$$c_p = \varepsilon c \qquad \text{at } r = 1 \tag{8-163}$$

where ε denotes the porosity of the particle, and c and c_p represent the species concentrations. This implies symmetry at the center of the particle. In addition, 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:

$$R = A_p(-D_{pe}\nabla c_p \cdot \mathbf{n}) \qquad (8\text{-}164)$$

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 solution exemplified here is general and can be used for very complex reaction mechanisms involving a large number of species.

Results and Discussion

Figure 8-72 shows the concentration of reacting species in the reactor as function of position. The levels of carbon monoxide and propylene are significantly reduced.
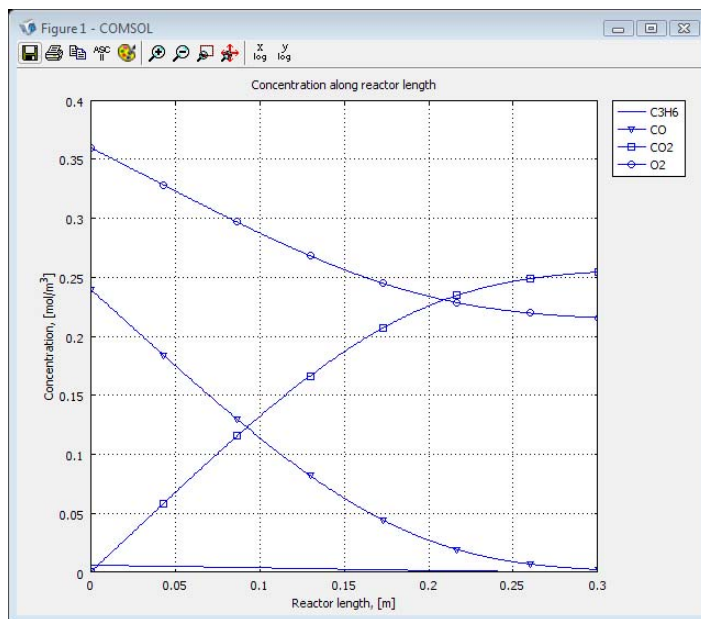

Figure 8-72: The concentration of reactants and products along the reactor length. The pellet radius r_p is 2.5mm.

The concentration can also be evaluated within each pellet, revealing whether or not the catalyst comes to efficient use. Figure 8-73 shows an example of this.
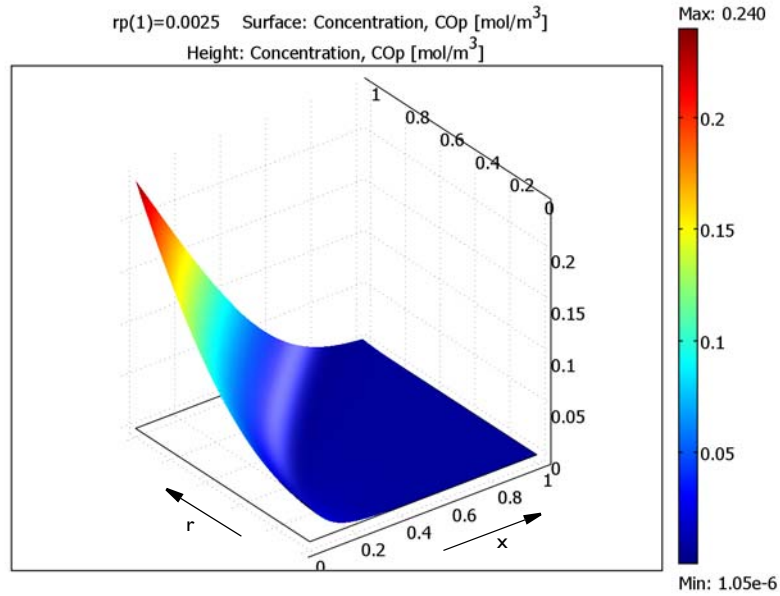

Figure 8-73: The concentration of in-pellet CO as function of reactor position. The scaled pellet radius is given on the r-axis and the reactor position along the x-axis.

