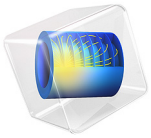


Model created in COMSOL Multiphysics 6.4

# 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 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.

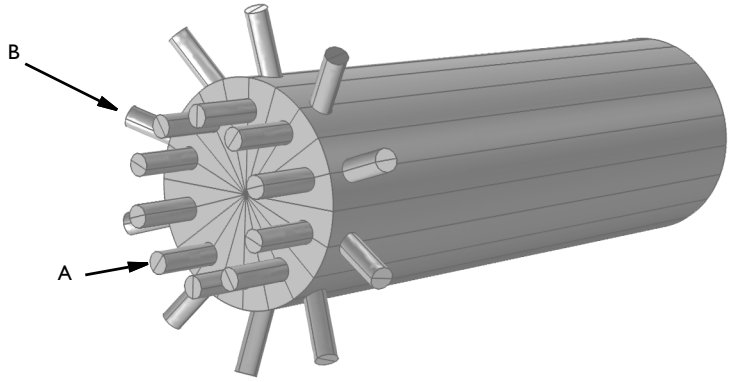



*Figure 1: Inlet section of a multijet tubular reactor. Monomer A (diol) enters through the axial inlets while monomer B (diacid) enters through the radial ports.*

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 $j$th 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 $\alpha$ AND $\beta$ |
|---|---|---|---|
| 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*

The polymerization reactions are first solved for using an ideal plug flow reactor model. This is performed using the *Reaction Engineering* interface, and produces the one dimensional development of the flow rates and temperature along the reactor.

To model the system in 3D, the *Generate Space-Dependent Model* feature, *Reaction Engineering* interface, is then used. A part from a 3D component, this also creates and a *Reacting Flow* multiphysics interface combining four physics interfaces. The *Chemistry*

interface implements the reaction kinetics, using the same reactions as in the plug flow model. The *Transport of Concentrated Species* interface and the *Heat Transfer in Fluids* interface solves for the mass transport and heat transfer respectively, including the mass sources and heat of reactions as defined by the *Chemistry* interface. The *Turbulent Flow k-ε* interface solves for the velocity, pressure, and turbulent mixing, used in the equations for mass transfer and the heat transfer. The *Reacting Flow* multiphysics node controls the coupling between the individual physics interfaces.

### STAGED SOLUTION

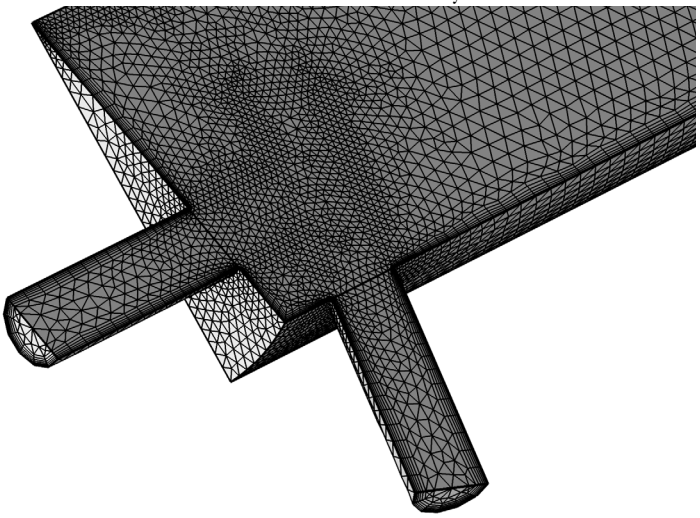
Since the chemical reactions are strongly dependent on the flow, the composition, and the temperature, the fully coupled system is often difficult to converge by starting from constant initial conditions. A faster and more robust solution procedure is to first solve for the velocity and pressure. And to use this as initial conditions, in a second step, to solve for the entire system.

### GEOMETRY

Due to symmetry, 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.



The results when solving for an ideal plug flow reactor of the same length as the 3D geometry are seen in Figure 2 below. As reactants are assumed fully mixed already when entering the reactor, the reactions go to completion over a small fraction of the reactor.

