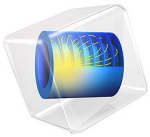

Packed Bed Reactor

Introduction

The packed bed reactor is used in heterogeneous catalytic processes and is one of the most common reactors in chemical industry. Its basic design is a column filled with porous catalyst particles, and these 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. In this example, volatile organic compounds (VOC) and CO are oxidized in a catalytic converter. Propylene is used as a representative for hydrocarbons present in the feed stream, which could, for example, be exhaust gas from a combustion process.

The structure of the packed catalyst particles makes the modeling of mass and energy transport in the reactor a challenge. The difficulty lies in the description of the porous structure, which gives transport of different orders of magnitudes within 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 1 and 10 micrometers.

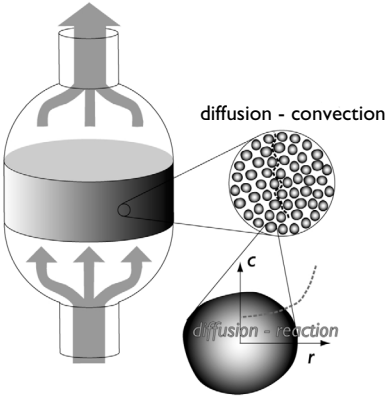

Figure 1: An example of the macro dimension (bed height) and the microdimension (pellet radial position) in a packed bed reactor.

This model presents a multigeometry approach to study microscale and macroscale mass balances in packed beds and other heterogeneous reactors with bimodal pore distribution. The example provides the mass and reaction distributions along the reactor and within each catalyst pellet along the reactor length. The Transport of Diluted Species and Chemistry interfaces are used and enable evaluation of the catalyst load utilization, optimal pellet size, or inlet temperature.

Model Definition

The following chemical reactions describe oxidation of carbon monoxide and an organic volatile by-product such as propylene in an automobile catalytic converter:

$$CO + \frac{1}{2}O_2 \rightarrow CO_2 \quad (1)$$

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3H_2O + 3CO_2 \quad (2)$$

For these heterogeneous catalytic reactions the rates (SI unit: mol/(m^3·s)) are given by (Ref. 2):

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

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

The rate and adsorption constants are defined by Arrhenius expressions which are available in the Chemistry interface. The values of the frequency factors and activation energies (SI unit: J/mol) are taken from the literature (Ref. 3) and listed in Table 1,

TABLE 1: ARRHENIUS PARAMETERS.

RATE/ADSORPTION CONSTANT	FREQUENCY FACTOR	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 in Equation 1 and Equation 2 describe a process limited by the second-order rate expression at high temperatures when the surface coverage is low. At low temperatures the adsorption reactions are slower and limit the reaction rate due to a shortage of free catalytic sites.

MACROSCALE EQUATIONS

The pressure drop along the reactor is described by the Ergun equation and is solved with a Coefficient Form PDE:

$$-\frac{dP}{dx} = \frac{150\mu u}{D_p^2} \cdot \frac{(1-\varepsilon_b)^2}{\varepsilon_b^3} + \frac{1.75\rho u^2}{D_p} \cdot \frac{(1-\varepsilon_b)}{\varepsilon_b^3} \quad (3)$$

In Equation 3, P is the pressure (SI unit: Pa), ε_b the porosity, D_p the particle diameter (SI unit: m), μ denotes the gas viscosity (SI unit: Pa·s), ρ the gas density (SI unit: kg/m^3), and x the reactor length coordinate (SI unit: m). u is the reactor flow velocity (SI unit: m/s) that depends on the pressure and velocity of the feed (SI unit: m/s), as described by Equation 4:

$$u = (\rho_{feed} u_{feed})/\rho = u_{feed} P_{feed}/P \quad (4)$$

This relation applies since the flux across the reactor is set as constant, the system is assumed to be isothermal, and the fluid (air) is considered to be an ideal gas.