From Figure 8-73 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 8-74 confirm this notion.
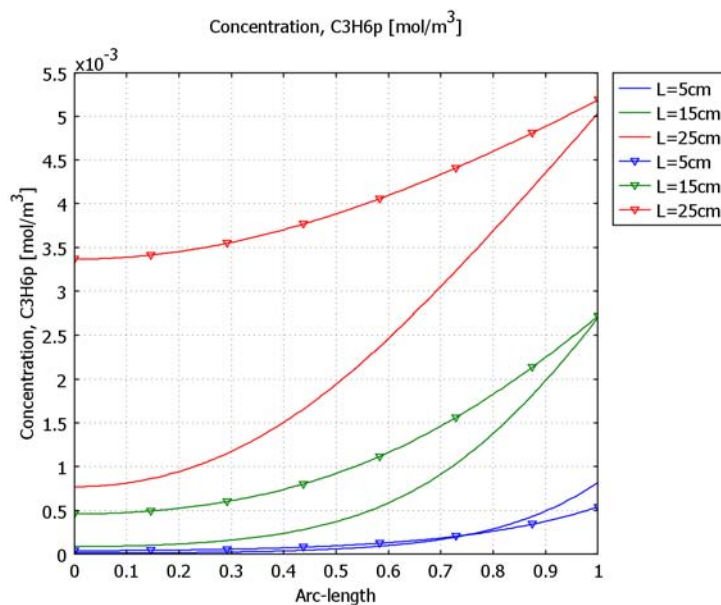

Figure 8-74: The concentration of in-pellet C_3H_6 at three different reactor positions (5, 15, and 25 cm). Solid lines represents a pellet radius of 2.5 mm and lines with triangular markers represents a pellet radius of 1.8 mm.

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 (6), pp. 935–943.

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

Model Library path: `Chemical_Engineering_Module/`
`Transport_and_Reactions/packed_bed_reactor`

*Modeling Using the Graphical User Interface*

The approach in this example is to treat the bed as a 1D model with independent variable x. At each x-coordinate, there is a model of a single pellet representative of all pellets at that position in the packed bed. Because the pellets are spherical and the surface concentrations can be considered constant around a particle, a 1D model with independent variable r is used for each particle. To model pellets along the packed bed, many such 1D models can be placed side by side, effectively creating a 2D geometry with independent variables x and r.

In the resulting model, all pellets can be modeled independently. There is therefore a 2D geometry for the pellets and a 1D geometry for the packed bed. The model involves a two-way coupling: the packed bed concentration enters the boundary condition for the particles, and the source term in the packed bed involves the flux at the particle surfaces.

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, click the **Multiphysics** button and select **2D** in the **Space dimension** list.

3 Click the **Add Geometry** button and enter `Particles` in the **Geometry name** edit field.

4 Change the independent variables to `x r z`, then click **OK** to close the dialog box.

5 Select the application mode **COMSOL Multiphysics>Chemical Engineering Module>Mass Transport>Diffusion**. Enter `C3H6p COp CO2p H2Op O2p` in the **Dependent variables** edit field. Click the **Add** button.

6 Click the **Add Geometry** button and type `Reactor` in the **Geometry name** edit field. Also set the **Space dimension** to **ID**. Close the dialog box by clicking **OK**.

7 Highlight the application mode **COMSOL Multiphysics>Chemical Engineering Module>Mass Transport>Convection and Diffusion**. Enter `C3H6 CO CO2 H2O O2` in the **Dependent variables** edit field.

8 Click the **Add** button.

9 Select the application mode **COMSOL Multiphysics>PDE Modes>PDE, Coefficient Form**. In the **Dependent variables** edit field, type P.
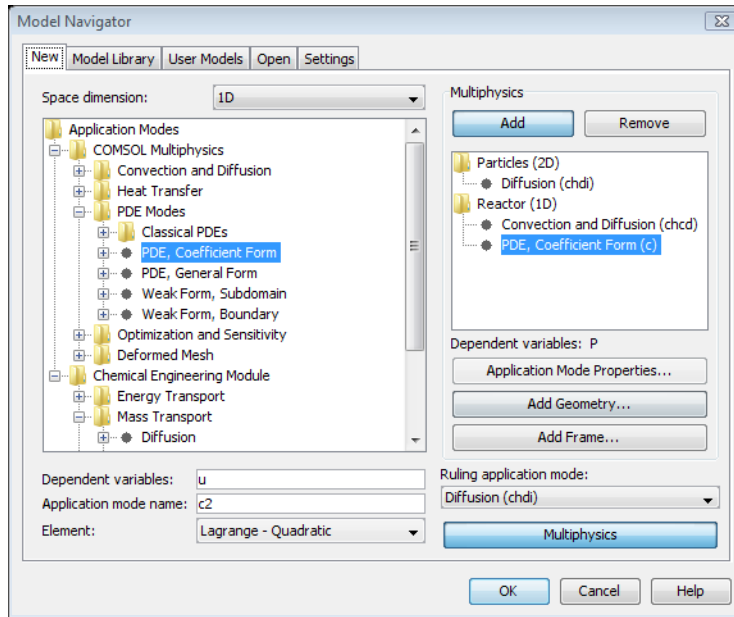
10 Click **OK** to close the **Model Navigator**.