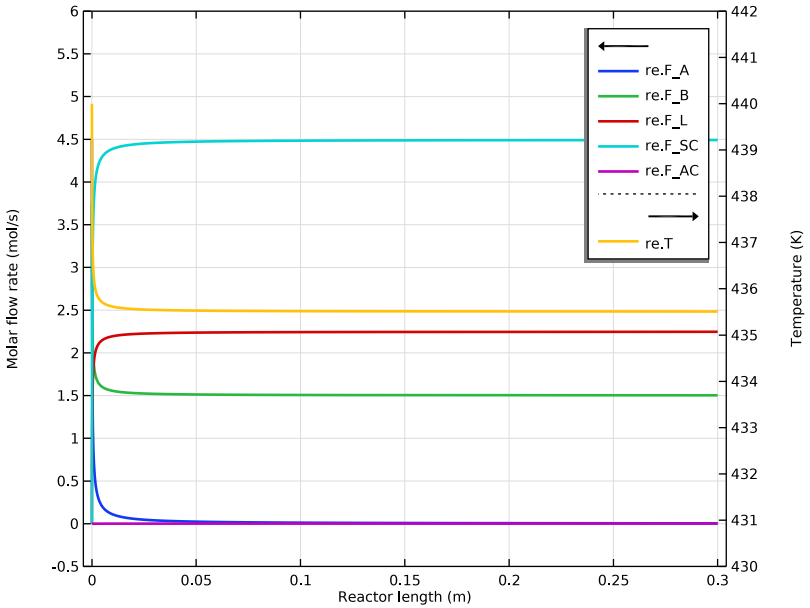



*Figure 2: Flow rates and temperature in an ideal plug flow reactor.*

In the 3D geometry the monomer reactants enter the reactor from different inlets and needs to be mixed before the reactions take place. Results from the 3D multijet tubular reactor model are shown below. Figure 3 shows the velocity field in a cut plane through the reactor. The figure indicates an intense mixing zone in the region were the axial and radial jets impinge. Plotting the streamlines of the velocity field Figure 4 provides more detailed information about the flow paths. Closer inspection at the entrance of the reactor reveals several recirculation zones.

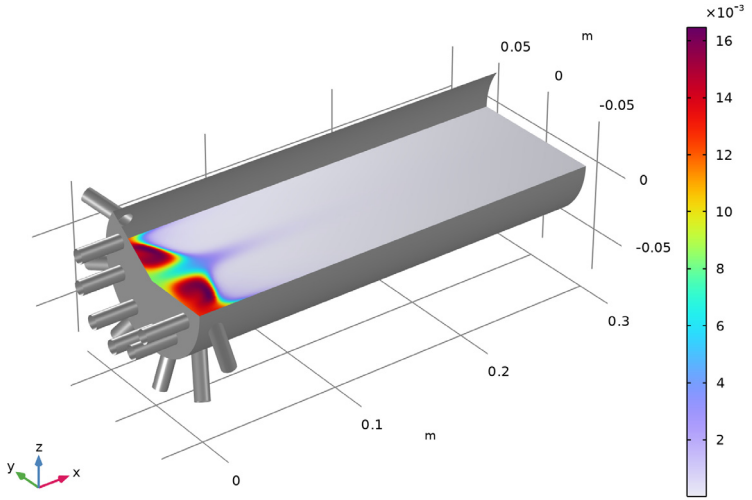



*Figure 3: Velocity field (m/s) in the multijet tubular reactor.*

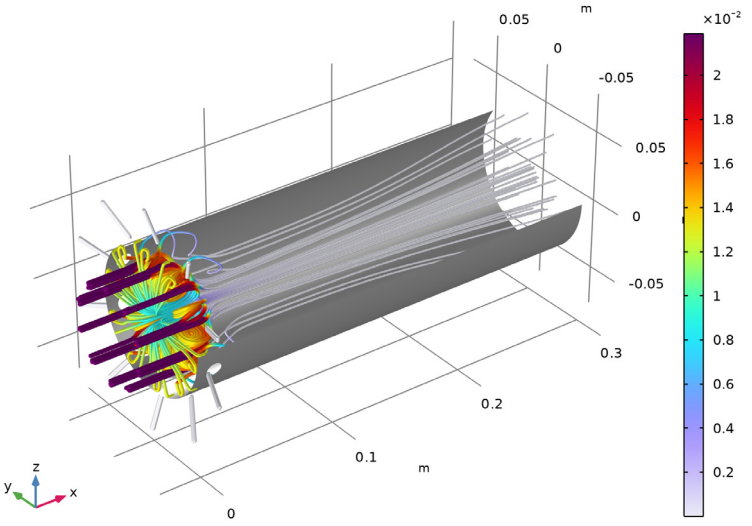



*Figure 4: Streamlines of the velocity field shows the recirculation zones near the inlet orifices. The concentration of reactants decrease rapidly at after the inlet stretch.*

The turbulent flow field transports and mixes the chemical species. Once monomer A comes into contact with the radial streams of monomer B, polymerization starts. Figure 5 shows the resulting concentration field of monomer A.