The mass transport on the macroscale level, along the reactor, takes place through convection and diffusion. This is easily accounted for using the Transport of Diluted Species interface in which the following equation (stationary) is solved:

$$\nabla \cdot (-D_i \nabla c_i + c_i u) = R_i \quad (5)$$

The reaction rate R source term (SI unit: mol/(m^3·s)) in Equation 5 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:

$$R = (1-\varepsilon_b) A_p (\mathbf{N} \cdot \mathbf{n}) \text{ at } r = r_p \quad (6)$$

In Equation 6, ε_b is the bed porosity, $\mathbf{N}$ denotes the flux vector inside the porous particle (SI unit: mol/(m^2·s)) and $\mathbf{n}$ is the outward unit vector normal to the particle surface. The equation 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 (SI unit: m^2/m^3). This property is related to the pellet radius as:

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

The boundary conditions for the macroscale mass balances are as follows:

At the inlet, the reactant concentrations are known:

$$c_{CO} = c_{COin}$$

$$c_{C3H6} = c_{C3H6in}$$

$$c_{O2} = c_{O2in}$$

$$c_{CO2} = 0$$

$$c_{H2O} = 0$$

At the outlet, the Outflow condition states that convective mass transport dominates the species transport across the boundary.

MICROSCALE EQUATIONS

To properly calculate R, mass balances are required for the catalyst pellet interior, that is, the microscale. In the catalyst pores, mass transport can be assumed to take place by diffusion only. If the pellets are selected with spherical and dimensionless coordinates the following equation applies:

$$\nabla \cdot \left(-\left(\frac{r}{r_p}\right)^2 D_{cp} \nabla c_p\right) + \left(\frac{r}{r_p}\right)^2 R_p = 0 \text{ for } 0 < r < 1 \tag{7}$$

Here, D_{cp} is the 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. r (SI unit: m) is the independent variable for the position along the radius of the particle. Equation 7 is modeled with a Transport of Diluted Species interface with corrections for spherical coordinates and dimensionless particle radius. The boundary conditions are symmetry at the center of the particle and concentration at the surface. The latter is described by $c_p = \varepsilon c$ where c and c_p represent the species concentrations in the bulk and in the particle, respectively, and ε is the catalyst porosity. 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 along the reactor. This implies that the source term (Equation 6) in the macroscale mass balance becomes:

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

This type of problem exists for many chemical reaction engineering applications and is often solved by using an analytical approximation of the solution to the microscale mass balance. However, such an approach cannot be used for complicated reaction mechanisms

involving several reaction species. The approach shown here is general and can be used for very complex reaction mechanisms involving a large number of species.

MACROSCALE AND MICROSCALE IMPLEMENTATION

A complication in solving the derived system of equations is that the macroscale and microscale balances are defined in different coordinate systems. In this example, the macroscale part (along the reactor length) is set up in 1D and the microscale (along the pellet radius) in 2D. In the latter part, the x direction represents the surface concentration of the pellet at each part along the reactor and the y direction the concentration distribution along the dimensionless pellet radius.

To achieve the coupling of the fluxes and concentrations between the two scales of the system, general extrusion features are used.

Results and Discussion

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

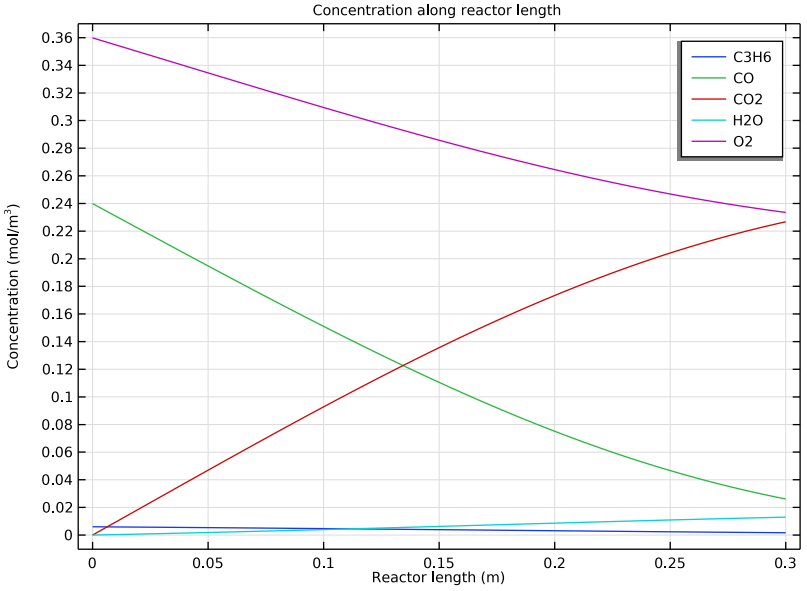

Figure 2: The concentration of reactants and products along the reactor length. The pellet radius r_p is 2.5 mm.