GEOMETRY MODELING

1 From the **Multiphysics** menu, choose **Reactor: Convection and Diffusion (chcd)**.

2 Hold the Shift key and click the **Line** button on the Draw toolbar to open the **Line** dialog box.

3 In the **x** edit field, type 0 0.3, then click **OK** to close the dialog box.

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

OPTIONS AND SETTINGS

1 From the **Options** menu, choose **Constants**.

2 Click the **Import Variables From File** button in the lower left of the **Constants** dialog box.

3 Select the file packed_bed_reactor_const.txt (located in the same Model Library folder as the MPH-file). Alternatively, enter the following parameter names and values in the **Constants** dialog box:

NAME	EXPRESSION	DESCRIPTION
P_feed	2[atm]	Feed Pressure
T	508[K]	Reactor Temperature
R	8.314[Pa*m^3/mol/K]	Gas constant
kmCO	3.90[cm/s]	External mass transfer coefficient for CO
kmO2	4.07[cm/s]	External mass transfer coefficient for O2
kmC3H6	3.90[cm/s]	External mass transfer coefficient for CO
D_CO	0.0487[cm^2/s]	Diffusion coefficient for CO
D_O2	0.0469[cm^2/s]	Diffusion coefficient for O2
D_C3H6	0.0487[cm^2/s]	Diffusion coefficient for C3H6
D_prod	0.0487[cm^2/s]	
E1	13108[K]	Activation energy for R1
E2	15109[K]	Activation energy for R2
A1	7.07e19[cm^3/mol/s]	Pre exponential factor for reaction 1
A2	1.47e21[cm^3/mol/s]	Pre exponential factor for reaction 2
Aco	8.099e6[cm^3/mol]	Eq constant for adsorption term
Ac3h6	2.579e8[cm^3/mol]	Eq constant for adsorption term
Eco	-409[K]	Activation energy for adsoption term
Ec3h6	191[K]	Activation energy for adsoption term
u_feed	75[cm/s]	Linear inflow velocity
dHr1	-67.63e3[cal/mol]	Heat of Reaction for R1
dHr2	-460.4e3[cal/mol]	Heat of Reaction for R2
Cp	0.25[cal/g/K]	Effective Heat capacity for bed
kp	0.779[W/(m*K)]	Thermal conductivity (ripped from other model)
por_b	1-rho_b/rho_p	Porosity of the bed (void/total)
rho_b	0.51[g/cm^3]	Density of bed

NAME	EXPRESSION	DESCRIPTION
rho_p	0.68[g/cm^3]	Density of pellet
Rr	5[cm]	reactor radius
Ra	pi*Rr^2	Reactor area
eta	0.028e-2[g/cm/s]	Fluid viscosity
rho_feed	1.292[kg/m^3]	Inlet gas density
Ctot_feed	P_feed/R/T	Total feed concentration
x_CO_feed	0.005	Molar fraction of CO in feed
x_O2_feed	0.0075	Molar fraction of O2 in feed
x_C3H6_feed	0.000125	Molar fraction of C3H6 in feed
Cinert_feed	(1-x_CO_feed-x_O2_feed-x_C3H6_feed)*Ctot_feed	Concentration of inert in feed
Ap	3/rp	Surface area of particles per unit volume
rp	0.25[cm]	particle radius

4 Choose **Options>Expressions>Global Expressions**.

5 Click the **Import Variables From File** button in the lower left of the **Global Expressions** dialog box and select the file packed_bed_reactor_expr.txt (located in the same Model Library folder as the MPH-file). Alternatively, enter the following parameter names and values in the **Global Expressions** dialog box:

NAME	EXPRESSION	DESCRIPTION
Ctot	(Cinert_feed+CO+O2+CO2+C3H6+H2O)	Total concentration
k1	A1*exp(-E1/T)	Rate constant for reaction 1
k2	A2*exp(-E2/T)	Rate constant for reaction 2
KCO	Aco*exp(-Eco/T)	Adsorbtion constant for CO
KC3H6	Ac3h6*exp(-Ec3h6/T)	Adsorbtion constant for C3H6
R1	k1*COp*O2p/(1+KCO*COp+KC3H6*C3H6p)^2	Rate expression for reaction 1
R2	k2*C3H6p*O2p/(1+KCO*COp+KC3H6*C3H6p)^2	Rate expression for reaction 2
u	u_feed*(Ctot/Ctot_feed)*(P_feed/P)	Linear velocity

NAME	EXPRESSION	DESCRIPTION
beta	G*(1-por_b)/ (rho_feed*2*rp*por_ b^3)*(150*(1-por_b) *eta/(2*rp)+1.75*G)	Ergun equation constant
G	u_feed*rho_feed	superficial mass velocity
F0	Ctot_feed*u_feed*Ra	Inlet molar flow
F	Ctot*u*Ra	Molar flow [mol/s]

6 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings—Convection and Diffusion

1 From the **Multiphysics** menu, select **2 Reactor: Convection and Diffusion (chcd)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1 in the **Subdomain Settings** dialog box.

4 Specify the settings as in the following table.

SETTINGS	C3H6	CO	CO2	H2O	O2
D	D_C3H6	D_CO	D_prod	D_prod	D_O2
R	-Ap*C3H6fl ux	-Ap*COflux	-Ap*CO2flu x	-Ap*H2Oflu x	-Ap*O2f lux
u	u	u	u	u	u

5 Click the **Init** tab and type 1e-6 in all edit fields.

6 Click **OK**.

Boundary Conditions—Convection and Diffusion

1 From the **Physics** menu, choose **Boundary Settings**.

2 Select Boundary 1.

3 Enter the species concentrations of the inlet stream. For each species in the table, find the **Boundary condition** list and select **Concentration**. Type in the entries from the following table:

BOUNDARY	C3H6	CO	CO2	H2O	O2
1	x_C3H6_feed* Ctot_feed	x_C3H6_feed *Ctot_feed	0	0	x_C3H6_feed *Ctot_feed

4 Select Boundary 2.

5 Set the **Boundary condition** to **Convective flux** for all species on the outlet boundary.

6 Click **OK**.

Subdomain Settings—PDE, Coefficient Form

1 From the **Multiphysics** menu, select **3 Reactor: Coefficient Form (c)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1 in the **Subdomain Settings** dialog box.

4 Specify the settings as in the following table.

SETTINGS	VALUE
f	Px+beta*(F/F0)*(P_feed/P)

5 Click the **Init** tab and type 1e5 in all edit fields.

6 Click **OK**.

Boundary Conditions—PDE, General Form

1 From the **Physics** menu, choose **Boundary Settings**.

2 Select Boundary 1, then type 1 in the **h** edit field.

3 In the **R** edit field, type P_feed.

4 Select Boundary 2, then click the **Neumann boundary condition** button.

5 Click **OK**.

The source terms in the reactor mass balances depend on fluxes from the catalyst pellets. To know this the catalyst model must also be set up. Once this is done the reaction rate can be calculated by coupling the two models.

GEOMETRY MODELING

1 From the **Multiphysics** menu, choose **1 Particles: Diffusion (chdi)**.

2 Draw a unit square with its lower left corner at (0,0).

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

PHYSICS SETTINGS

Subdomain Settings—Convection and Diffusion

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1 in the **Subdomain Settings** dialog box.