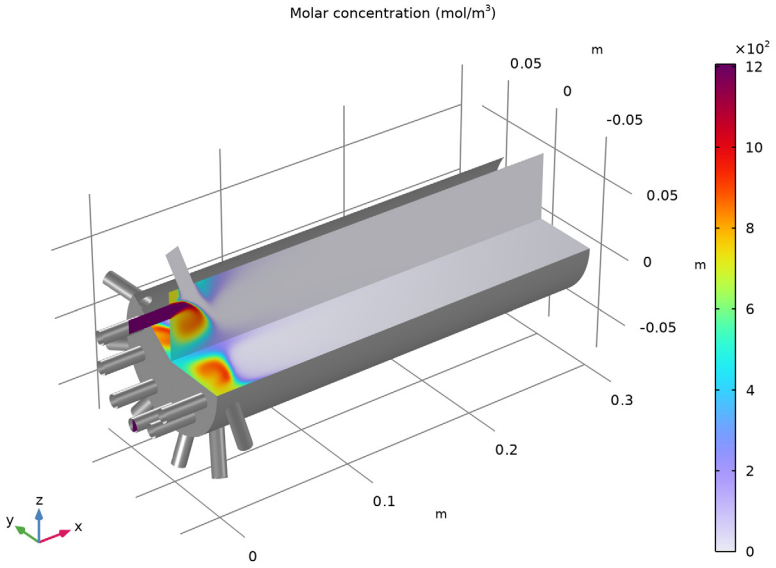



*Figure 5: Concentration distribution of monomer A ($mol/m^3$).*

Figure 6 shows isosurfaces of the polymer linkage L concentration. Concentrated isolevels clearly mark the positions of where the inlet streams meet. But isolevels are also present throughout the recirculation zones.

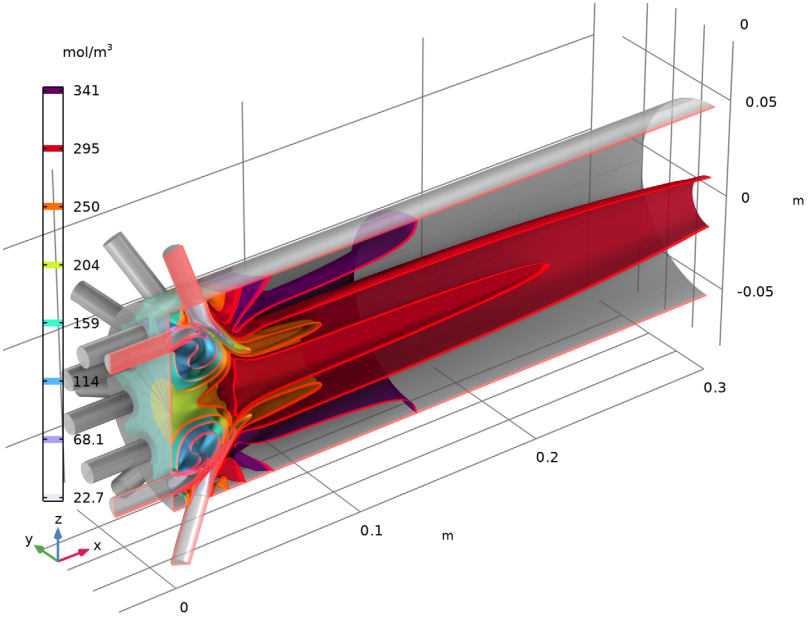



*Figure 6: Isosurfaces for the concentration of L (mol/m$^3$) visualized using a clip plane.*

As mentioned above, recirculation is evident in the entrance of the reactor. Recirculation will increase the effective residence time of the reactor. Figure 7 shows the concentration of polymer linkage, $c_L$, with a surface slice plot. 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.