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

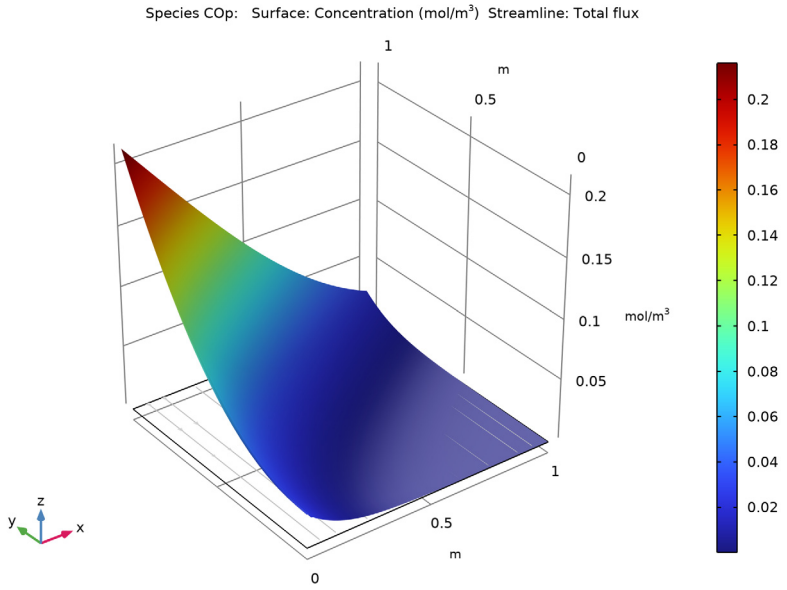

Figure 3: The concentration of in-pellet CO as a function of reactor position. The scaled pellet radius is given on the y-axis and the reactor position along the x-axis.

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 is not used. Reducing the pellet diameter could potentially fix this situation and simulation results (see Figure 4) confirm this.

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.

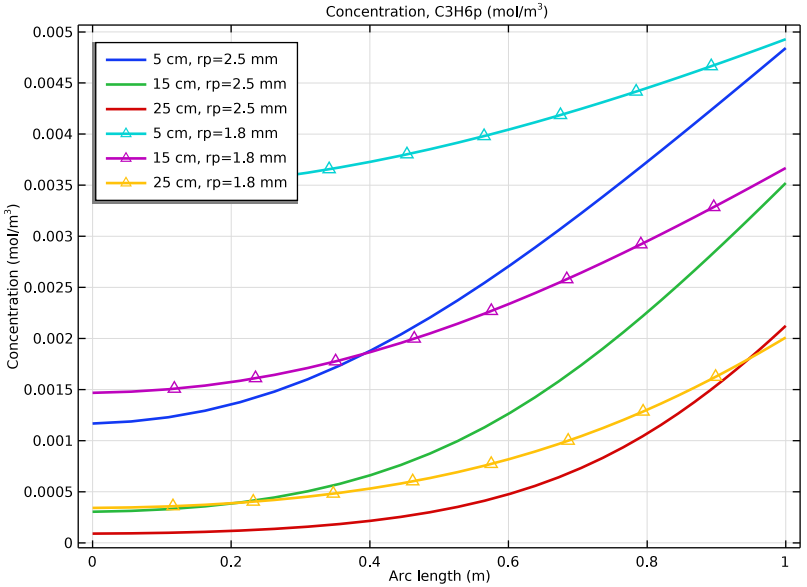

Figure 4: The concentration of in-pellet C_3H_6 at different reactor positions (5, 15, and 25 cm). Solid lines represent a pellet radius of 2.5 mm and lines with triangular markers represent a pellet radius of 1.8 mm.

References

1. J.M. Coulson and J.F. Richardson, *Chemical Engineering*, vol. 2, 4th ed., Pergamon Press, 1990.

2. 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.

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

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/packed_bed_reactor`

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, Start by adding the necessary 1D physics interfaces: **Transport of Diluted Species** and **Coefficient Form PDE**.

