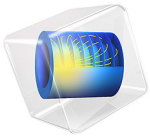

Hydrocarbon Dehalogenation in a Tortuous Microreactor

Introduction

Removing halogen groups from hydrocarbons is an important reaction step in several chemical processes. One application is water purification. Other examples involve organic synthesis, where the removal of halogen groups serves as a starting point for carbon-carbon coupling reactions. Typically, the carbon-halogen bond scission is activated by precious metal catalysts based on platinum or palladium.

The model presented here shows hydrocarbon dehalogenation as it occurs in a microreactor. The reactants are transported from the fluid bulk to the catalytic surfaces at the reactor walls, where they react. First you set up a space-independent model, analyzing two competing reactions, using the Reaction Engineering interface. Then, you export the reaction kinetics and set up and solve a space-dependent model of the microreactor.

Model Definition

The adsorption of halogenated hydrocarbons onto the surface of a platinum catalyst leads to cleavage of the carbon halogen bond. The hydrocarbon fragments then undergo either hydrogenation or coupling reactions. The scheme below illustrates the overall reactions for a brominated hydrocarbon species.

$$\text{R-Br} \xrightarrow[[\text{Pt}]]{k_1} \text{R-H}$$

$$2\text{R-Br} \xrightarrow[[\text{Pt}]]{k_2} \text{R-R}$$

Figure 1: The dehalogenation of RBr can result either in hydrogenation or coupling of the hydrocarbon fragments.

The reaction rates are:

$$r_1 = k_1 c_{\text{RBr}}$$

and

$$r_2 = k_2 c_{\text{RBr}}^2$$

where the rate constants are given by the Arrhenius expression:

$$k_j = A_j \exp\left(-\frac{E_j}{R_g T}\right) \tag{1}$$

In Equation 1, A is the frequency factor, and E the activation energy (SI unit: J/mol). The bulk species are said to be dissolved in water. The table below lists the values of the Arrhenius parameters for the two reactions.

TABLE 1: ARRHENIUS PARAMETERS.

	Frequency factor	Activation energy
Reaction 1	`2e-3[m/s]`	`10e3[J/mol]`
Reaction 2	`1e-3[m^4/(mol*s)]`	`30e3[J/mol]`

IDEAL REACTOR MODEL

The mass balance equation for a flow-through reactor is given by

$$\frac{dF_i}{dV} = R_i \tag{2}$$

where F is the molar flow rate (SI unit: mol/s), V the reactor volume (SI unit: m^3), and R_i the net reaction term (SI unit: mol/(m^3·s)). If the reactor has constant cross-section and constant flow velocity, the left-hand side of Equation 2 can be rewritten as

$$\frac{dF_i}{dV} = u\frac{dc_i}{dx} = \frac{dc_i}{d\tau}$$

The reactor mass balance thus becomes

$$\frac{dc_i}{d\tau} = R_i \tag{3}$$

where τ represents the residence time (SI unit: s). The assumption of constant flow velocity is valid for incompressible liquids or liquids where the effect of temperature on the density is small. Equation 3 is identical to the balance equation of the batch reactor, except that residence time replaces the reaction time. You can therefore make use of the Batch reactor type when solving the model in the Chemical Reaction Engineering Module.

The ideal reactor model assumes by default that reactions take place in the entire reactor volume. In the 3D microreactor model, reactions occur at catalytic surfaces located at the reactor walls. In order to make the ideal model represent a reactor with surface reactions, Equation 3 has to be scaled by the reactive area per reactor volume. Scaling the ideal reactor equations by the dimensions of the microreactor makes the 1D and 3D models comparable. The area to volume ratio is

$$\frac{WL}{WLH} = \frac{1}{H}$$

where W is the width of the channel (SI unit: m), H the channel height (SI unit: m), and L the length of a reactive section (SI unit: m). The scaled ideal reactor equation is then

$$\frac{dc_i}{d\tau} = \frac{R_i}{H}$$

Note that the net reaction term (R_i) in this case represents surface reactions (SI unit: mol/(m^2·s)).

SPACE-DEPENDENT MODEL

The microreactor considered in this example consists of a tortuous channel, fitted with inlet and outlet adapter sections, as illustrated in Figure 2.

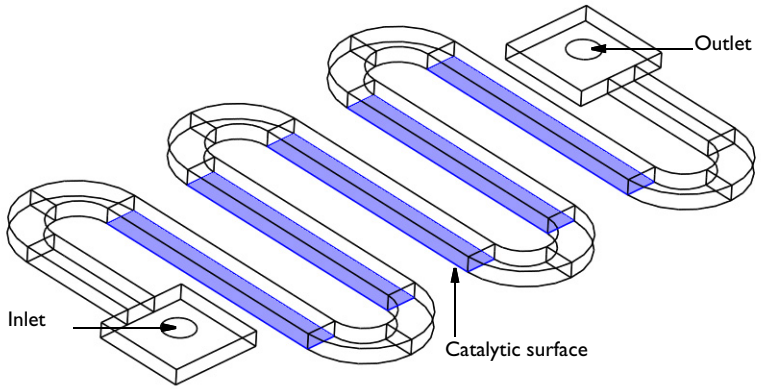

Figure 2: Microreactor geometry.

In the straight sections of the reactor, the channel walls are in part coated with platinum catalyst. As water with small amounts of a brominated hydrocarbon flows through the reactor, dehalogenation reactions occur at the catalytic surfaces.

MOMENTUM BALANCES

The flow in the channel is modeled with the Laminar Flow interface by solving the stationary incompressible Navier-Stokes equations:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2\mu}{3}(\nabla\cdot\mathbf{u})\mathbf{I}\right]$$

$$\rho\nabla\cdot\mathbf{u} = 0$$

Here, μ denotes the dynamic viscosity (SI unit: N·s/m^2), $\mathbf{u}$ the velocity (SI unit: m/s), ρ the density of the fluid (SI unit: kg/m^3), and p the pressure (SI unit: Pa).