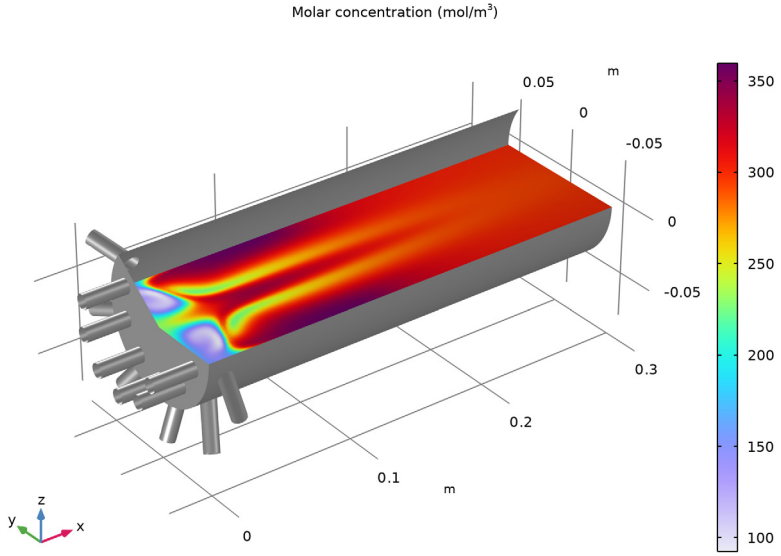



*Figure 7: Concentration distribution of polymer linkage, $c_L$ ($mol/m^3$).*

Figure 8 shows the axial development of the flow rates though the multijet tubular reactor. The flow rate of monomer B is initially zero since it is injected through radial inlets attached about 1.3 cm into the reactor. Following the injection, monomer B attains a maximum around 2 cm into the reactor. The other species evolve monotonically in the axial direction. It can be noted that the reaction zone in the 3D reactor is significantly longer compared to that in Figure 2 using the plug flow assumption.

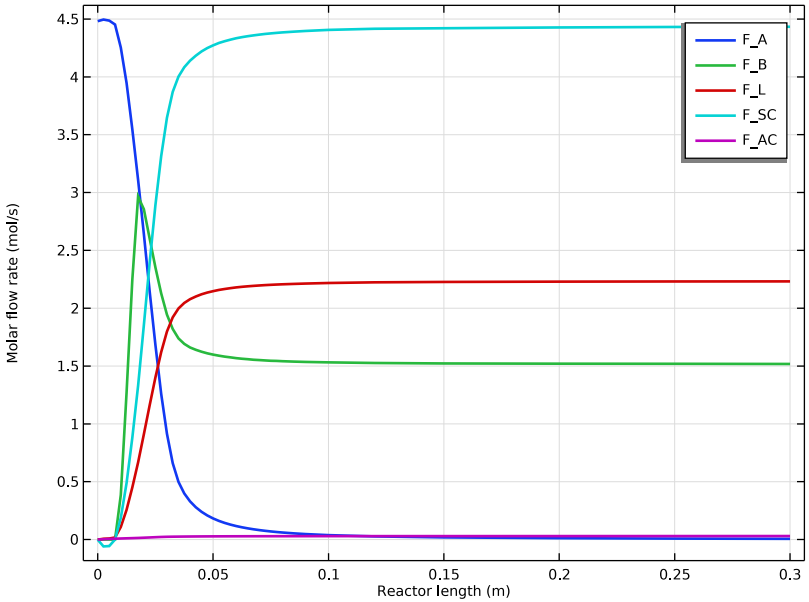



*Figure 8: Axial development of flow rates through the multijet tubular reactor.*

The total condensation chemistry is endothermic. Figure 9 displays the resulting temperature field in the reactor.

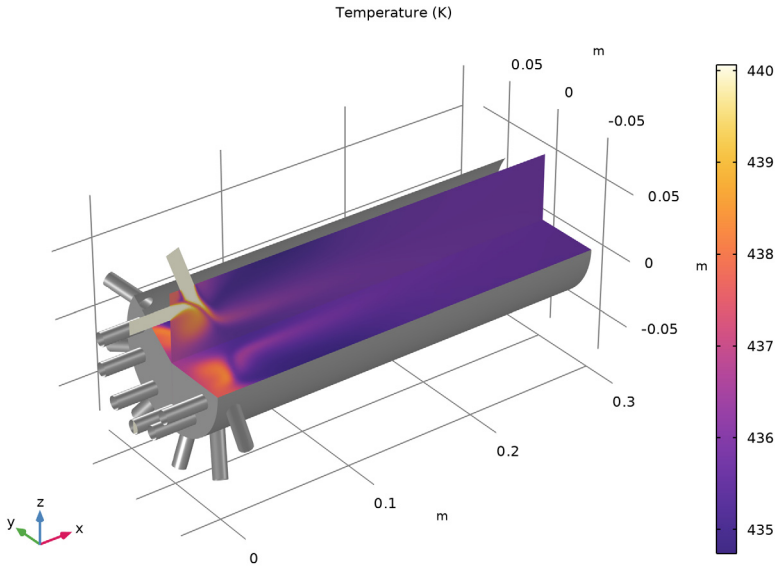



*Figure 9: Temperature distribution in the multijet tubular reactor. The inlet temperatures of radial and axial streams are 440 K.*

## *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. en.wikipedia.org/wiki/Polyester.

**Application Library path:** `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/polymerization_multijet`

## *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 **Preset Studies for Selected Physics Interfaces** > **Stationary Plug Flow**.

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 `polymerization_multijet_parameters.txt`.