2 click **1D**.

3 In the **Select Physics** tree, select **Chemical Species Transport> Transport of Diluted Species (tds)**.

4 Click **Add**.

5 In the **Number of species** text field, type 5.

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

C3H6
C0
C02
H20
02

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

8 Click **Add**.

9 In the **Field name** text field, type P.

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

P

11 Click **Study**.

12 In the **Select Study** tree, select **General Studies>Stationary**.

13 Click **Done**.

GEOMETRY 1

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

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

3 In the table, enter the following settings:

Coordinates (m)
0
0.3

4 Click **Build Selected**.

ROOT

Add the model parameters from a text file.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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

3 Click **Load from File**.

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

Variables 1

1 In the **Home** toolbar, click **Variables** and choose **Global Variables**.

Import also the global variables from a text file.

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

3 Click **Load from File**.

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

Follow these steps to set up mass transport equations for the packed bed. Start with the **Transport of Diluted Species**.

TRANSPORT OF DILUTED SPECIES (TDS)

Transport Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>** **Transport of Diluted Species (tds)** click **Transport Properties 1**.

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

3 Specify the **u** vector as

u	x

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

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

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

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

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

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

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

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

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

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

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

Reactions 1

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

2 Select Domain 1 only.

3 In the **Settings** window for **Reactions**, locate the **Reaction Rates** section.

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

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

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

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

8 In the R_{O2} text 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 the reactor is `(1-por_b)`.

Inflow 1

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Inflow**, locate the **Concentration** section.

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

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

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

7 Locate the **Boundary Condition Type** section. From the list, choose **Flux (Danckwerts)**.

Outflow 1

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

2 Select Boundary 2 only.

COEFFICIENT FORM PDE: ERGUN EQUATION

Follow the steps below to specify the Ergun equation in the **Coefficient Form PDE**.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Coefficient Form PDE (c)**.

2 In the **Settings** window for **Coefficient Form PDE**, type `Coefficient Form PDE: Ergun Equation` in the **Label** text field.

3 Locate the **Units** section. Click **Select Dependent Variable Quantity**.

4 In the **Physical Quantity** dialog box, type `pressure` in the text field.

5 Click **Filter**.

6 In the tree, select **General>Pressure (Pa)**.

7 Click **OK**.

8 In the **Settings** window for **Coefficient Form PDE**, locate the **Units** section.

9 In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	`N/m^3`

Coefficient Form PDE 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Coefficient Form PDE: Ergun Equation (c)** click **Coefficient Form PDE 1**.

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

3 In the c text field, type `0`.

4 Locate the **Source Term** section. In the f text field, type `Px+(150*mu*u/(2*Rr)^2*(1-por_b)^2/por_b^3+1.75*rho_feed*u^2/(2*Rr)*(1-por_b)/por_b^3)`.

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

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

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

Dirichlet Boundary Condition 1

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

2 Select Boundary 1 only.

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

4 In the r text field, type `P_feed`.

The source terms in the reactor mass balances depend on the surface fluxes from the catalyst pellets. Therefore, set up a separate model component calculating the mass transport and reaction in the pellets.The model geometry is in 2D. The x-coordinate represents reactor length and the y-coordinate the pellet radius.

ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component>2D**.

ADD PHYSICS

1 In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

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

Select a **Chemistry** interface handling the reactions and a **Transport of Diluted Species** interface for the mass transport within the pellets.

3 In the tree, select **Chemical Species Transport>Chemistry (chem)**.

4 Click **Add to Component 2** in the window toolbar.

5 In the tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

6 Click to expand the **Dependent Variables** section. In the **Number of species** text field, type `5`.

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

C3H6p
COp
CO2p
H2Op
O2p

8 Click **Add to Component 2** in the window toolbar.

9 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

GEOMETRY 2

Square 1 (sq1)

1 In the **Geometry** toolbar, click **Square**.

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

CHEMISTRY (CHEM)

Start setting up the **Chemistry** interface for the two reactions present in the system.

In the **Model Builder** window, under **Component 2 (comp2)** click **Chemistry (chem)**.

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 `CO+1/2O2=>CO2`.