A pressure difference drives the flow through the reactor, as indicated by the boundary conditions

$$p = p_{\text{inlet}} \qquad \text{inlet}$$
$$p = 0 \qquad \text{outlet}$$

Each pressure condition is specified along with a vanishing viscous stress condition at the boundary

$$\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\mathbf{n} = \mathbf{0}$$

At the wall the velocity is zero

$$\mathbf{u} = 0 \qquad \text{walls}$$

MASS BALANCES

The mass balances are set up with the Transport of Diluted Species interface and solves the diffusion-convection equations at steady state:

$$\mathbf{u} \cdot \nabla c_i + \nabla \cdot (-D_i \nabla c_i) = 0$$

Here D_i denotes the diffusion coefficient (SI unit: m^2/s), c_i is the species concentration (SI unit: mol/m^3), and $\mathbf{u}$ equals the velocity (SI unit: m/s).

The diffusivity of the reacting species is assumed to depend on the temperature according to

$$D = 5 \cdot 10^{-7} \cdot \exp\left(-\frac{2000\ \text{K}}{T}\right)\ \text{m}^2/\text{s}$$

No reactions take place in the fluid bulk. Rather, the reactions take place on the catalytic surfaces. The boundary fluxes at the catalytic surfaces thus become

$$\mathbf{n} \cdot (-D_i \nabla c_i) = R_i$$

where R_i represents the reaction term.

Inlet conditions are equal to the inlet concentrations

$$c = c_{\text{in}}$$

At the outlet, the mass transport is prescribed to be dominated by convection by setting the diffusive flux to zero.

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

The same no flux condition is also applied on all boundaries where the velocity is zero.

Results and Discussion

First review the results of the ideal reactor model, which you set up and solve using the Reaction Engineering interface.

Figure 3 through Figure 5 show concentration profiles of reactant and products as function of residence time, evaluated at 288 K, 343 K, and 363 K.

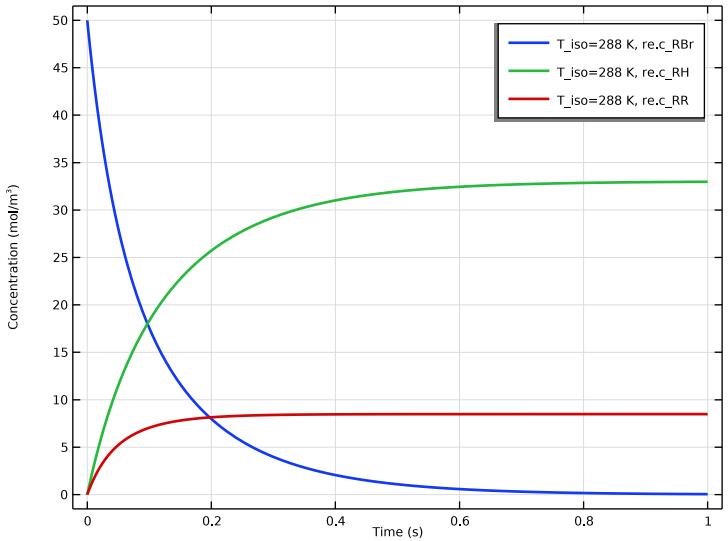

Figure 3: Concentration of the RBr, RH, and RR species as function of residence time. Reactions occur at 288 K.

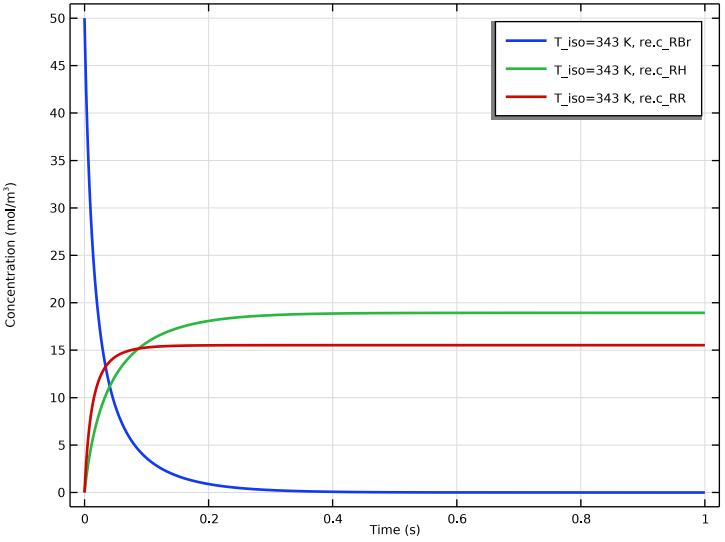

Figure 4: Concentration of the RBr, RH, and RR species as function of residence time. Reactions occur at 343 K.

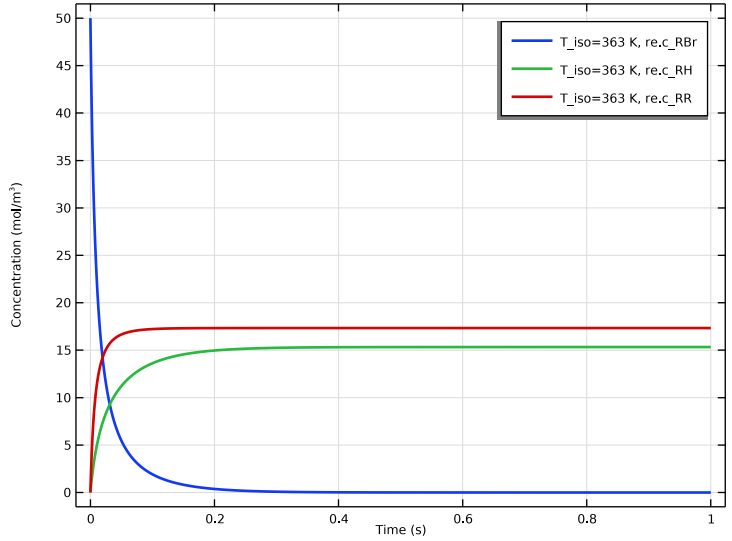

Figure 5: Concentration of the RBr, RH, and RR species as function of residence time. Reactions occur at 363 K.

The hydrocarbon coupling reaction has the higher activation energy and is hence more temperature sensitive than the hydrogenation reaction (see Table 1). The concentration plots of the ideal reactors outline the effect quite clearly. At 288 K, the hydrogenation product RH is dominant, while at 363 K the coupling product is the more prominent. Notably, at 343 K, the concentration dependency on the reaction rates becomes accentuated, so that RBr dominates only at shorter τ and RH at longer τ.