### DEFINITIONS

*Variables 1*

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

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

3 In the table, enter the following settings:

| Name | Expression | Unit | Description |
|---|---|---|---|
| `r_len` | `re.Vr/A_r` | m | `Reactor length` |

### 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**, click to expand the **Equation** section.

3 Locate the **Reactor** section. From the **Reactor type** list, choose **Plug flow**.

4 Locate the **Energy Balance** section. From the **Energy balance** list, choose **Include**.

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

*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 `2 A + B + S => L + 2 SC`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** checkbox.

6 In the $A^{\mathrm{f}}$ text field, type `Af1`.

7 In the $E^{\mathrm{f}}$ text field, type `Ef1`.

8 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

9 In the $H$ text field, type `H1`.

*Species: A*

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

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

3 In the $M$ text field, type `MwA`.

4 Click to expand the **Thermodynamic Expressions** section. From the list, choose **User defined**.

*Species: B*

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

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

3 In the $M$ text field, type `MwB`.

4 Locate the **Thermodynamic Expressions** section. From the list, choose **User defined**.

*Species: S*

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

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

3 In the $M$ text field, type `MwS`.

4 In the ρ text field, type `rho_S`.

5 Locate the **Thermodynamic Expressions** section. From the list, choose **User defined**.

6 In the $C_p$ text field, type `Cp_S*MwS`.

*Species: L*

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

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

3 In the $M$ text field, type `MwL`.

4 Locate the **Thermodynamic Expressions** section. From the list, choose **User defined**.

*Species: SC*

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

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

3 In the $M$ text field, type `MwSC`.

4 Locate the **Thermodynamic Expressions** section. From the list, choose **User defined**.

*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 `A + SC <=> S + AC`.

4 Click **Apply**.

5 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** checkbox.

6 In the $A^{\mathrm{f}}$ text field, type `Af2`.

7 In the $E^{\mathrm{f}}$ text field, type `Ef2`.

8 In the $A^{\mathrm{r}}$ text field, type `Ar2`.

9 In the $E^{\mathrm{r}}$ text field, type `Er2`.

10 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

11 In the $H$ text field, type `H2`.

*Species: AC*

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

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

3 In the $M$ text field, type `MwAC`.

4 Locate the **Thermodynamic Expressions** section. From the 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 **General Parameters** section.

3 In the $T_{0,\text{in}}$ text field, type `T_in`.

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

| Species | Molar flow rate (mol/s) |
|---|---|
| A | `F_A_feed` |
| B | `F_B_feed` |
| S | `F_mass/MwS` |

## STUDY 1

### *Step 1: Stationary Plug Flow*

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary Plug Flow**.

2 In the **Settings** window for **Stationary Plug Flow**, locate the **Study Settings** section.

3 In the **Output volumes** text field, type `range(0,0.1,1)*V_r`.

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

Create a plot showing the flow rates and temperature in a plug flow reactor.

## RESULTS

### *Plug Flow: Flow Rate and Temperature*

1 In the **Settings** window for **1D Plot Group**, type `Plug Flow: Flow Rate and Temperature` in the **Label** text field.

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

3 Locate the **Plot Settings** section. In the **x-axis label** text field, type `Reactor length (m)`.

4 Select the **Two y-axes** checkbox.

5 Select the **Secondary y-axis label** checkbox. In the associated text field, type `Temperature (K)`.

### *Global 1*

1 In the **Model Builder** window, expand the **Plug Flow: Flow Rate and Temperature** node, then click **Global 1**.

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

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| | | |

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

5 In the **Expression** text field, type `r_len`.

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

*Plug Flow: Flow Rate and Temperature*

In the **Plug Flow: Flow Rate and Temperature** toolbar, click **Global**.

*T*

1 In the **Settings** window for **Global**, type `T` in the **Label** text field.

2 Locate the **y-Axis Data** section. Click **Clear Table**.

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `re.T` | `K` | `Temperature` |

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

5 In the **Expression** text field, type `r_len`.

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

*Plug Flow: Flow Rate and Temperature*

1 In the **Model Builder** window, click **Plug Flow: Flow Rate and Temperature**.

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

3 In the table, select the **Plot on secondary y-axis** checkbox for **T**.

4 Locate the **Axis** section. Select the **Manual axis limits** checkbox.

5 In the **y minimum** text field, type `-0.5`.

6 In the **y maximum** text field, type `6`.

7 In the **Secondary y minimum** text field, type `430`.

8 In the **Secondary y maximum** text field, type `442`.

9 In the **Plug Flow: Flow Rate and Temperature** toolbar, click **Plot**.

*Temperature (re)*

In the **Model Builder** window, right-click **Temperature (re)** and choose **Delete**.