3 Specify the settings according to the following table.

SETTINGS	C3H6P	COP	CO2P	H2OP	O2P
D (anisotropic)	0 0 0 (D_C3H6/ rp^2)*r^2	0 0 0 (D_CO/ rp^2)*r^2	0 0 0 (D_prod/ rp^2)*r^2	0 0 0 (D_prod/ rp^2)*r^2	0 0 0 (D_O2/ rp^2)*r ^2
R	-r^2*R2	-r^2*R1	r^2*(R1+3* R2)	r^2*3*R2	-r^2*(0 .5*R1+4 .5*R2)

4 On the **Init** page, type 1e-6 in all edit fields.

5 Click **OK**.

Boundary Conditions—Diffusion

1 From the **Physics** menu, choose **Boundary Settings**.

2 Select Boundary 3.

3 Enter the species concentration on the pellet surface. This can be taken from the reactor model through a coupling variable. For now, find the **Boundary condition** list and select **Concentration**, then type the entries from the following table:

BOUNDARY	C3H6P	COP	CO2P	H2OP	O2P
3	C3H6bulk	CObulk	CO2bulk	H2Obulk	O2bulk

4 Leave Boundaries 1, 2, and 4 with the default boundary condition **Insulation/ Symmetry**.

5 Click **OK**.

The species concentration at the pellet boundary can be taken from the reactor model. Each position along the x-axis, in the reactor model, corresponds to a position along the x-axis in the pellet model. So the concentration at pellet-bulk interface can be taken form the reaction model with a Subdomain Extrusion coupling variable. This concentration at the pellet surface will give rise to mass flux at the interface. This mass flux can be coupled back to give the total reactor reaction rate for all species. To set up the coupling follow these steps:

1 From the **Multiphysics** menu, select **2 Reactor: Convection and Diffusion (chcd)**.

2 Select **Options>Extrusion Coupling Variables>Subdomain Variables**.

3 Define the coupling variables by entering names and expressions according to the following table:

NAME	EXPRESSION
CObulk	CO
O2bulk	O2
CO2bulk	CO2
C3H6bulk	C3H6
H2Obulk	H2O

4 For each entry also select **General transformation**. This must be done for all 5 species.

5 Click the **Destination** tab.

6 In the **Geometry** list, choose **Particles**. Make sure that the **Level** list is set to **Boundary**.

7 Select **CObulk** in the **Variable** list.

8 Select Boundary 3

9 Enter x*0.30 in the **Destination transformation** edit field. This correspond to that the reactor length is only 30% of the pellet domain because the pellet domain is scaled.

10 Repeat Steps 8 and 9 for all other species in the **Variable** list.

11 Click **OK**.

To uphold the concentration constraint on the particle surface there will be a diffusive flux out through the top boundary of the pellet. This flux is equal to the total reaction rate if it is multiplied by the specific surface area, at steady state. But to make this flux available this must be coupled back to the reactor geometry.

1 From the **Multiphysics** menu, select **1 Particles: Diffusion (chdi)**.

2 Select **Options>Extrusion Coupling Variables>Boundary Variables**.

3 Mark Boundary 3 in the **Boundary Selection** list.

4 Define the coupling variables by entering names and expressions according to the following table:

NAME	EXPRESSION
COflux	D_CO*COpr*r/rp
O2flux	D_O2*O2pr*r/rp
CO2flux	D_prod*CO2pr*r/rp

NAME	EXPRESSION
C3H6flux	D_C3H6*C3H6pr*r/rp
H2Oflux	D_prod*H2Opr*r/rp

5 For each entry also click the **General transformation** button. This must be done for all 5 species.

6 Click the **Destination** tab.

7 In the **Geometry** list, choose **Reactor** and make sure that the **Level** list is set to **Subdomain**.

8 Select **COflux** in the **Variable** list.

9 Select Subdomain 1. In the **Destination transformation** edit field, type x/0.30. This transformation accounts for the fact that the reactor length is only 30% of the pellet domain because the pellet domain is scaled.

10 Repeat Steps 8 and 9 for all other species in the **Variable** list.

11 Click **OK**.

MESH GENERATION

1 From the **Multiphysics** menu, select **2 Reactor: Convection and Diffusion (chcd)**.

2 From the **Mesh** menu, choose **Free Mesh Parameters**.

3 In the **Maximum Element Size** edit field, enter 0.0025.

4 Click the **Remesh** button and close the dialog box.

5 From the **Multiphysics** menu, select **1 Particles: Diffusion (chdi)**.

6 From the **Mesh** menu, choose **Mapped Mesh Parameters**.

7 Click the **Boundary** tab. Select Boundaries 1 and 4 by Ctrl-clicking their entries in the **Boundary selection** list.

8 Select the **Constrain element distribution** check box, then enter 30 in the **Number of edge elements** edit field. Also enter 0.2 in the **Element ratio** edit field. This makes the mesh finer near the pellet surface.

