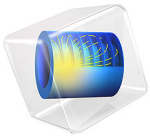


Polymerization in Multijet Tubular Reactor

Introduction

Production processes for polymers often involve turbulent flows and rapid reaction kinetics. The sophisticated interplay between fluid dynamics and fast chemical reactions can significantly impact the reactor performance, and thereby affect conversion and yield. Furthermore, the turbulent fluid mixing and its effects on the reaction can influence the average length of polymer chains, the molecular weight distribution, cross-linking, and chain-branching. All these properties are important for the integrity of the final material. This example demonstrates a polyester reactor, with multiple inlets, and includes heat transfer and temperature dependent kinetics. It employs the eddy dissipation concept (EDC), a model for the mean reaction rate in turbulent flows.

Note: This application requires both the Chemical Reaction Engineering Module and the CFD Module.

Model Definition

GEOMETRY

The geometry of the inlet section of a multijet tubular reactor is illustrated in Figure 1.

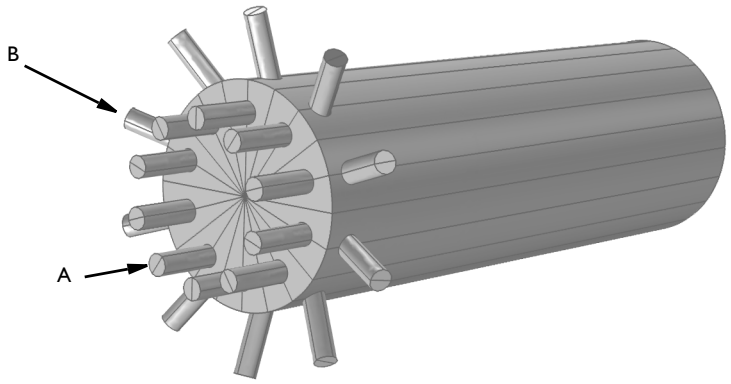


Figure 1: Inlet section of a multijet tubular reactor. Monomer A (diol) enters through the axial inlets while monomer B (diacid) enters through the radial ports.

Two reacting monomers enter through separate inlet ports. Monomer A enters through the axial inlets while monomer B enters through the radial ports.

CHEMISTRY

Condensation reactions are fundamental to the production of many important polymers, such as polyamides, polyesters, polyurethanes, and silicones.

This model simulates a polyester reactor. Condensation polymerization of monomers A (a diol) and B (a diacid), forms the polyester linkage, L (Ref. 1, Ref. 2). The reactions take place in the presence of a solvent catalyst, S.

TABLE 1: SPECIES USED ON THE MODEL.

NAME	DESCRIPTION
A	Diol monomer
B	Diacid monomer
L	Polyester linkage (product)
S	Solvent catalyst ($TiCl_3$)
C	Complexating water

The catalytic species, S, is temporarily trapped in an intermediary H_2O complex, S · C, where C represents the complex-forming water in the irreversible reaction

$$2\mathrm{A} + \mathrm{B} + \mathrm{S} \xrightarrow{k_1^f} \mathrm{L} + 2\mathrm{SC} \tag{1}$$

The regeneration of solvent is governed by the reversible reaction

$$\mathrm{A} + \mathrm{SC} \underset{k_2^r}{\overset{k_2^f}{\Leftrightarrow}} \mathrm{S} + \mathrm{AC} \tag{2}$$

The reaction rates for each chemical reaction is determined by the law of mass action and the eddy dissipation concept (EDC) model. The law of mass action gives the rates (mol/(m^3·s))

$$r_1 = k_1^f c_\mathrm{A}^2 c_\mathrm{B} c_\mathrm{S} \tag{3}$$

and

$$r_2 = k_2^f c_\mathrm{A} c_\mathrm{SC} - k_2^r c_\mathrm{S} c_\mathrm{AC} \tag{4}$$

for reactions Equation 1and Equation 2, respectively, where the rate constants are given by the Arrhenius expression

$$k_j = A_j \exp\left(-\frac{E_j}{R_g T}\right) \tag{5}$$

In Equation 5, A_j is the frequency factor and E_j the activation energy (J/mol) for the jth reaction. The table below lists the values of the Arrhenius parameters for the reactions. The rates are adjusted for turbulent conditions according to the EDC model: If the time scale of the turbulent mixing is larger than the reaction kinetics derived by the law of mass action above, the turbulent mixing will be rate determining. For detailed information, see the section *Eddy Dissipation Model* in the *CFD Module User's Guide*.

TRANSPORT

The 3D model geometry is illustrated in Figure 1.

Velocities and Pressure

The average velocities at the radial and axial inlets are set to 5 m/s. Furthermore, a constant pressure is set at the outlet and logarithmic wall functions are specified at the solid walls.

Mass Transport

Concentration boundary conditions apply at the inlets:

$$\begin{aligned} c_A &= 1200 \text{ mol/m}^3 \text{ at axial inlets} \\ c_B &= 1000 \text{ mol/m}^3 \text{ at radial inlets} \end{aligned} \tag{6}$$

The catalytic solvent S is set as solvent in the mass transport model.

Energy Transport

The reactor is assumed to be insulated at the walls and all inlet streams are specified to 440 K temperature.

Summary of Input Data

For the rate expressions in Equation 3 and Equation 4 the following data is used (Ref. 1):

TABLE 2: KINETIC DATA.

QUANTITY	FREQUENCY FACTOR	ACTIVATION ENERGY	TURBULENT PARAMETERS α AND β
Forward Reaction 1	25.6	61.3[kJ/mol]	4, 0.5
Forward reaction 2	3.9e3	56.8[kJ/mol]	4, 0.5
Reverse reaction 2	4.7e3	102[kJ/mol]	4, 0.5

The material properties and boundary conditions used are (Ref. 1 and Ref. 2).