4 Click **Apply**.

5 Locate the **Reaction Rate** section. In the r_j text field, type `chem.kf_1*chem.c_CO*chem.c_O2/(1+KCO*chem.c_CO+KC3H6*chem.c_C3H6)^2`.

6 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `2`.

7 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

8 In the A^{f} text field, type `A1`.

9 In the E^{f} text field, type `E1`.

Reaction 2

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 `C3H6+9/2O2=>3H2O+3CO2`.

4 Click **Apply**.

5 Locate the **Reaction Rate** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `2`.

6 In the r_j text field, type `chem.kf_2*chem.c_C3H6*chem.c_O2/(1+KCO*chem.c_CO+KC3H6*chem.c_C3H6)^2`.

7 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

8 In the A^f text field, type `A2`.

9 In the E^f text field, type `E2`.

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 `N2`.

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

5 In the **Model Builder** window, collapse the **Chemistry (chem)** node.

Note that the molar masses are computed from the chemical formula.

6 In the **Model Builder** window, click **Chemistry (chem)**.

7 In the **Settings** window for **Chemistry**, locate the **Model Input** section.

8 From the T list, choose **User defined**. In the associated text field, type `Tr`.

9 From the p list, choose **User defined**. In the associated text field, type `P_feed`.

10 Locate the **Species Matching** section. From the **Species solved for** list, choose **Transport of Diluted Species 2**.

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

Species	Type	Molar concentration	Value (mol/m^3)
C3H6	Variable	C3H6p	Solved for
CO	Variable	COp	Solved for
CO2	Variable	CO2p	Solved for
H2O	Variable	H2Op	Solved for
N2	Solvent	User defined	`Cinert_feed`
O2	Variable	O2p	Solved for

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

TRANSPORT OF DILUTED SPECIES 2 (TDS2)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Transport of Diluted Species 2 (tds2)**.

2 In the **Settings** window for **Transport of Diluted Species**, locate the **Transport Mechanisms** section.

3 Clear the **Convection** check box.

Transport Properties 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, under **Component 2 (comp2)> Transport of Diluted Species 2 (tds2)** click **Transport Properties 1**.

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

3 From the list, choose **Diagonal**.

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

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

5 From the list, choose **Diagonal**.

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

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

7 From the list, choose **Diagonal**.

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

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

9 From the list, choose **Diagonal**.

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

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

11 From the list, choose **Diagonal**.

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, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

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

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

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

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

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

Reactions 1

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

Use the reaction rates calculated for each species in the **Chemistry** node.

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

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

4 Locate the **Reaction Rates** section. In the R_{C3H6p} text field, type `y^2/1[m^2]*chem.R_C3H6`.

5 In the R_{COp} text field, type `y^2/1[m^2]*chem.R_CO`.

6 In the R_{CO2p} text field, type `y^2/1[m^2]*chem.R_CO2`.

7 In the R_{H2Op} text field, type `y^2/1[m^2]*chem.R_H2O`.

8 In the R_{O2p} text field, type `y^2/1[m^2]*chem.R_O2`.

Concentration 1

1 In 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 **Settings** window for **Concentration**, locate the **Concentration** section.

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

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

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

7 In the $c_{0,COp}$ text field, type `CObulk`.

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

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

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

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

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

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

14 Click the **Show More Options** button in the **Model Builder** toolbar.

15 In the **Show More Options** dialog box, in the tree, select the check box for the node **Physics>Advanced Physics Options**.

16 Click **OK**.

17 In the **Settings** window for **Concentration**, click to expand the **Constraint Settings** section.

18 From the **Apply reaction terms on** list, choose **Individual dependent variables**.

Complete the model setup by coupling the reactor and pellet models. First use a nonlocal general extrusion coupling to make the reactor species concentrations available in the pellet model. A correction of 0.30 is required since the 2D model uses the 1-by-1 dimension.

DEFINITIONS (COMP1)

In the **Model Builder** window, under **Component 1 (comp1)** click **Definitions**.

General Extrusion 1 (genext1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **General Extrusion**.

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

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

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

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

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

DEFINITIONS (COMP2)

In the **Model Builder** window, under **Component 2 (comp2)** click **Definitions**.

General Extrusion 2 (genext2)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **General Extrusion**.