9 Select Boundary 3 in the **Boundary selection** list. Select the **Constrain element distribution** check box, then enter 120 in the **Number of edge elements** edit field.

10 Click **Remesh**. When the mesher has finished, click **OK** to close the dialog box.

Now there are equally many numbers of elements on the coupled lines, which is good for stability reasons when coupling in both directions.

To evaluate the conversion of C_3H_6 and CO it is convenient to set up dedicated expressions for this.

1 From the **Multiphysics** menu, select **2 Reactor: Convection and Diffusion (chcd)**.

2 From the **Options** menu, choose **Integration Coupling Variables>Boundary Variables**.

3 Select **2** in the **Boundary Selection** list.

4 Create the following variables:

NAME	EXPRESSION
X_C3H6	1-C3H6/(x_C3H6_feed*Ctot_feed)
X_CO	1-CO/(x_CO_feed*Ctot_feed)

5 Click **OK**.

COMPUTING THE SOLUTION

To save memory the Stationary Segregated Solver will be used. This solver alternates between solving for the species in the Reactor geometry and the pellet each iteration. To avoid feedback from the variables that are currently not being solved for a strict one way coupling will be enforced for the couplings between the geometries. This is not default when the coupling takes place on a boundary condition, which is the case for the Particles geometry.

1 From the **Multiphysics** menu, select **1 Particles: Diffusion (chdi)**.

2 Go to **Properties** in the **Physics** menu.

3 Set the **Constraint type** drop down list to **Non-Ideal**. Click **OK** to close the dialog box.

4 Click the **Solver Parameters** button on the toolbar.

5 Select the **Stationary Segregated** solver in the **Solver** list. Click **OK** to close.

6 Click the **Solve** button.

The remaining solving stages continue after the postprocessing section.

POSTPROCESSING AND VISUALIZATION

To create Figure 8-72 perform the following steps

1 From the **Postprocessing** menu, open the **Domain Plot Parameters** dialog box.

2 On the **General** page, select the **Keep current plot** check box.

3 Click the **Title/Axis** button.

4 In the **Title** edit field, enter Concentration along reactor length.

5 Enter Reactor length, [m] in the **First axis label** and Concentration, [mol/m³] in the **Second axis label** edit field.

6 Click the **Line/Extrusion** tab.

7 Select **Concentration, C3H6** in the **Predefined quantities** list.

8 Click the **Line Settings** button. Select **Color** in the **Line color** list.

9 Click the **Color** button and select black. Click **OK** twice to close the dialog boxes.

10 Click **Apply** to plot the concentration.

11 Repeat Steps 7 to 10 for the species CO, CO_2, and O_2 giving each line a different color.

12 Click **OK**.

To create Figure 8-73 preform the following steps

1 From the **Postprocessing** menu open the **Plot Parameters** dialog box.

2 Click the **Surface** tab.

3 Select **Concentration, O2p** in the **Predefined quantities** list.

4 Click the **Height Data** tab.

5 Select the **Height data** check box.

6 From the **Predefined quantities** list, select **Concentration, O2p**. Click **OK**.

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

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 From the **Solver** list, select **Parametric segregated**.

3 To vary the pellet radius, type rp in the **Parameter names** edit field.

4 In the **Parameter values** edit field, type 0.0025 0.0018.

5 On the **Parametric** page, select the **Manual tuning of parameter step size** check box.

6 Enter the values in the following table:

SETTINGS	C3H6
Initial Step size	0.0002
Minimum Step size	1e-6
Maximum step size	0.0003

This ensures that the solver does not jump from 0.0025 to 0.0018 in a single step; taking small steps can increase the solver stability.

7 Click **OK** to close the **Solver Parameters** dialog box.

8 Click the **Restart** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To reproduce the plot in Figure 8-74, perform the following steps:

1 From the **Postprocessing** menu, open the **Cross-Section Plot Parameters** dialog box.

2 On the **General** page, select **0.0025** in the **Solutions to use** list.

3 Select the **Keep current plot** check box.

4 On the **Line/Extrusion** page, select **Concentration, C3H6** from the **Predefined quantities** list.

5 In the **Cross-section line data** area, set **x1** to 0 and **r1** to 1.

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

7 Set the **Number of lines** to 3, then click **Apply**.

8 On the **General** page, select **0.0018** in the **Solutions to use** list.

9 Click **OK**.