TABLE 3: INPUT DATA.

PROPERTY	VALUE
Diffusivity	1e-8[m^2/s]
Density of catalyst solvent	2640[kg/m^3]
Heat capacity of catalyst solvent	2550[J/kg/K]
Inlet velocity	5[m/s]
Inlet temperature	440[K]
Molar mass, monomer A	48[g/mol]
Molar mass, monomer B	104[g/mol]
Molar mass, complexating H_2O	18[g/mol]
Molar mass, polymer L	164[g/mol]
Molar mass, catalyst S	154[g/mol]
Molar mass, catalytic species complex SC	172[g/mol]
Molar mass, species complex AC	66[g/mol]
Heat of reaction, Reaction 1	100[kJ/mol]
Heat of reaction, Reaction 2	40[kJ/mol]

Modeling in COMSOL

- For the 3D model, the *Reacting Flow, Turbulent* interface is used for the mass transport, reactions, and fluid flow simulation. The *Heat Transfer in Fluids* interface is used to do the heat transfer simulation including the heat of reactions, coupled with the reacting flow.

STAGED SOLUTION

Since the chemical reactions are strongly depending on the fluid movement, the fully coupled system may be difficult to converge in the first iterations due insufficient start guesses on the velocity field. Therefore the following staged solutions is used. Each study step uses the converged solution from the previous step as a start guess:

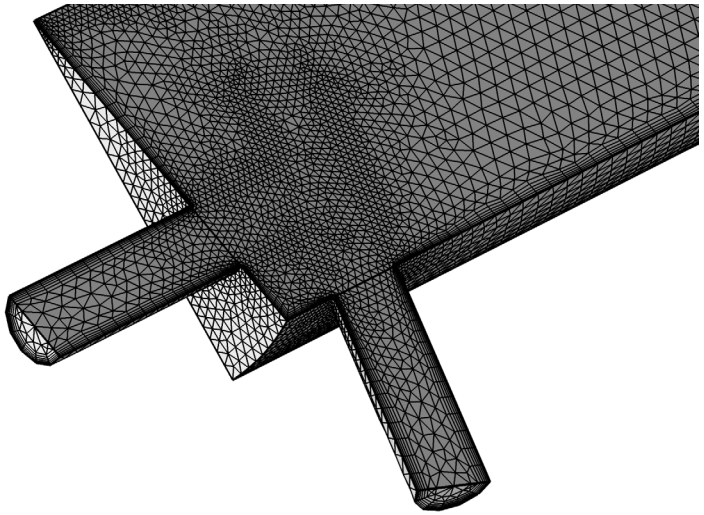
1. Velocity and pressure only.
2. Velocity, pressure, concentrations distribution including reactions. Isothermal.
3. Temperature only, including heat of reaction.
4. All variables.

GEOMETRY

Thanks to symmetry observations, a sector of one 1/20 of the geometry shown in Figure 1 is modeled. The modeling results are rotated to the full geometry by sector datasets.

MESH

The mesh is calibrated to resolve the shear layers that appear near the inlets of the reactor. Further downstream where the flow profile is expected to be more uniform, a simpler extruded mesh is used to save time and memory.



Results of the flow field calculations are presented first. Figure 2 shows the velocity field in the multijet tubular reactor, plotted in two perpendicular planes through the reactor.

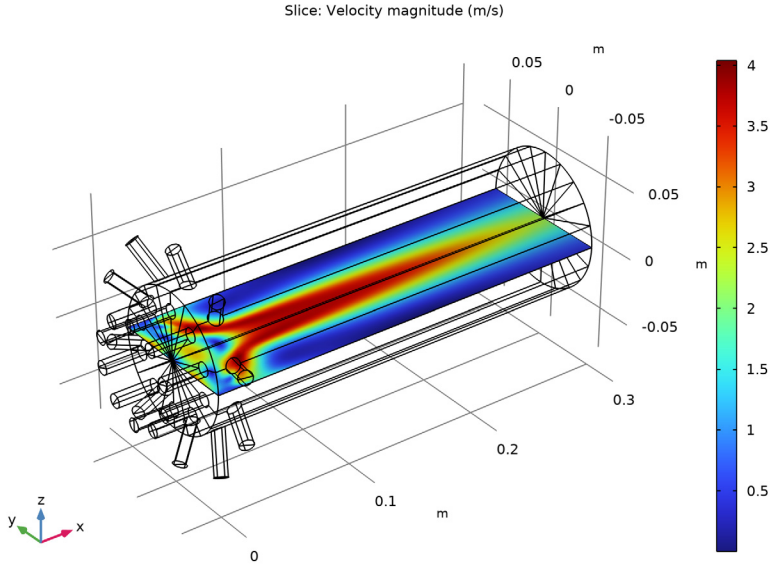


Figure 2: Velocity field (m/s) in the multijet tubular reactor.

The plot illustrates the impinging axial and radial jets.

Plotting the streamlines of the velocity field provides additional information, indicating flow paths. Figure 3 shows such a plot. Closer inspection at the entrance of the reactor reveals several recirculation zones.