Although the primary goal may be to remove the halogenated reactant, RBr, it may also be important to set reaction conditions in such a way that the most favorable by-product is formed. The present model shows how such design aspects can readily be investigated with the Chemical Reaction Engineering Module.

The next set of results refer to the space-dependent model of a tortuous microreactor.

Figure 6 shows the velocity of the laminar flow field in the reactor running at 363 K. The flow is driven by a pressure difference of 1500 Pa between inlet and outlet. The resulting maximum velocity is approximately 18 mm/s.

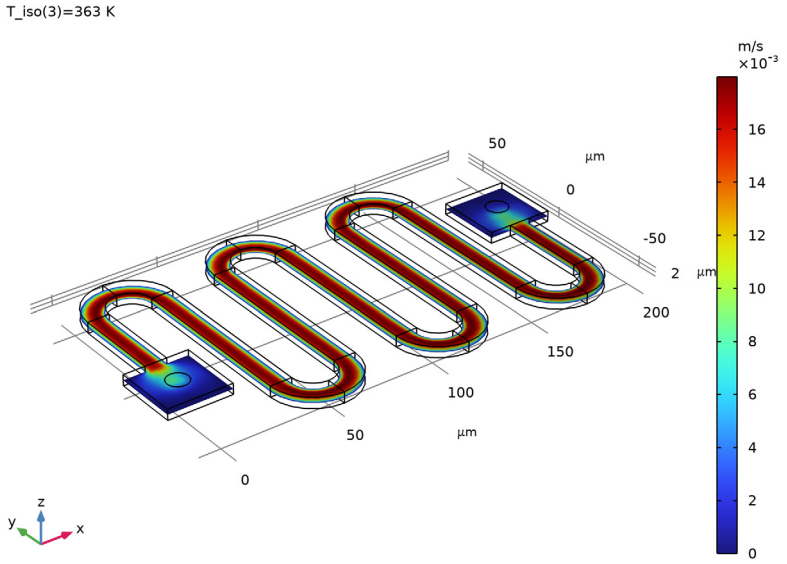

Figure 6: Velocity field in the reactor where the pressure difference between inlet and outlet is 1500 Pa.

Figure 7 shows the concentration distribution of the reactant RBr in the reactor. At relatively high temperature, 363 K, the outlet concentration is 7.7 mol/m^3.

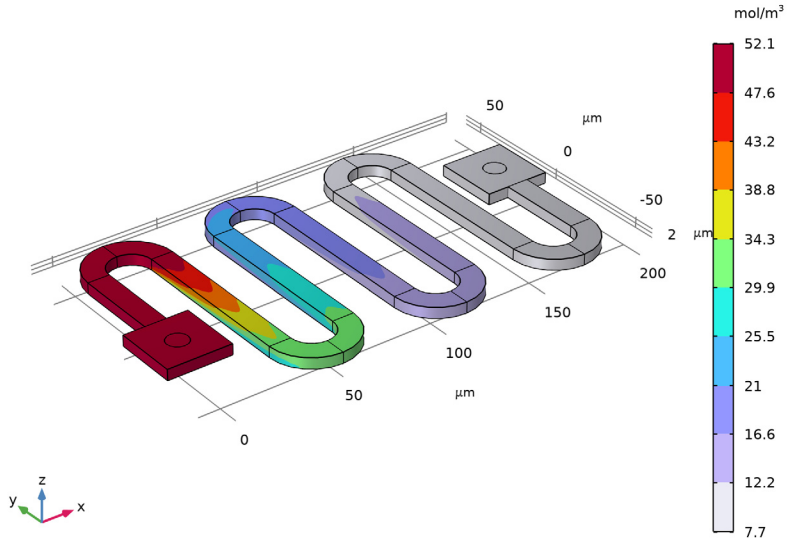

Figure 7: Concentration distribution of the halogenated reactant RBr. Transport properties and reaction rates are evaluated at 363 K.

Running the reactor at 288 K, the outlet concentration of RBr is 11.5 mol/m^3.

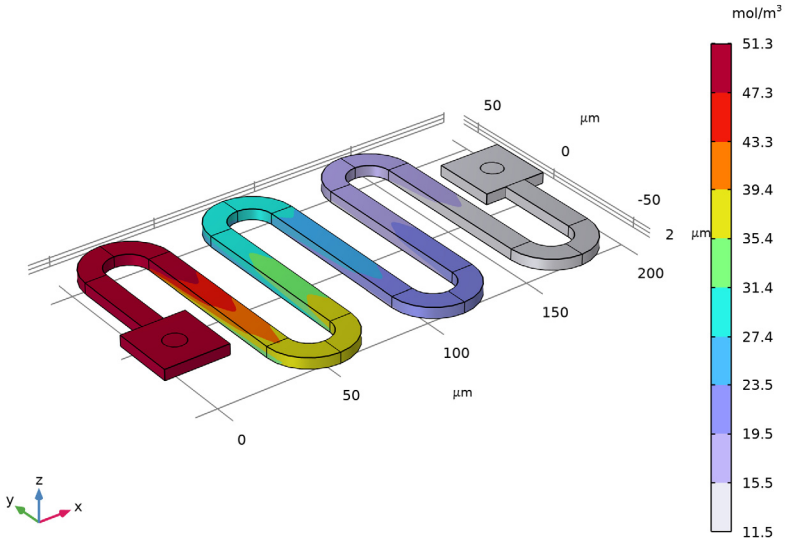

Figure 8: Concentration distribution of the halogenated reactant RBr. Transport properties and reaction rates are evaluated at 288 K.

Judging from the results of the ideal reactor models, a more pronounced temperature effect would be expected, as both reaction rates and species diffusivities increase notably at higher temperatures. The reason for this apparently moderate influence on conversion is that the increased temperature also affects the flow.

Increasing the temperature from 282 K to 363 K decreases the viscosity of water from $1.2 \cdot 10^{-3}$ to $3.2 \cdot 10^{-4}$ Pa·s. This is automatically taken into account by the temperature-dependent fluid properties. As the flow through the reactor is driven by a constant pressure difference, the velocity increases as viscosity decreases. Results also show that the maximum fluid velocity at 363 K is greater than at 282 K, resulting in a shorter residence time.