## REACTION ENGINEERING (RE)

*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 **Chemical species transport** subsection. From the list, choose **Nonisothermal Reacting Flow: New**.

4 From the list, choose **Turbulent Flow**.

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

## GEOMETRY 1 (3D)

For the 3D model, start by building the geometry of the multijet reactor. 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 **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 `polymerization_multijet_geom_sequence.mph`.

4 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 Click to select the **Activate Selection** toggle button for **Domains to include**.

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

### TURBULENT FLOW, K-ε (SPF)

*Initial Values 1*

1 In the **Model Builder** window, expand the **Component 2 (comp2)** > **Turbulent Flow, k-ε (spf)** node, then 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 **Model Builder** window, click **Inlet 1**.

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 $U_{\text{av}}$ text field, type `5`.

*Outlet 1*

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

2 Select Boundary 11 only.

### CHEMISTRY (CHEM)

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

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

3 From the **Density** list, choose **User defined**.

4 In the ρ text field, type `rho_S`.

5 Click to expand the **Calculate Transport Properties** section. From the **Heat capacity** list, choose **User defined**.

6 In the $C_p$ text field, type `Cp_S`.

7 From the **Thermal conductivity** list, choose **User defined**.

8 In the $k$ text field, type `0.21+Cp_S*spf.muT/0.72`.

9 In the μ text field, type `0.001*(1.17817558982837+(-298[K]+T)/223[K])^(-3.758)[Pa*s]`.

### TRANSPORT OF CONCENTRATED SPECIES (TCS)

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

*Fluid 1*

1 In the **Model Builder** window, expand the **Transport of Concentrated Species (tcs)** node, then click **Fluid 1**.

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

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

4 Locate the **Diffusion** section. In the $D^{\mathrm{f}}_{\mathrm{wA}}$ text field, type `D`.

5 In the $D^{\mathrm{f}}_{\mathrm{wAC}}$ text field, type `D`.

6 In the $D^{\mathrm{f}}_{\mathrm{wB}}$ text field, type `D`.

7 In the $D^{\mathrm{f}}_{\mathrm{wL}}$ text field, type `D`.

8 In the $D^{\mathrm{f}}_{\mathrm{wS}}$ text field, type `D`.

9 In the $D^{\mathrm{f}}_{\mathrm{wSC}}$ 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 $\omega_{0,\mathrm{wA}}$ text field, type `1e-6`.

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

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

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

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

*Inflow 1*

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

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

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

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

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

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

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

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

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

*Outflow 1*

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

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 Sources 1*

1 In the **Model Builder** window, click **Reaction Sources 1**.

2 Select Domain 1 only.

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

4 From the **Chemistry** list, choose **Chemistry (chem)**.

5 Clear the **Mass transfer to other phases** checkbox.

## HEAT TRANSFER IN FLUIDS (HT)

*Initial Values 1*

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Heat Transfer in Fluids (ht)** 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 **Model Builder** window, click **Temperature 1**.

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 **Model Builder** window, click **Outflow 1**.

2 Select Boundary 11 only.

*Symmetry 1*

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

2 Select Boundaries 4 and 8 only.

## 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**.

When solving reacting flow problems it is often efficient to start by solving for the fluid flow only. This ensures good initial flow conditions when solving the full problem.

## 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 **Solve for** column of the table, under **Component 2 (comp2)**, clear the checkboxes for **Transport of Concentrated Species (tcs)** and **Heat Transfer in Fluids (ht)**.

4 In the **Solve for** column of the table, under **Component 2 (comp2)** > **Multiphysics**, clear the checkbox for **Reacting Flow 1 (nirf1)**.

*Step 2: Stationary 2*

In the **Study** toolbar, click **Stationary**.

*Solution 2 (sol2)*

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

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

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

4 Clear the **Generate default plots** checkbox.

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 2/Solution 2 (3) (sol2)**.

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**.

*Sector 3D 2*

1 Right-click **Sector 3D 1** and choose **Duplicate**.

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

3 From the **Sectors to include** list, choose **Manual**.

4 In the **Start sector** text field, type 5.

5 In the **Number of sectors to include** text field, type 12.

6 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 3 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**.

4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

*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 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prism**.

*Velocity, xy-Plane*

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

*Surface 1*

1 In the **Settings** window for **Surface**, locate the **Data** section.

2 From the **Dataset** list, choose **Sector 3D 2**.

*Selection 1*

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

2 Select Boundaries 2, 3, 6, 7, 9, and 10 only.

*Surface 1*

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

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

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

*Material Appearance 1*

1 Right-click **Surface 1** and choose **Material Appearance**.

2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.