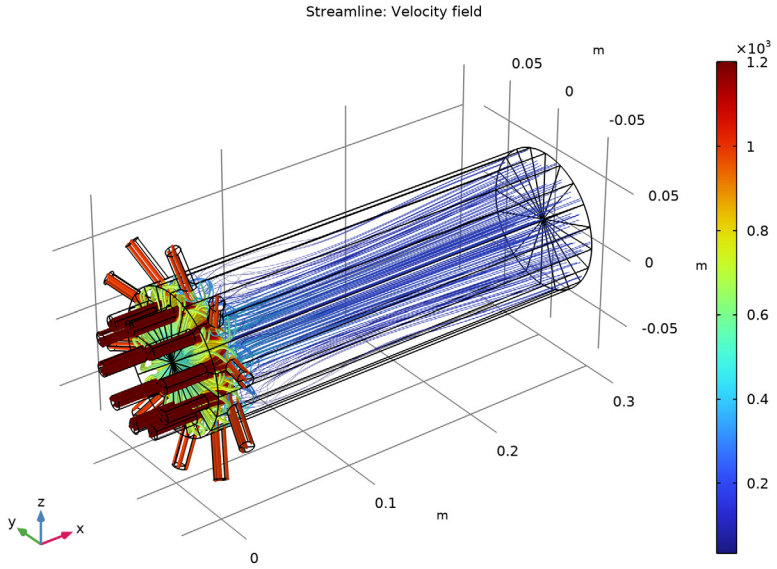


Figure 3: Streamlines of the velocity field shows some recirculation behavior near the inlet orifices. The concentration of reactants decrease rapidly at after the inlet stretch.

Next, mass is transported with the calculated flow field. Once monomer A comes into contact with the radial streams of monomer B, polymerization starts. Figure 4 shows the concentration field of monomer A.

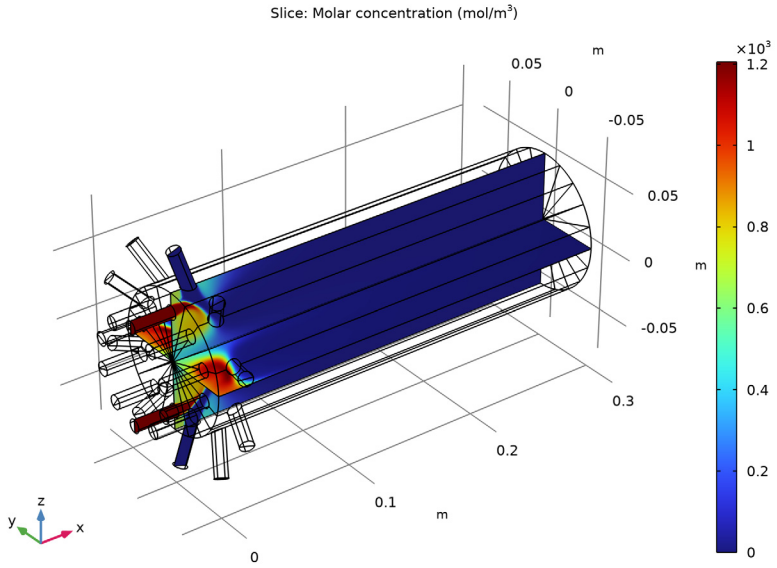


Figure 4: Concentration distribution of monomer A (mol/m^3).

Figure 5 shows isosurfaces for the polymer linkage L concentration. Isolevels at the entrance of the reactor clearly mark the positions of where the inlet streams mix. However, the azimuthal concentration gradients increase quickly with axial position, indicating that

inlet streams are well mixed for reaction to take place approximately 5 cm down the reactor.

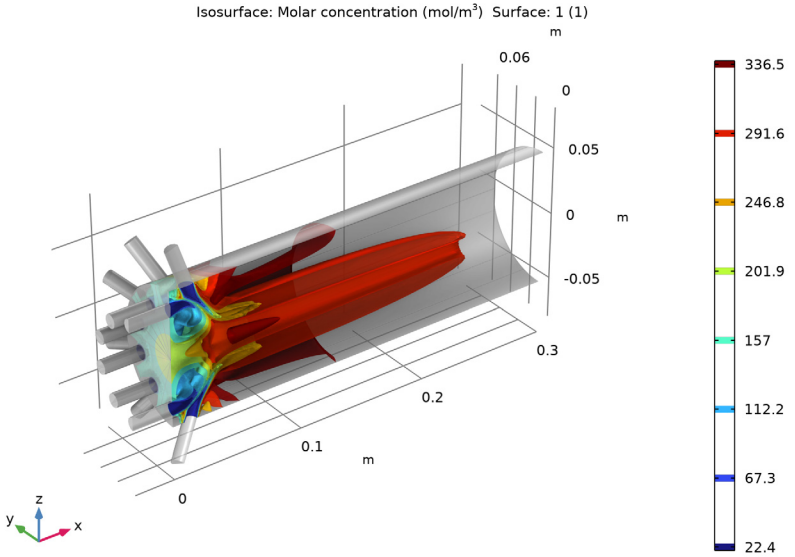


Figure 5: Isosurfaces for the concentration of L (mol/m^3) visualized using a clip plane.

As mentioned above, recirculation is evident in the entrance of the reactor. Recirculation will increase the effective residence time of the reactor. Figure 6 shows the concentration of polymer linkage, c_L, with a surface slice plot.