Finally, compare the concentrations of the reactant and products along the reactor length in the 3D model, with those predicted by the 0D model (Figure 9). The overall trends are similar for both the 0D and the 3D model. The results for the concentration of RH in the 3D model closely matches the prediction of the 0D model. However, the concentration of the reactant RBr is higher, and the concentration of RR is lower, in the 3D reactor than

in the 0D prediction. The reason is that, in 3D, the diffusion of reactant RBr toward the catalytically active surfaces is modeled. As the reaction at the surface proceeds, the reactant concentration is limited by the diffusion rate. However, in the 0D model, the reactions are assumed to occur at the bulk concentrations. A concentration approaching zero at the catalytic surface reduces the rate for a second-order reaction more than for a first-order reaction. Thus, the real reactor has a higher selectivity for the RH product than what the 0D model predicts.

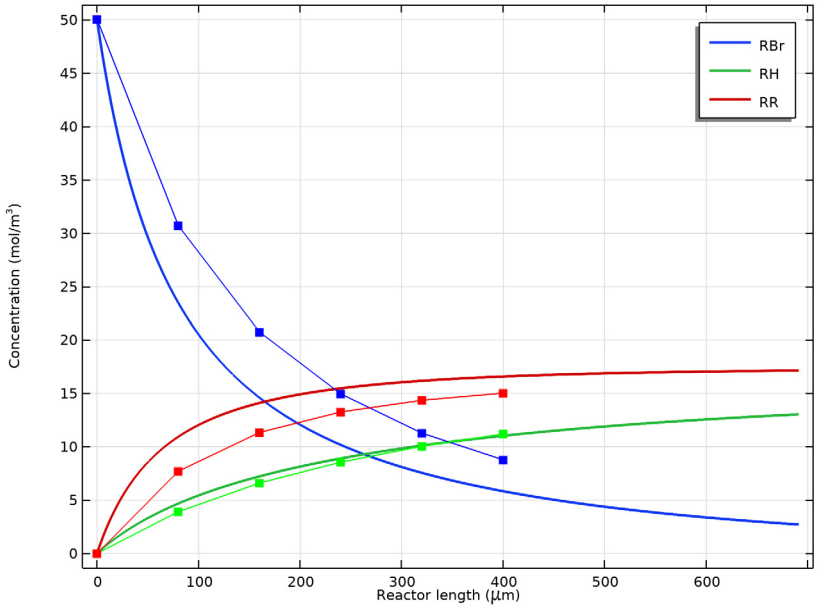

Figure 9: Concentrations of reactant RBr and products RH and RR, from both the 0D model (lines) and the 3D model (lines with markers). All data is for the highest temperature, 363 K. The reactor length only includes the length of each catalytic section, and not the turns between them where no reaction occurs.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_Transfer/tortuous_reactor`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **0D**.

2 In the **Select Physics** tree, select **Chemical Species Transport>Reaction Engineering (re)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

6 Click **Done**.

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 `tortuous_reactor_parameters.txt`.

REACTION ENGINEERING (RE)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering (re)**.

2 In the **Settings** window for **Reaction Engineering**, locate the **Energy Balance** section.

3 In the T text field, type `T_iso`.

You will solve for an isothermal system at three different temperatures.

4 Locate the **Mixture Properties** section. From the **Phase** list, choose **Liquid**.

As explained by Equation 3, you can use a batch reactor to model a flow-through system if the velocity is constant. The **Batch** reactor type is the default selection of the **Reaction Engineering** interface.

In order to set up the chemical reactions describing the dehalogenation process, a surface species `AS(ads)` is introduced into the following two surface reactions. In **Reaction Engineering**, a reaction is defined as a surface reaction if there are any surface species participating in the reaction.

Reaction 1

1 In the **Reaction Engineering** toolbar, click **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `RBr+AS(ads)=>RH`.

4 Locate the **Reaction Rate** section. From the list, choose **User defined**.

5 In the r_j text field, type `re.kf_1*re.c_RBr`.

6 Locate the **Reaction Orders** section. Find the **Surface overall reaction order** subsection. In the **Forward** text field, type `0`.

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 **Reaction Engineering** toolbar, click  **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `2RBr+AS(ads)=>RR`.

4 Locate the **Reaction Rate** section. From the list, choose **User defined**.

5 Locate the **Reaction Orders** section. Find the **Surface overall reaction order** subsection. In the **Forward** text field, type `0`.

6 Locate the **Reaction Rate** section. In the r_j text field, type `re.kf_2*re.c_RBr^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`.

Surface species: AS(ads)

The surface species `AS(ads)` acts as catalyst. Its concentration is constant.

1 In the **Model Builder** window, click **Surface species: AS(ads)**.

2 In the **Settings** window for **Species**, locate the **Constant Concentration/Activity** section.

3 Select the **Keep concentration/activity constant** check box.

The catalytic reaction only takes place on the reactor walls, and not in the whole reactor volume. This is accounted for by defining the surface area to volume ratio. Doing so allows you to compare this ideal 1D reactor with the 3D reactor that you model in the second part of this example.

4 In the **Model Builder** window, click **Reaction Engineering (re)**.

5 In the **Settings** window for **Reaction Engineering**, locate the **Reactor** section.

6 Find the **Surface reaction area** subsection. Click the **Surface area to volume ratio** button.

7 In the a_s text field, type `1/H`.

Initial Values 1

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

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

3 In the table, enter the following settings:

Species	Concentration (mol/m^3)
RBr	c_RBr0
RH	c_RH0
RR	c_RR0

4 Locate the **Surface Species Initial Values** section. In the table, enter the following settings:

Species	Surface concentration (mol/m^2)	Site occupancy number (1)
AS(ads)	c_As0_ads	1

STUDY 1

With the selection of reactor type and the input of the chemical kinetics you are ready to solve the ideal reactor model. Following the steps below you will set up an auxiliary sweep to solve the model for three different temperatures.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, 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
T_iso (Reactor temperature (K))	288 343 363	K

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

RESULTS

Concentrations 0D model

In the **Settings** window for **1D Plot Group**, type `Concentrations 0D model` in the **Label** text field.

Global 1

1 In the **Model Builder** window, expand the **Concentrations 0D model** node, then click **Global 1**.

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

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

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

This dataset contains the stored results from the auxiliary sweep. You can review the results by choosing entries in the **Parameters selection** lists and then clicking **Plot** button.

5 Locate the **Data** section. From the **Parameter selection (T_iso)** list, choose **From list**.

6 In the **Parameter values (T_iso (K))** list, select **288**.

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

This selection will give you the (residence) time on the x-axis of the plot.