3 From the **Appearance** list, choose **Custom**.

4 From the **Material type** list, choose **Steel (anodized)**.

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

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

Figure 5 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 2 (comp2)** > **Transport of Concentrated Species** > **Species wA** > **tcs.c_wA - Molar concentration - mol/m³**.

*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 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Slice 1**.

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 2 (comp2)** > **Transport of Concentrated Species** > **Species wL** > **tcs.c_wL - Molar concentration - mol/m³**.

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

*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 showing 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 2 (comp2)** > **Heat Transfer in Fluids** > **Temperature** > **T - Temperature - K**.

3 Locate the **Coloring and Style** section. From the **Color table** list, choose **HeatCameraLight**.

*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 2 (comp2)** > **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 8, showing the axial flow rates in the reactor. First create a **Cut Plane** dataset with cut planes perpendicular to axial direction.

*Cut Plane 2*

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

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

3 Select the **Additional parallel planes** checkbox.

4 In the **Distances** text field, type `range(0.0025,0.0025,0.08) 0.085 0.09 0.1 0.12 0.15 0.2 0.25 0.3`.

*Evaluation Group 1*

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

Create an **Evaluation Group** to compute the axial flow rates at the positions defined in the **Cut Plane**.

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

3 From the **Dataset** list, choose **Cut Plane 2**.

*Surface Average 1*

1 Right-click **Evaluation Group 1** and choose **Average** > **Surface Average**.

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

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `x` | `m` | `x-coordinate` |

4 Locate the **Multiple Surfaces** section. Select the **Evaluate each plane separately** checkbox.

*Evaluation Group 1*

In the **Evaluation Group 1** toolbar, click  **Integration** and choose **Surface Integration**.

*Surface Integration 1*

1 In the **Settings** window for **Surface Integration**, locate the **Multiple Surfaces** section.

2 Select the **Evaluate each plane separately** checkbox.

3 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 2 (comp2)** > **Transport of Concentrated Species** > **Species wA** > **Fluxes** > **Total flux - kg/(m²·s)** > **tcs.tflux_wAx - Total flux, x-component**.

4 Locate the **Expressions** section. In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `tcs.tflux_wAx/tcs.M_wA*nSectors*(sqrt(y^2+z^2)<r_r)` | `mol/s` | `F_A` |

5 Right-click **Surface Integration 1** and choose **Copy**.

*Surface Integration 2*

Right-click **Results** > **Evaluation Group 1** > **Surface Integration 1** and choose **Duplicate**.

Duplicate the node and edit the resulting nodes to compute the molar flow rates of the remaining species.

*Surface Integration 3*

Right-click **Surface Integration 1** and choose **Duplicate**.

*Surface Integration 4*

Right-click **Surface Integration 1** and choose **Duplicate**.

*Surface Integration 5*

Right-click **Surface Integration 1** and choose **Duplicate**.

*Surface Integration 2*

1 In the **Model Builder** window, click **Surface Integration 2**.

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

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `tcs.tflux_wBx/tcs.M_wB*nSectors*(sqrt(y^2+z^2)<r_r)` | `mol/s` | `F_B` |

*Surface Integration 3*

1 In the **Model Builder** window, click **Surface Integration 3**.

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

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| tcs.tflux_wLx/tcs.M_wL*nSectors*(sqrt(y^2+z^2)<r_r) | mol/s | F_L |

*Surface Integration 4*

1 In the **Model Builder** window, click **Surface Integration 4**.

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

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| nSectors*tcs.cflux_wSCx/tcs.M_wSC*(sqrt(y^2+z^2)<r_r) | mol/s | F_SC |

*Surface Integration 5*

1 In the **Model Builder** window, click **Surface Integration 5**.

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

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| nSectors*tcs.cflux_wACx/tcs.M_wAC*(sqrt(y^2+z^2)<r_r) | mol/s | F_AC |

*Evaluation Group 1*

1 In the **Model Builder** window, click **Evaluation Group 1**.

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

3 Select the **Transpose** checkbox.

4 Click to expand the **Format** section. From the **Concatenation** list, choose **Vertical**.

5 In the **Evaluation Group 1** toolbar, click = **Evaluate**.

Use the table data to plot the flow rates in a line graph.