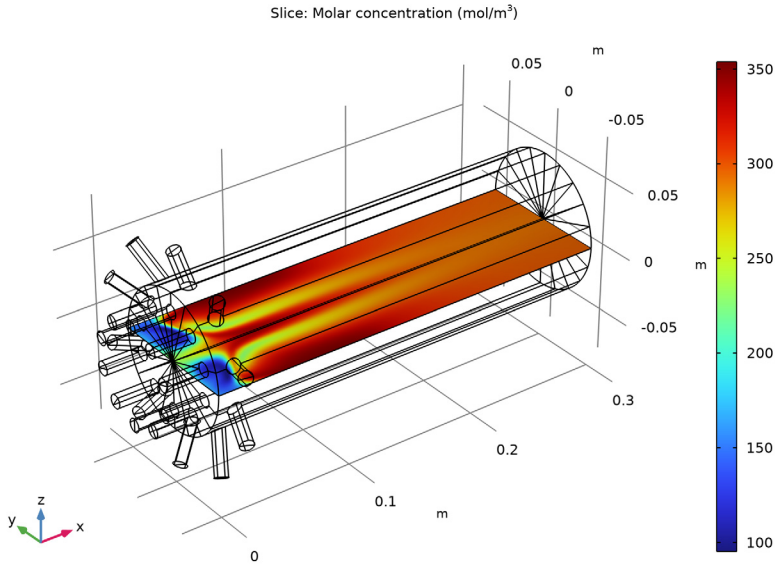


Figure 6: Concentration distribution of polymer linkage, c_L (mol/m^3).

Clearly, the concentration of L is relatively low in the recirculation region. In polymerization processes, increasing linkage concentration can lead to dramatic changes in the properties of the reacting fluid, particularly viscosity. This in turn may cause fouling or even reactor failure.

Figure 7 shows the concentration of product L in a cross section plot along the axis of the reactor. The recirculation effects in the beginning of the multijet tubular model are evident. Results also point to the influence of mixing on the reaction rate. The mixing in the space-dependent reactor is influenced by the detailed flow field.

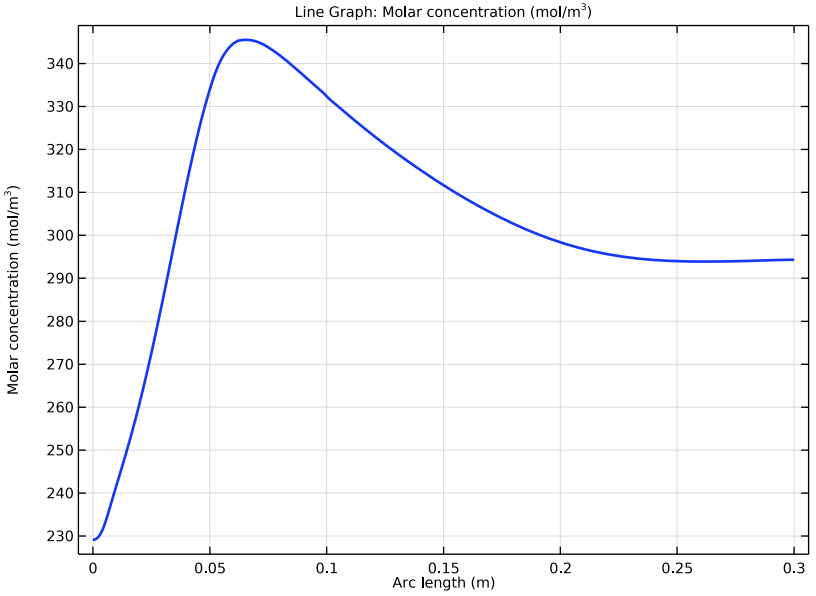


Figure 7: Concentration of polymer linkage, c_L, as a function of axial position in the reactor. The space-dependent model accounts for recirculation effects near the reactor inlet.

The total condensation chemistry is endothermic. Figure 8 displays the resulting temperature field in the reactor.

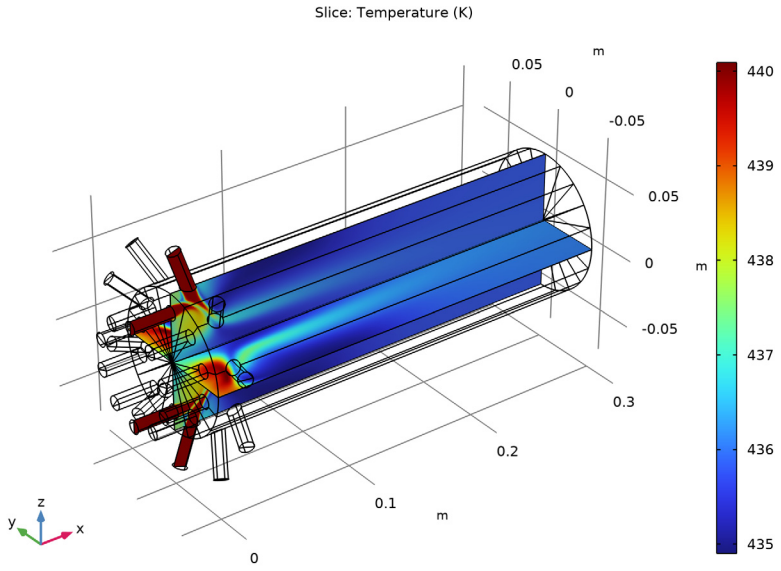


Figure 8: Temperature distribution in the multijet tubular reactor. The inlet temperatures of radial and axial streams are 440 K.

The endothermic reactions efficiently cool down the reacting flow.

References

1. N.H. Kolhapure, J.N. Tilton, and C.J. Pereira, "Integration of CFD and condensation polymerization chemistry for a commercial multi-jet tubular reactor," *Chem. Eng. Sci.*, vol. 59, p. 5177, 2004.

2. http://en.wikipedia.org/wiki/Polyester.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/polymerization_multijet`

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

2 In the **Select Physics** tree, select **Chemical Species Transport>Reacting Flow> Turbulent Flow>Turbulent Flow, k-ε**.