8 In the **Concentrations 0D model** toolbar, click **Plot**.

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

10 Locate the **Data** section. In the **Parameter values (T_iso (K))** list, select **343**.

11 In the **Concentrations 0D model** toolbar, click **Plot**.

12 In the **Parameter values (T_iso (K))** list, select **363**.

13 In the **Concentrations 0D model** toolbar, click **Plot**.

REACTION ENGINEERING (RE)

The **Generate Space-Dependent Model** feature automatically sets up physics interfaces for modeling space- and time-dependent systems. This process uses the model in the **Reaction Engineering** interface as reference to set up transport interfaces, transferring variable names, reaction kinetics, as well as property expressions. By default the **Generate Space-Dependent Model** feature sets up a **Transport of Diluted Species** interface to describe a space-dependent reacting system and a **Chemistry** node with all reaction and species properties. The default settings are used in this example.

Generate Space-Dependent Model 1

1 In the **Reaction Engineering** toolbar, click **Generate Space-Dependent Model**.

2 In the **Settings** window for **Generate Space-Dependent Model**, locate the **Physics Interfaces** section.

3 Find the **Fluid flow** subsection. From the list, choose **Laminar Flow: New**.

4 Locate the **Space-Dependent Model Generation** section. Click **Create/Refresh**.

Note how the model generation creates a new component node, **Component 2**. By expanding this node you will find the **Transport of Diluted Species** and **Laminar Flow** interfaces that have been set up automatically.

GEOMETRY 1 (3D)

Import a geometry for the tortuous microreactor.

1 In the **Model Builder** window, expand the **Component 2 (comp2)** node, then click **Geometry 1(3D)**.

2 In the **Geometry** toolbar, click **Insert Sequence** and choose **Insert Sequence**.

3 Browse to the model's Application Libraries folder and double-click the file `tortuous_reactor_geom_sequence.mph`.

4 In the **Geometry** toolbar, click **Build All**.

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

ADD MATERIAL

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

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

3 In the tree, select **Liquids and Gases>Liquids>Water**.

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

5 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

By default, the first material you add applies on all domains. Associating a material with the geometry makes the predefined property expressions of the material available to the physics interfaces. In this case the temperature dependent expressions for the density and viscosity of water will be automatically included in the definition of the **Laminar Flow** interface.

CHEMISTRY 1 (CHEM)

Species: RBr

1 In the **Model Builder** window, expand the **Chemistry 1 (chem)** node, then click **Species: RBr**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the M text field, type `Mn_RBr`.

Surface species: AS(ads)

1 In the **Model Builder** window, click **Surface species: AS(ads)**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the M text field, type `Mn_As`.

Species: RH

1 In the **Model Builder** window, click **Species: RH**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the M text field, type `Mn_RH`.

Species: RR

1 In the **Model Builder** window, click **Species: RR**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the M text field, type `Mn_RR`.

TRANSPORT OF DILUTED SPECIES (TDS)

Transport Properties 1

1 In the **Model Builder** window, expand the **Transport of Diluted Species (tds)** node, then click **Transport Properties 1**.

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

3 In the D_{cRBr} text field, type `D`.

4 In the D_{cRH} text field, type `D`.

5 In the D_{cRR} text field, type `D`.

Surface Reactions 1

This feature takes surface reaction rates as boundary fluxes. The parameter is a **Feature Input** and matched automatically with variables from the **Chemistry** set up by the model generation process.

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

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

3 From the **Selection** list, choose **Catalytic Surfaces**.

Concentration 1

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

2 In the **Settings** window for **Concentration**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Concentration** section. Select the **Species cRBr** check box.

5 In the $c_{0,\mathrm{cRBr}}$ text field, type `c_RBr0`.

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

7 In the $c_{0,\mathrm{cRH}}$ text field, type `c_RH0`.

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

9 In the $c_{0,\mathrm{cRR}}$ text field, type `c_RR0`.

Outflow 1

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

2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

Recall that the reactions take place solely on the catalytic surfaces. Therefore the generated **Reactions** and **Flux Discontinuity** nodes can be removed.

Reactions 1

In the **Model Builder** window, right-click **Reactions 1** and choose **Delete**.

Flux Discontinuity 1

In the **Model Builder** window, under **Component 2 (comp2)>**
Transport of Diluted Species (tds) right-click **Flux Discontinuity 1** and choose **Delete**.

LAMINAR FLOW 1 (SPF)

Fluid Properties 1

1 In the **Model Builder** window, expand the **Component 2 (comp2)>Laminar Flow 1 (spf)** node, then click **Fluid Properties 1**.

2 In the **Settings** window for **Fluid Properties**, locate the **Model Input** section.

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

Note that both the fluid density and dynamic viscosity are taken from the water material.

Inlet 1

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

2 In the **Settings** window for **Inlet**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Boundary Condition** section. From the list, choose **Pressure**.

5 Locate the **Pressure Conditions** section. In the p_0 text field, type `delta_p`.

Outlet 1

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

2 In the **Settings** window for **Outlet**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

MULTIPHYSICS

Reacting Flow, Diluted Species 1 (rfd1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain>Reacting Flow, Diluted Species**.

This completes the setup of the physics interfaces. Following the steps below, discretize the reactor geometry with a mesh. With chemistry occurring on reactor walls, mass transport gradients are expected to be most pronounced perpendicular to the direction of the flow. Using a swept mesh will allow you to maintain high mesh resolution in the cross section of the reactor channel while setting a lower resolution in the direction of the flow. Analyzing the chemistry and physics of your system and distributing the mesh accordingly will often allow you to reduce memory requirements and computational time.

MESH 1

Free Triangular 1

1 In the **Mesh** toolbar, click **More Generators** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, locate the **Boundary Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `8` in the **Selection** text field.

5 Click **OK**.

Size 1

1 Right-click **Free Triangular 1** and choose **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.

5 Select the **Maximum element size** check box. In the associated text field, type `1`.

Swept 1

1 In the **Mesh** toolbar, click **Swept**.

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

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

4 From the **Selection** list, choose **Channel**.

Distribution 1

1 Right-click **Swept 1** and choose **Distribution**.

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

3 In the **Number of elements** text field, type 6.

Free Tetrahedral 1

1 In the **Mesh** toolbar, click  **Free Tetrahedral**.

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

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

4 From the **Selection** list, choose **Adapter Sections**.

Size 1

1 Right-click **Free Tetrahedral 1** and choose **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.

5 Select the **Maximum element size** check box. In the associated text field, type 2.

6 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.