### EVALUATION GROUP 1

1 Go to the **Evaluation Group 1** window.

2 Click the **Table Graph** button in the window toolbar.

## RESULTS

*Axial Flow Rates*

1 In the **Model Builder** window, under **Results** click **1D Plot Group 6**.

2 In the **Settings** window for **1D Plot Group**, type `Axial Flow Rates` in the **Label** text field.

*Table Graph 1*

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

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

3 From the **x-axis data** list, choose **Column 1**.

4 Click to expand the **Legends** section. Select the **Show legends** checkbox.

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

6 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

| Legends |
|---|
| F_A |
| F_B |
| F_L |
| F_SC |
| F_AC |

*Axial Flow Rates*

1 In the **Model Builder** window, click **Axial Flow Rates**.

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

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

4 Select the **y-axis label** checkbox. In the associated text field, type `Molar flow rate (mol/s)`.

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

*Velocity Streamlines*

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

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

5 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

6 Locate the **Color Legend** section. Select the **Show units** checkbox.

*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 `100`.

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 `sqrt(tcs.c_wA)+sqrt(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 **Coloring and Style** section.

3 From the **Color table** list, choose **Prism**.

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

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

*Velocity Streamlines*

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

*Surface 1*

1 In the **Settings** window for **Surface**, locate the **Data** section.

2 From the **Dataset** list, choose **Sector 3D 2**.

*Material Appearance 1*

1 Right-click **Surface 1** and choose **Material Appearance**.

2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.

3 From the **Appearance** list, choose **Custom**.

4 From the **Material type** list, choose **Steel (anodized)**.

*Selection 1*

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

2 Select Boundary 9 only.

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 **Results** toolbar, click **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**.

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

5 Locate the **Color Legend** section. Select the **Show units** checkbox.

*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 2 (comp2)** > **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 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prism**.

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

6 In the **Concentration, L (Isosurface)** toolbar, click **Plot**.

Add a clip plane 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** checkbox.

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 Right-click **Concentration, L (Isosurface)** and choose **Align to y-Axis**.

8 Right-click **Concentration, L (Isosurface)** and choose **Invert Clipping**.

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

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

10 From the gizmo context menu, select **Align to y-Axis**.

11 From the gizmo 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, hide the gizmo for a tidier view.

12 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 Find the **Transparency** subsection. 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 Find the **Transparency** subsection. 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**.

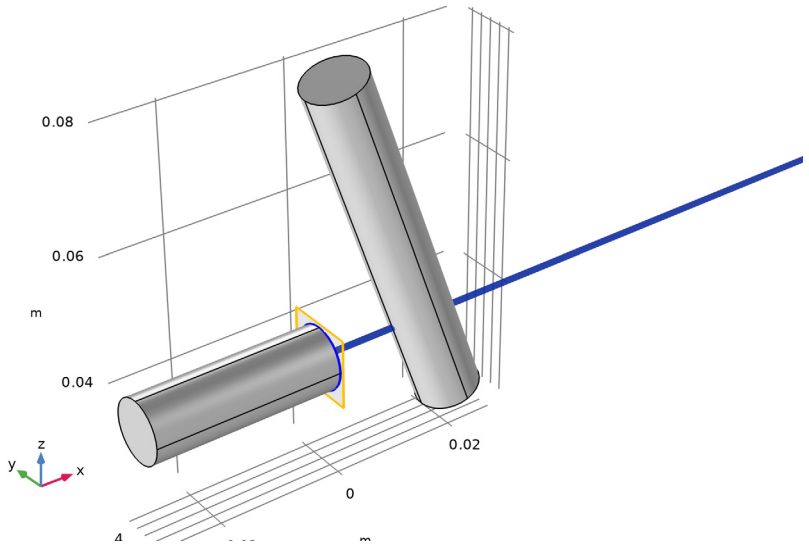
8 Click **Build Selected**.

*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** checkbox.

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.

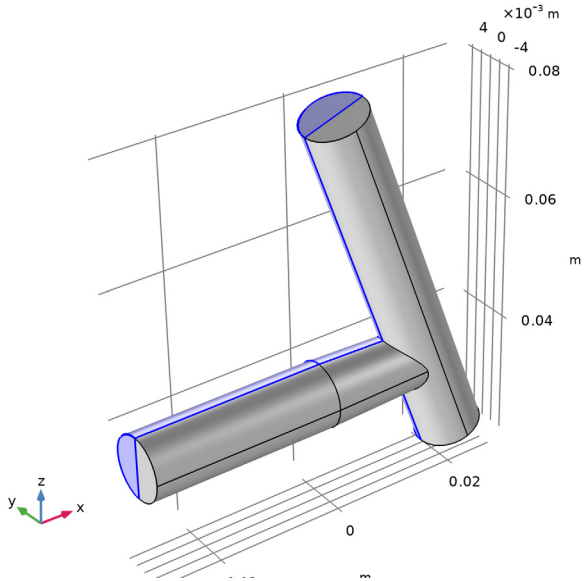
3 In the **Settings** window for **Partition Objects**, locate the **Partition Objects** section.

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 **Go to Plane Geometry**.

*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**.