3 Click **Add**.

4 In the **Added physics interfaces** tree, select **Transport of Concentrated Species (tcs)**.

5 In the **Number of species** text field, type 6.

6 In the **Mass fractions** table, enter the following settings:

wA
wB
wS
wL
wSC
wAC

7 In the **Select Physics** tree, select **Heat Transfer>Heat Transfer in Fluids (ht)**.

8 Click **Add**.

9 Click **Study**.

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

11 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 `polymerization_multijet_parameters.txt`.

GEOMETRY 1

Start by creating the geometry. You can simplify this by inserting a prepared geometry sequence from file. You can read the instruction for building the geometry in the appendix.

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

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

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

Mesh Control Domains 1 (mcd1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Mesh Control Domains**.

2 On the object **fin**, select Domain 4 only.

Mesh Control Faces 1 (mcf1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Mesh Control Faces**.

2 On the object **mcd1**, select Boundary 11 only.

Mesh Control Domains 1 (mcd1)

1 In the **Model Builder** window, click **Mesh Control Domains 1 (mcd1)**.

2 In the **Settings** window for **Mesh Control Domains**, locate the **Input** section.

3 Find the **Domains to include** subsection. Click to select the **Activate Selection** toggle button.

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

TURBULENT FLOW, K-ε (SPF)

Fluid Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Turbulent Flow, k-ε (spf)** click **Fluid Properties 1**.

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

3 From the μ list, choose **User defined**. In the associated text field, type `0.001*(1.17817558982837+(-298[K]+T)/223[K])^(-3.758)[Pa*s]`.

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 k text field, type `7e-8`.

4 In the *ep* text field, type `1e-11`.

Symmetry 1

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

2 Select Boundaries 4 and 8 only.

Inlet 1

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

2 Select Boundaries 1 and 5 only.

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

4 From the list, choose **Fully developed flow**.

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `5`.

Outlet 1

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

2 Select Boundary 11 only.

TRANSPORT OF CONCENTRATED SPECIES (TCS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Concentrated Species (tcs)**.

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

3 From the **Diffusion model** list, choose **Fick's law**.

4 Locate the **Species** section. From the **From mass constraint** list, choose **wS**.

Transport Properties 1

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

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

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

4 In the M_{wA} text field, type `MwA`.

5 In the M_{wB} text field, type `MwB`.

6 In the M_{wS} text field, type `MwS`.

7 In the M_{wL} text field, type `MwL`.

8 In the M_{wSC} text field, type `MwSC`.

9 In the M_{wAC} text field, type `MwAC`.

10 Locate the **Diffusion** section. In the D^{f}_{wA} text field, type `D`.

11 In the D^{f}_{wB} text field, type `D`.

12 In the D^{f}_{wS} text field, type `D`.

13 In the D^{f}_{wL} text field, type `D`.

14 In the D^{f}_{wSC} text field, type `D`.

15 In the D^{f}_{wAC} text field, type `D`.

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 $\omega_{0,wA}$ text field, type `1e-6`.

4 In the $\omega_{0,wB}$ text field, type `1e-6`.

5 In the $\omega_{0,wL}$ text field, type `1e-6`.

6 In the $\omega_{0,wSC}$ text field, type `1e-6`.

7 In the $\omega_{0,wAC}$ text field, type `1e-6`.

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 **Inflow** section.

4 From the **Mixture specification** list, choose **Molar concentrations**.

5 In the $c_{0,wA}$ text field, type `1200[mol/m^3]`.

6 In the $c_{0,wB}$ text field, type `1e-3[mol/m^3]`.

7 In the $c_{0,wL}$ text field, type `1e-3[mol/m^3]`.

8 In the $c_{0,wSC}$ text field, type `1e-3[mol/m^3]`.

9 In the $c_{0,wAC}$ text field, type `1e-3[mol/m^3]`.

Inflow 2

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

2 Select Boundary 5 only.

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

4 From the **Mixture specification** list, choose **Molar concentrations**.

5 In the $c_{0,wA}$ text field, type `1e-3[mol/m^3]`.

6 In the $c_{0,wB}$ text field, type `1000[mol/m^3]`.

7 In the $c_{0,\mathrm{wL}}$ text field, type `1e-3[mol/m^3]`.

8 In the $c_{0,\mathrm{wSC}}$ text field, type `1e-3[mol/m^3]`.

9 In the $c_{0,\mathrm{wAC}}$ text field, type `1e-3[mol/m^3]`.

Outflow 1

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

2 Select Boundary 11 only.

Symmetry 1

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

2 Select Boundaries 4 and 8 only.

Reaction 1

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

2 Select Domain 1 only.

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

4 In the ν_{wA} text field, type `-2`.

5 In the ν_{wB} text field, type `-1`.

6 In the ν_{wS} text field, type `-1`.

7 In the ν_{wL} text field, type `1`.

8 In the ν_{wSC} text field, type `2`.

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

10 In the A^{f} text field, type `25.6`.

11 In the E^{f} text field, type `61.3e3`.

12 In the A^{r} text field, type `0`.

13 Locate the **Turbulent Flow** section. From the **Turbulent-reaction model** list, choose **Eddy-dissipation**.

Reaction 2

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

2 Select Domain 1 only.

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

4 In the ν_{wA} text field, type `-1`.

5 In the ν_{wS} text field, type `1`.

6 In the ν_{wSC} text field, type `-1`.

7 In the ν_{wAC} text field, type `1`.

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

9 In the A^{f} text field, type `3.9e3`.

10 In the E^{f} text field, type `56.8e3`.

11 In the A^{r} text field, type `4.7e3`.

12 In the E^{r} text field, type `102e3`.

13 Locate the **Turbulent Flow** section. From the **Turbulent-reaction model** list, choose **Eddy-dissipation**.

HEAT TRANSFER IN FLUIDS (HT)

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Fluids (ht)** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Heat Convection** section.