The instructions below detail how to solve the model. As was the case for the perfectly mixed reactor model, you will set up auxiliary sweeps to solve for three different temperatures. The temperature affects not only reaction rates but also the diffusivity for the mass balance equations. The fluid flow is also affected, as the fluid density and viscosity are both temperature dependent.

Set up two study steps to solve the model. The first step solves for the fluid flow. The second step solves for the mass transport, using the flow field calculated in the first step for the convective mass transport. There is no need to solve the fully coupled problem as the mass transport does not influence the fluid flow in this example.

STUDY 2

Step 1: Stationary

1 In the **Model Builder** window, expand the **Study 2** node, then click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check boxes for **Reaction Engineering (re)** and **Transport of Diluted Species (tds)**.

4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

5 Click + **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
T_iso (Reactor temperature (K))	288 343 363	K

Step 2: Stationary 2

1 In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check boxes for **Reaction Engineering (re)** and **Laminar Flow 1 (spf)**.

4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

5 Click + **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
T_iso (Reactor temperature (K))	288 343 363	K

In this study step, do not solve for the laminar flow. However, to have all solutions from the previous step (flow at all temperatures) available when solving for the concentrations at different temperatures in the present step, change the settings for the values of variables not solved for.

7 Click to expand the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

8 From the **Method** list, choose **Solution**.

9 From the **Study** list, choose **Study 2, Stationary**.

10 From the **Selection** list, choose **Automatic (all solutions)**.

11 In the **Study** toolbar, click = **Compute**.

RESULTS

Concentration, RBr, Surface (tds)

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

2 In the **Settings** window for **3D Plot Group**, click to expand the **Title** section.

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

4 Locate the **Color Legend** section. Select the **Show units** check box.

Surface 1

1 In the **Model Builder** window, expand the **Concentration, RBr, Surface (tds)** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 Click **Change Color Table**.

4 In the **Color Table** dialog box, select **Rainbow>Prism** in the tree.

5 Click **OK**.

6 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

7 From the **Color table type** list, choose **Discrete**.

Concentration, RBr, Surface (tds)

The default surface plot shows the concentration of species RBr evaluated at 363 K. Select from the **Parameter** value list to look at other results.

1 In the **Model Builder** window, click **Concentration, RBr, Surface (tds)**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Parameter value (T_iso (K))** list, choose **288**.

4 In the **Concentration, RBr, Surface (tds)** toolbar, click **Plot**.

Velocity (spf1)

1 In the **Model Builder** window, click **Velocity (spf1)**.

2 In the **Settings** window for **3D Plot Group**, locate the **Color Legend** section.

3 Select the **Show units** check box.

Slice

1 In the **Model Builder** window, expand the **Velocity (spf1)** node, then click **Slice**.

2 In the **Settings** window for **Slice**, click to expand the **Title** section.

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

4 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.

5 In the **Planes** text field, type 1.

6 In the **Velocity (spf1)** toolbar, click **Plot**.

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

For future use of Study 1 and the 0D model, turn off all interfaces except **Reaction Engineering** in the table describing what physics interfaces to solve for.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check boxes for **Chemistry 1 (chem)**, **Transport of Diluted Species (tds)**, and **Laminar Flow 1 (spf)**.

To compare the results of the 3D model with the 0D Reaction Engineering model, first define a number of integration operators, and then use them to calculate the integrated total flux of each species, entering each section of the tortuous reactor. By dividing the resulting flux by the integrated flow velocity at the same position, the concentrations of each species will be obtained. These concentrations will correspond to the 0D concentrations for different residence times.

Prepare integration operators for the cross-sectional boundary at the entrance of each catalytic section of the reactor. The last operator is defined after the last catalytic section.

DEFINITIONS (COMP2)

Integration 1 (intop1)

1 In the **Model Builder** window, expand the **Component 2 (comp2)>Definitions** node.

2 Right-click **Component 2 (comp2)>Definitions** and choose **Nonlocal Couplings> Integration**.

3 In the **Settings** window for **Integration**, locate the **Source Selection** section.

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type 31 in the **Selection** text field.

6 Click **OK**.

7 In the **Settings** window for **Integration**, locate the **Source Selection** section.

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

9 Click  **Copy Selection**.

10 Click  **Paste Selection**.

11 In the **Paste Selection** dialog box, type 31 in the **Selection** text field.

12 Click **OK**.

Integration 2 (intop2)

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

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

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

4 Click  **Paste Selection**.

5 In the **Paste Selection** dialog box, type 40 in the **Selection** text field.

6 Click **OK**.

Integration 3 (intop3)

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

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

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

4 Click  **Paste Selection**.

5 In the **Paste Selection** dialog box, type 61 in the **Selection** text field.

6 Click **OK**.

Integration 4 (intop4)

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

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

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

4 Click  **Paste Selection**.

5 In the **Paste Selection** dialog box, type 70 in the **Selection** text field.

6 Click **OK**.

Integration 5 (intop5)

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

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

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

4 Click  **Paste Selection**.

5 In the **Paste Selection** dialog box, type 91 in the **Selection** text field.

6 Click **OK**.

Integration 6 (intop6)

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

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

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

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `85` in the **Selection** text field.

6 Click **OK**.

Update the solution to make the integral operators usable in expressions.

STUDY 2

In the **Study** toolbar, click **Update Solution**.

Now, create three evaluation groups. Each group is used to compute the concentration of one species, creating a table of concentrations for each cross-sectional entrance boundary. For each entrance boundary, the corresponding integration operator is used to calculate the concentration, as the total flux integral divided by the velocity times the Y-axis normal vector. Using just the Y-component works because the catalytic sections are parallel to the Y-axis. In general, for boundaries not aligned with an axis, an expression of the following form can be used for the velocity: `u*spf.nx+v*spf.ny+w*spf.nz`. Perform the comparison for the last, and highest, temperature in the sweep.