2 In the **Settings** window for **General Extrusion**, 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** text field, type `x/0.30`.

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

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

8 Clear the y^i**-expression** text field.

DEFINITIONS (COMP1)

In the **Model Builder** window, under **Component 1 (comp1)** click **Definitions**.

Variables 2

1 In the **Definitions** toolbar, click a= **Local Variables**.

Import a variable file that defines the species fluxes at the pellet boundary in the 1D model.

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

3 Click **Load from File**.

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

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

DEFINITIONS (COMP2)

Now, read in the variable file that defines the bulk species concentrations in the 2D model.

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Definitions**.

Variables 3

1 In the **Definitions** toolbar, click a= **Local Variables**.

2 In the **Settings** window for **Variables**, 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 Application Libraries folder and double-click the file `packed_bed_reactor_variables_2d.txt`.

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

MESH 1

Set up meshes for both the 1D and 2D geometries. A distributed mapped mesh is suitable in the 2D geometry to minimize the number of mesh elements solved for.

In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

Edge 1

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

Size

1. In the **Model Builder** window, click **Size**.
2. In the **Settings** window for **Size**, locate the **Element Size** section.
3. Click the **Custom** button.
4. Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `0.0025`.
5. Click  **Build All**.

MESH 2

In the **Model Builder** window, under **Component 2 (comp2)** click **Mesh 2**.

Mapped 1

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

Distribution 1

1. Right-click **Mapped 1** and choose **Distribution**.
2. Select Boundaries 1 and 4 only.
3. In the **Settings** window for **Distribution**, locate the **Distribution** section.
4. From the **Distribution type** list, choose **Predefined**.
5. In the **Number of elements** text field, type `30`.
6. In the **Element ratio** text field, type `0.2`.

Distribution 2

1. In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.
2. Select Boundary 3 only.
3. In the **Settings** window for **Distribution**, locate the **Distribution** section.
4. In the **Number of elements** text field, type `120`.
5. Click  **Build All**.

STUDY 1

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

RESULTS

Concentrations, All Species (tds)

The first default plot shows the concentrations of all species in the reactor as functions of the position.

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

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

3 Locate the **Plot Settings** section.

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

5 In the **Concentrations, All Species (tds)** toolbar, click **Plot**.

Now modify the default plot of the concentration of CO within the pellets.

Height Expression 1

1 In the **Model Builder** window, expand the **Results>Concentration, COp (tds2)** node.

2 Right-click **Surface 1** and choose **Height Expression**.

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

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, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
rp (Particle radius)	`0.0025 0.0018`	`m`

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

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

RESULTS

Cut Line 2D 1

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

2 In the **Settings** window for **Cut Line 2D**, 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` and **y** to `1`.

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

6 In the **Distances** text field, type `-10/30 -20/30`.

7 Click **Plot**.

Pellet size comparison

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

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

For rp=2.5 mm

1 Right-click **Pellet size comparison** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `For rp=2.5 mm` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.

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

5 In the **Parameter values (rp (m))** list, select **0.0025**.

6 Locate the **y-Axis Data** section. In the **Expression** text field, type `C3H6p`.

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

8 Click to expand the **Legends** section. Select the **Show legends** check box.

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

10 In the **Legend** text field, type `eval(x*0.3,cm) cm, rp=eval(rp,mm) mm`.

For rp=1.8 mm

1 Right-click **For rp=2.5 mm** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type `For rp=1.8 mm` in the **Label** text field.

3 Locate the **Data** section. In the **Parameter values (rp (m))** list, select **0.0018**.

4 Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Triangle**.

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

Pellet size comparison

1 In the **Model Builder** window, click **Pellet size comparison**.

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

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

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

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

6 In the **Pellet size comparison** toolbar, click **Plot**.

The following steps fix the rest of the plot groups.

Pressure drop

1 In the **Model Builder** window, under **Results** click **Coefficient Form PDE: Ergun Equation**.

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

3 Locate the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** check box. In the associated text field, type `Pressure (Pa)`.

6 In the **Pressure drop** toolbar, click **Plot**.

Concentrations, All Species (tds)

1 In the **Model Builder** window, click **Concentrations, All Species (tds)**.

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

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

4 In the **Concentrations, All Species (tds)** toolbar, click **Plot**.