3 From the $\mathbf{u}$ list, choose **Velocity field (spf)**.

4 Locate the **Heat Conduction, Fluid** section. From the k list, choose **User defined**. In the associated text field, type `0.21+Cp_S*spf.muT/0.72`.

5 Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Gas/Liquid**.

6 From the ρ list, choose **Density (tcs/cdm1)**.

7 From the C_p list, choose **User defined**. In the associated text field, type `Cp_S`.

8 From the γ list, choose **User defined**.

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 T text field, type `440[K]`.

Temperature 1

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

2 Select Boundaries 1 and 5 only.

3 In the **Settings** window for **Temperature**, locate the **Temperature** section.

4 In the T_0 text field, type `440[K]`.

Outflow 1

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

2 Select Boundary 11 only.

Symmetry 1

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

2 Select Boundaries 4 and 8 only.

Heat Source 1

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

2 Select Domain 1 only.

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

4 In the Q_0 text field, type `-100[kJ/mol]*tcs.treac1.r-40[kJ/mol]*tcs.treac2.r`.

MESH 1

Free Tetrahedral 1

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

Size

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

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Calibrate for** list, choose **Fluid dynamics**.

Free Tetrahedral 1

1 In the **Model Builder** window, click **Free Tetrahedral 1**.

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

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

4 Select Domains 1 and 3–5 only.

Size 1

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

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

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

4 Select Edges 13, 14, 22, 23, 31, 33–35, 38, 40, 42, and 43 only.

5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

6 From the **Predefined** list, choose **Extra fine**.

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 Select Domain 2 only.

Distribution 1

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

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

3 From the **Distribution type** list, choose **Predefined**.

4 In the **Number of elements** text field, type `40`.

5 In the **Element ratio** text field, type `4`.

Boundary Layers 1

1 In the **Mesh** toolbar, click **Boundary Layers**.

2 In the **Settings** window for **Boundary Layers**, click to expand the **Corner Settings** section.

3 In the **Maximum angle per split** text field, type `50`.

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.

2 Select Boundaries 2, 3, 6, 7, 9, 10, 14, 19, and 22–24 only.

3 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.

4 In the **Number of layers** text field, type `6`.

5 In the **Thickness adjustment factor** text field, type `2.4`.

6 Click **Build All**.

STUDY 1

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** 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 **Transport of Concentrated Species (tcs)** and **Heat Transfer in Fluids (ht)**.

4 In the table, clear the **Solve for** check box for **Reacting Flow 1 (nirf1)**.

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 **Turbulent Flow, k-ε (spf)** and **Heat Transfer in Fluids (ht)**.

Stationary 3

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 **Turbulent Flow, k-ε (spf)** and **Transport of Concentrated Species (tcs)**.

4 In the table, clear the **Solve for** check box for **Reacting Flow 1 (nirf1)**.

Stationary 4

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

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, click **Study 1**.

3 In the **Settings** window for **Study**, locate the **Study Settings** section.

4 Clear the **Generate default plots** check box.

5 In the **Study** toolbar, click **Compute**.

RESULTS

Sector 3D 1

1 In the **Model Builder** window, expand the **Results** node.

2 Right-click **Results>Datasets** and choose **More 3D Datasets>Sector 3D**.

3 In the **Settings** window for **Sector 3D**, locate the **Data** section.

4 From the **Dataset** list, choose **Study 1/Solution Store 3 (sol4)**.

5 Locate the **Axis Data** section. In row **Point 2**, set **x** to 1 and **z** to 0.

6 Locate the **Symmetry** section. In the **Number of sectors** text field, type 20.

7 From the **Transformation** list, choose **Rotation and reflection**.

8 Find the **Radial direction of reflection plane** subsection. In the **x** text field, type 0.

9 In the **z** text field, type 1.

10 Click **Plot**.

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

Cut Plane 1

1 In the **Results** toolbar, click **Cut Plane**.

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

3 From the **Dataset** list, choose **Sector 3D 1**.

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

5 Click **Plot**.

Cut Line 3D 1

1 In the **Results** toolbar, click **Cut Line 3D**.

2 In the **Settings** window for **Cut Line 3D**, locate the **Data** section.

3 From the **Dataset** list, choose **Sector 3D 1**.

4 Locate the **Line Data** section. In row **Point 2**, set **x** to `0.4`.

5 Click **Plot**.

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

Figure 2 is created with the following steps.

Velocity, xy-plane

1 In the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Velocity, xy-plane` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Sector 3D 1**.

Slice 1

1 Right-click **Velocity, xy-plane** and choose **Slice**.

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

3 From the **Plane** list, choose **xy-planes**.

4 In the **Planes** text field, type `1`.

5 In the **Velocity, xy-plane** toolbar, click **Plot**.

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

Figure 4 showing the monomer A concentration is reproduced in the following way.

Concentration, A

1 In the **Model Builder** window, right-click **Velocity, xy-plane** and choose **Duplicate**.

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

Slice 1

1 In the **Model Builder** window, expand the **Concentration, A** node, then click **Slice 1**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Transport of Concentrated Species>Species wA>tcs.c_wA - Molar concentration - mol/m³**.

3 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

Slice 2

1 Right-click **Results>Concentration, A>Slice 1** and choose **Duplicate**.

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 **zx-planes**.

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

6 Locate the **Coloring and Style** section. Select the **Color legend** check box.

7 In the **Concentration, A** toolbar, click **Plot**.

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

Figure 6 showing the polymer linkage L concentration is reproduced in the following way.

Concentration, L

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

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

Slice 1

1 In the **Model Builder** window, expand the **Concentration, L** node, then click **Slice 1**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Transport of Concentrated Species>Species wL>tcs.c_wL - Molar concentration - mol/m³**.