RESULTS

Concentration of RBr

1 In the **Results** toolbar, click **Evaluation Group**.

2 In the **Settings** window for **Evaluation Group**, type `Concentration of RBr` in the **Label** text field.

Concentration of RH

1 In the **Results** toolbar, click **Evaluation Group**.

2 In the **Settings** window for **Evaluation Group**, type `Concentration of RH` in the **Label** text field.

Concentration of RR

1 In the **Results** toolbar, click **Evaluation Group**.

2 In the **Settings** window for **Evaluation Group**, type `Concentration of RR` in the **Label** text field.

Global Evaluation 1

1 In the **Model Builder** window, right-click **Concentration of RBr** and choose **Global Evaluation**.

Next, set the evaluation groups to use the dataset corresponding to the final temperature sweep, and transpose the tables to simplify plotting later on. Then, import the expressions to use in each evaluation group. The last expression has a negative sign, since the normal of the y axis points in the opposite direction, relative to the other positions, at that boundary. Finally, for each case, evaluate each group to display the results.

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

3 From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

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

5 Locate the **Expressions** section. Click **Clear Table**.

6 Click **Load from File**.

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

Concentration of RBr

1 In the **Model Builder** window, click **Concentration of RBr**.

2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.

3 Select the **Transpose** check box.

4 Click to expand the **Format** section. From the **Include parameters** list, choose **Off**.

5 In the **Concentration of RBr** toolbar, click **Evaluate**.

Global Evaluation 1

1 In the **Model Builder** window, right-click **Concentration of RH** and choose **Global Evaluation**.

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

3 From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

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

5 Locate the **Expressions** section. Click **Clear Table**.

6 Click **Load from File**.

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

Concentration of RH

1 In the **Model Builder** window, click **Concentration of RH**.

2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.

3 Select the **Transpose** check box.

4 Locate the **Format** section. From the **Include parameters** list, choose **Off**.

5 In the **Concentration of RH** toolbar, click **Evaluate**.

Global Evaluation 1

1 In the **Model Builder** window, right-click **Concentration of RR** and choose **Global Evaluation**.

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

3 From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

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

5 Locate the **Expressions** section. Click **Clear Table**.

6 Click **Load from File**.

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

Concentration of RR

1 In the **Model Builder** window, click **Concentration of RR**.

2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.

3 Select the **Transpose** check box.

4 Locate the **Format** section. From the **Include parameters** list, choose **Off**.

5 In the **Concentration of RR** toolbar, click **Evaluate**.

Finally, create a plot comparing the 0D and the 3D results. Compare the results using the distance along the reactor as X axis. However, the 0D model data is a function of time, so to obtain it as a function of distance through the reactor, multiply it with the average value of the y-axis normal vector times the flow velocity. First, create an operator to calculate the average y-axis flow velocity. Since there is a steady flow through the reactor, you can arbitrarily choose to calculate the average at the cross-sectional boundary at the start of the first catalytic section.

DEFINITIONS (COMP2)

Average 1 (aveop1)

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

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

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

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `31` in the **Selection** text field.

6 Click **OK**.

Update the solution to make the average operator usable in expressions.

STUDY 2

In the **Study** toolbar, click **Update Solution**.

Now create the 1D plot, with 0D data and 3D data for each species.

RESULTS

0D versus 3D concentrations

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

2 In the **Settings** window for **1D Plot Group**, type `0D versus 3D concentrations` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **None**.

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

5 Locate the **Plot Settings** section.

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

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

Global 1

1 Right-click **0D versus 3D concentrations** and choose **Global**.

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

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

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

5 From the **Time selection** list, choose **Manual**.

6 In the **Parameter indices (1-210)** text field, type `range(1,1,90)`.

7 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

Convert residence time into distance along the reactor by multiplying residence time by the average flow velocity in the 3D reactor model. Use the `withsol` operator to select the final temperature dataset of the 3D model to get the velocity.

8 In the **Expression** text field, type `t*withsol('sol3',comp2.aveop1(-comp2.v*comp2.spf.ny))`.

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

10 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
RBr
RH
RR

12 In the **0D versus 3D concentrations** toolbar, click **Plot**.

Table Graph 1

1 In the **Model Builder** window, right-click **0D versus 3D concentrations** and choose **Table Graph**.

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

3 From the **Source** list, choose **Evaluation group**.

4 From the **x-axis data** list, choose **Row index**.

Use linear preprocessing of the x-axis data (the table indices) so that the indices correspond to the increasing cumulative total length along the reactor. Each catalytic section has the length of 80 μm.

5 Click to expand the **Preprocessing** section. Find the **x-axis column** subsection. From the **Transformation** list, choose **Linear**.

6 In the **Scaling** text field, type `80`.

7 In the **Shift** text field, type `-80`.

8 Locate the **Coloring and Style** section. From the **Color** list, choose **Blue**.

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

10 Right-click **Table Graph 1** and choose **Duplicate**.

Table Graph 2

1 In the **Model Builder** window, click **Table Graph 2**.

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

3 From the **Evaluation group** list, choose **Concentration of RH**.

4 Locate the **Coloring and Style** section. From the **Color** list, choose **Green**.

5 Right-click **Table Graph 2** and choose **Duplicate**.

Table Graph 3

1 In the **Model Builder** window, expand the **Table Graph 2** node, then click **Results> 0D versus 3D concentrations>Table Graph 3**.

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

3 From the **Evaluation group** list, choose **Concentration of RR**.

4 Locate the **Coloring and Style** section. From the **Color** list, choose **Red**.

Finally, plot the results.

0D versus 3D concentrations

1 In the **Model Builder** window, click **0D versus 3D concentrations**.

2 In the **0D versus 3D concentrations** toolbar, click **Plot**.

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

Appendix — Geometry Modeling Instructions

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

NEW

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

ADD COMPONENT

In the **Home** toolbar, click **Add Component** and choose **3D**.

GEOMETRY 1

1 In the **Settings** window for **Geometry**, locate the **Units** section.

2 From the **Length unit** list, choose **µm**.

Block 1 (blk1)

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

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Width** text field, type 10.

4 In the **Depth** text field, type 80.

5 In the **Height** text field, type `5`.

6 Locate the **Position** section. In the **x** text field, type `30`.

7 In the **y** text field, type `-40`.

8 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. Click **New**.

9 In the **New Cumulative Selection** dialog box, type `Channel` in the **Name** text field.

10 Click **OK**.

Array 1 (arr1)

1 In the **Geometry** toolbar, click **Transforms** and choose **Array**.

2 In the **Settings** window for **Array**, locate the **Input** section.

3 From the **Input objects** list, choose **Channel**.

4 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Channel**.