3 Locate the **Coloring and Style** section. Select the **Color legend** check box.

Slice 2

In the **Model Builder** window, right-click **Slice 2** and choose **Disable**.

Concentration, L

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

2 In the **Model Builder** window, click **Concentration, L**.

3 In the **Concentration, L** toolbar, click **Plot**.

Concentration, A

Figure 8 shows the temperature within the reactor and is created with these steps.

Temperature

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

2 In the **Settings** window for **3D Plot Group**, type `Temperature` in the **Label** text field.

Slice 1

1 In the **Model Builder** window, expand the **Temperature** node, then click **Slice 1**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Heat Transfer in Fluids>Temperature>T - Temperature - K**.

Slice 2

1 In the **Model Builder** window, click **Slice 2**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Heat Transfer in Fluids>Temperature>T - Temperature - K**.

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

4 In the **Temperature** toolbar, click  **Plot**.

Use a **1D Plot Group** to create Figure 7, showing the axial concentration distribution of L.

Concentration, L (axial)

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

2 In the **Settings** window for **1D Plot Group**, type `Concentration, L (axial)` in the **Label** text field.

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

Line Graph 1

1 Right-click **Concentration, L (axial)** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Transport of Concentrated Species>Species wL>tcs.c_wL - Molar concentration - mol/m³**.

3 Click to expand the **Coloring and Style** section. In the **Width** text field, type `2`.

4 In the **Concentration, L (axial)** toolbar, click  **Plot**.

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

Figure 3, showing the velocity field streamlines, can be reproduced using the following steps.

Velocity streamlines

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Velocity streamlines` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Sector 3D 1**.

Streamline 1

1 Right-click **Velocity streamlines** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

3 In the **Points** text field, type `150`.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Tube**.

5 In the **Tube radius expression** text field, type `tcs.c_wA+tcs.c_wB`.

Color Expression 1

1 Right-click **Streamline 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

3 In the **Expression** text field, type `tcs.c_wA+tcs.c_wB`.

4 In the **Velocity streamlines** toolbar, click **Plot**.

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

Adjust the view angle of the plot with the mouse.

Velocity streamlines

1 In the **Model Builder** window, under **Results** click **Velocity streamlines**.

2 In the **Velocity streamlines** toolbar, click **Plot**.

Figure 7 shows the isosurface concentration of L. Follow these step to create this figure.

Concentration, L (isosurface)

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Concentration, L (isosurface)` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Sector 3D 1**.

Isosurface 1

1 Right-click **Concentration, L (isosurface)** and choose **Isosurface**.

2 In the **Settings** window for **Isosurface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Transport of Concentrated Species>Species wL>tcs.c_wL - Molar concentration - mol/m³**.

3 Locate the **Levels** section. In the **Total levels** text field, type `8`.

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

5 In the **Concentration, L (isosurface)** toolbar, click  **Plot**.

Add a clip plane in order to visualize the solution inside the reactor. First add a separate view to be used in the current plot group only.

Concentration, L (isosurface)

1 In the **Model Builder** window, click **Concentration, L (isosurface)**.

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

3 From the **View** list, choose **New view**.

4 Clear the **Plot dataset edges** check box.

5 In the **Concentration, L (isosurface)** toolbar, click  **Plot**.

6 In the **Graphics** window toolbar, click ▾ next to  **Clipping**, then choose **Add Clip Plane**.

7 In the **Graphics** window toolbar, click ▾ next to  **Scene Light**, then choose **Ambient Occlusion**.

Use the mouse to hover over the frame outlining the clip plane. Right-clicking the frame displays a context menu with clip plane options.

8 From the clip plane context menu, select **Align to y-axis**.

9 From the clip plane context menu, select **Invert Clipping**.

Using the clip plane, the solution can be traversed by dragging the frame in the normal direction of the plane. The Gizmo can be used to interactively change the cut plane orientation.

For the time being, for a more tidy view, hide the Gizmo.

10 In the **Graphics** window toolbar, click ▾ next to  **Clipping Active**, then choose **Show Gizmos**.

Add transparency to the concentration isosurfaces. Also plot the exterior of the reactor to visualize the full geometry.

Transparency 1

1 In the **Model Builder** window, right-click **Isosurface 1** and choose **Transparency**.

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

3 In the **Transparency** text field, type `0.1`.

Surface 1

1 In the **Model Builder** window, right-click **Concentration, L (isosurface)** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

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

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

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

Transparency 1

1 Right-click **Surface 1** and choose **Transparency**.

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

3 In the **Transparency** text field, type `0.3`.

Filter 1

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

2 In the **Settings** window for **Filter**, locate the **Element Selection** section.

3 In the **Logical expression for inclusion** text field, type `(sqrt(y^2+z^2)>r_r*0.995)||(x<r_r*0.005)`.

4 In the **Concentration, L (isosurface)** toolbar, click  **Plot**.

5 Right-click **Filter 1** and choose **Copy**.

Filter 1

1 In the **Model Builder** window, right-click **Isosurface 1** and choose **Paste Filter**.

2 In the **Settings** window for **Filter**, locate the **Element Selection** section.

3 In the **Logical expression for inclusion** text field, type `(sqrt(y^2+z^2)<r_r*0.995)&&(x>r_r*0.005)`.

4 In the **Concentration, L (isosurface)** toolbar, click  **Plot**.

Appending — Geometry Modeling Instructions

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

2 Click **Done**.

GEOMETRY 1

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 `0.005`.

4 In the **Height** text field, type `0.06`.

5 Locate the **Position** section. In the **x** text field, type `0.01318`.

6 In the **z** text field, type `0.0205`.

7 Click **Build Selected**.

Rotate 1 (rot1)

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

2 Click the object to select it.

3 Select the object **cyl1** only.

4 In the **Settings** window for **Rotate**, locate the **Rotation** section.

5 In the **Angle** text field, type `-19.2`.

6 Locate the **Point on Axis of Rotation** section. In the **x** text field, type `0.01318`.

7 In the **z** text field, type `0.05`.

8 Locate the **Rotation** section. From the **Axis type** list, choose **y-axis**.

9 Click **Build Selected**.

Cylinder 2 (cyl2)

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 `0.005`.

4 In the **Height** text field, type `0.03`.

5 Locate the **Position** section. In the **x** text field, type `-0.03`.

6 In the **z** text field, type `0.036`.

7 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

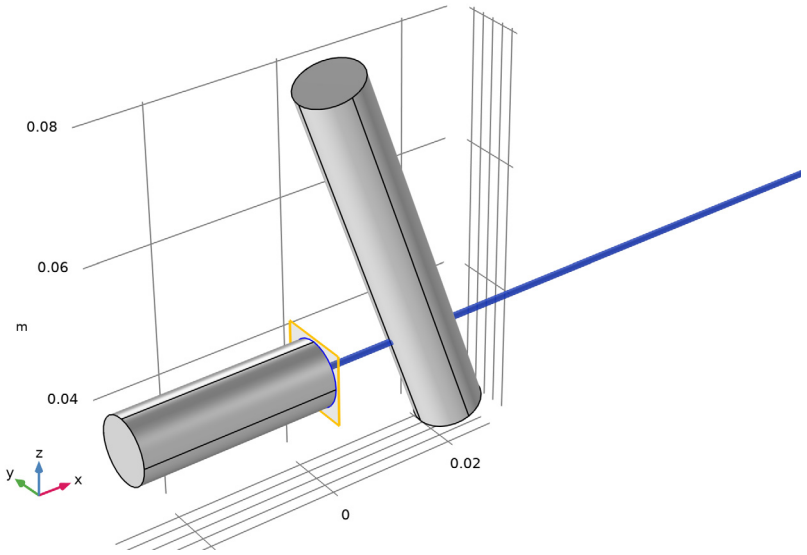
8 Click **Build Selected**.

Extrude 1 (ext1)

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

Select the far edge of the lying cylinder to add face 4 to the list.

2 On the object **cyl2**, select Boundary 4 only.



3 In the **Settings** window for **Extrude**, locate the **Distances** section.

4 In the table, enter the following settings:

Distances (m)
0.016

5 Click to expand the **Scales** section. In the table, enter the following settings:

Scales xw	Scales yw
.9	.9

The scales creates a slightly tapered cylinder section.

6 Click **Build Selected**.

Union 1 (uni1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

Now click both geometry parts to add them to the selection list.

2 Click in the **Graphics** window and then press Ctrl+A to select both objects.

3 In the **Settings** window for **Union**, locate the **Union** section.

4 Clear the **Keep interior boundaries** check box.

5 Click **Build Selected**.

Work Plane 1 (wp1)

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

2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.

3 From the **Plane** list, choose **zx-plane**.

Partition Objects 1 (par1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Partition Objects**.

2 Select the object **uni1** only.

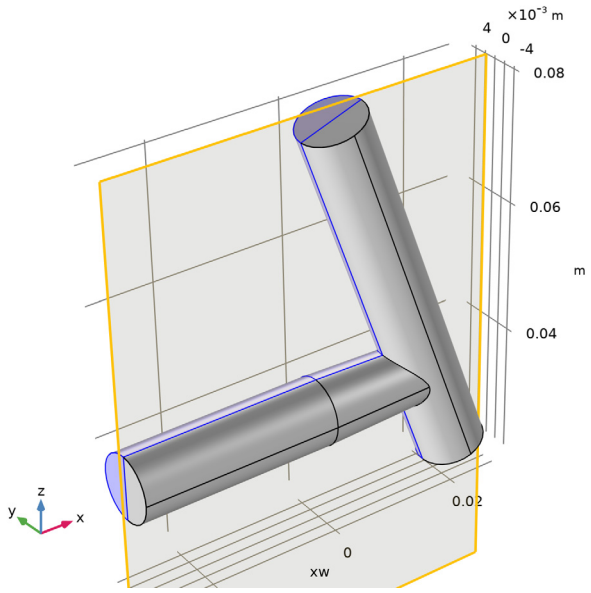
3 In the **Settings** window for **Partition Objects**, locate the **Partition Objects** section.

4 From the **Partition with** list, choose **Work plane**.

5 Click **Build Selected**.

6 In the **Graphics** window toolbar, click next to **Select Objects**, then choose **Select Domains**.

7 On the object **par1**, select Domain 2 only.



Delete Entities 1 (del1)

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

Work Plane 2 (wp2)

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

2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.

3 From the **Plane** list, choose **yz-plane**.

4 Click **Show Work Plane**.

Work Plane 2 (wp2)>Circle 1 (c1)

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

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

3 In the **Radius** text field, type `0.05`.

4 In the **Sector angle** text field, type `18`.

5 Locate the **Rotation Angle** section. In the **Rotation** text field, type `90`.

6 Click **Build Selected**.

Extrude 2 (ext2)

1 In the **Model Builder** window, under **Component 1 (comp1)>Geometry 1** right-click **Work Plane 2 (wp2)** and choose **Extrude**.

2 In the **Settings** window for **Extrude**, locate the **Distances** section.

3 In the table, enter the following settings:

Distances (m)
.1
.3

4 Click **Build Selected**.

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**.