5 Locate the **Size** section. In the **x size** text field, type `5`.

6 Locate the **Displacement** section. In the **x** text field, type `30`.

Cylinder 1 (cyl1)

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

2 In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.

3 In the **Radius** text field, type `20`.

4 In the **Height** text field, type `5`.

5 Locate the **Position** section. In the **x** text field, type `50`.

6 In the **y** text field, type `-40`.

7 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (μm)
`Layer 1`	`10`

8 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Channel**.

9 Right-click **Cylinder 1 (cyl1)** and choose **Duplicate**.

Cylinder 2 (cyl2)

1 In the **Model Builder** window, click **Cylinder 2 (cyl2)**.

2 In the **Settings** window for **Cylinder**, locate the **Position** section.

3 In the **x** text field, type `20`.

4 In the **y** text field, type `40`.

Array 2 (arr2)

1 In the **Geometry** toolbar, click  **Transforms** and choose **Array**.

2 Select the objects **cyl1** and **cyl2** only.

3 In the **Settings** window for **Array**, locate the **Selections of Resulting Entities** section.

4 Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Channel**.

5 Locate the **Size** section. In the **x size** text field, type `3`.

6 Locate the **Displacement** section. In the **x** text field, type `60`.

Block 2 (blk2)

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

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Width** text field, type `30`.

4 In the **Depth** text field, type `30`.

5 In the **Height** text field, type `5`.

6 Locate the **Position** section. In the **x** text field, type `-10`.

7 In the **y** text field, type `-30`.

8 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. Click **New**.

9 In the **New Cumulative Selection** dialog box, type `Adapter Sections` in the **Name** text field.

10 Click **OK**.

Work Plane 1 (wp1)

1 In the **Geometry** toolbar, click  **Work Plane**.

2 In the **Settings** window for **Work Plane**, locate the **Selections of Resulting Entities** section.

3 Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Adapter Sections**.

4 Locate the **Plane Definition** section. In the **z-coordinate** text field, type `5`.

Work Plane 1 (wp1)>Plane Geometry

In the **Model Builder** window, click **Plane Geometry**.

Work Plane 1 (wp1)>Circle 1 (c1)

1 In the **Work Plane** toolbar, click **Circle**.

2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.

3 In the **Radius** text field, type `5`.

4 Locate the **Position** section. In the **xw** text field, type `4.6`.

5 In the **yw** text field, type `-15.4`.

Rotate 1 (rot1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Geometry 1** right-click **Work Plane 1 (wp1)** and choose **Transforms>Rotate**.

2 In the **Settings** window for **Rotate**, locate the **Input** section.

3 From the **Input objects** list, choose **Adapter Sections**.

4 Select the **Keep input objects** check box.

5 Locate the **Rotation** section. In the **Angle** text field, type `180`.

6 Locate the **Point on Axis of Rotation** section. In the **x** text field, type `95`.

7 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Adapter Sections**.

Block 3 (blk3)

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

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Width** text field, type `10`.

4 In the **Depth** text field, type `40`.

5 In the **Height** text field, type `5`.

6 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Channel**.

7 Right-click **Block 3 (blk3)** and choose **Duplicate**.

Block 4 (blk4)

1 In the **Model Builder** window, click **Block 4 (blk4)**.

2 In the **Settings** window for **Block**, locate the **Position** section.

3 In the **x** text field, type `180`.

4 In the **y** text field, type `-40`.

5 Click **Build Selected**.

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

Delete Entities 1 (del1)

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

2 In the **Settings** window for **Delete Entities**, locate the **Entities or Objects to Delete** section.

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

4 On the object **arr2(1,1,1,1)**, select Domains 2, 3, and 5 only.

5 On the object **arr2(1,1,1,2)**, select Domains 1, 3, and 4 only.

6 On the object **arr2(2,1,1,1)**, select Domains 2, 3, and 5 only.

7 On the object **arr2(2,1,1,2)**, select Domains 1, 3, and 4 only.

8 On the object **arr2(3,1,1,1)**, select Domains 2, 3, and 5 only.

9 On the object **arr2(3,1,1,2)**, select Domains 1, 3, and 4 only.

Form Union (fin)

1 In the **Model Builder** window, click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, click **Build Selected**.

Inlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Inlet` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 6 only.

Outlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Outlet` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 109 only.

Catalytic Surfaces

1 In the **Geometry** toolbar, click **Selections** and choose **Box Selection**.

2 In the **Settings** window for **Box Selection**, locate the **Geometric Entity Level** section.

3 From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. From the **Entities** list, choose **From selections**.

5 Click **Add**.

6 In the **Add** dialog box, select **Channel** in the **Selections** list.

7 Click **OK**.

8 In the **Settings** window for **Box Selection**, locate the **Box Limits** section.

9 In the **x minimum** text field, type `20`.

10 In the **x maximum** text field, type `170`.

11 In the **y minimum** text field, type `-41`.

12 In the **y maximum** text field, type `41`.

13 In the **z maximum** text field, type `0.01`.

14 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside box**.

15 In the **Label** text field, type `Catalytic Surfaces`.

Adjacent Selection - Walls

1 In the **Geometry** toolbar, click **Selections** and choose **Adjacent Selection**.

2 In the **Settings** window for **Adjacent Selection**, locate the **Input Entities** section.

3 Click **Add**.

4 In the **Add** dialog box, in the **Input selections** list, choose **Channel** and **Adapter Sections**.

5 Click **OK**.

6 In the **Settings** window for **Adjacent Selection**, type `Adjacent Selection - Walls` in the **Label** text field.

Exterior Walls

1 In the **Geometry** toolbar, click **Selections** and choose **Difference Selection**.

2 In the **Settings** window for **Difference Selection**, type `Exterior Walls` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Click the **Add** button for **Selections to add**.

5 In the **Add** dialog box, select **Adjacent Selection - Walls** in the **Selections to add** list.

6 Click **OK**.

7 In the **Settings** window for **Difference Selection**, locate the **Input Entities** section.

8 Click the **Add** button for **Selections to subtract**.

9 In the **Add** dialog box, in the **Selections to subtract** list, choose **Inlet** and **Outlet**.

10 Click **OK**.