Created in COMSOL Multiphysics 5.6

Fine Chemical Production in a Plate Reactor

Introduction

Plate reactors running under continuous conditions have emerged as candidates to replace batch reactors, primarily in fine chemicals and pharmaceuticals production. One of the advantages of the plate reactor design is that it allows for efficient temperature control of the reacting fluid. For instance, this means that the heat released from strongly exothermic reactions can be readily dissipated and more concentrated reaction mixtures can be run through the system. Plate reactors show promise to provide more energy-efficient production in a smaller package.

The model presented here shows you how to set up and solve the coupled flow, mass, and energy transport equations describing the reacting flow in a plate reactor.

Model Definition

A plate reactor is similar to a heat exchanger in design, where reactor plates and cooling/heating plates are stacked on top of one another. Figure 1 shows the winding interior of a reactor plate treated in the present model. Reactants enter the system through two inlet streams. Two heat exchange zones affect the outer boundaries.

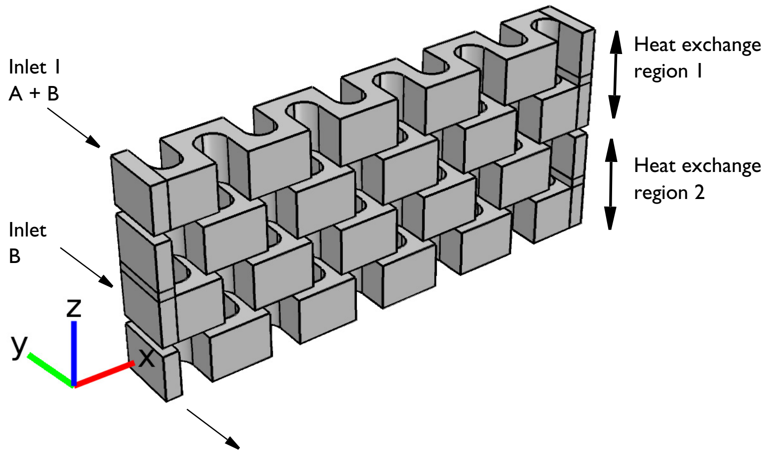

Figure 1: 3D geometry of a reactor plate. Two inlet streams are indicated as are the two heat exchange zones.

CHEMISTRY

Two exothermic chemical reactions take place in aqueous solution. The first reaction generates the desired product D. In the second reaction the desired product proceeds to react with B to generate the unwanted product U.

$$\mathrm{A} + \mathrm{B} \xrightarrow{k_1} \mathrm{D}$$

$$\mathrm{D} + \mathrm{B} \xrightarrow{k_2} \mathrm{U}$$

The reaction rates (mol/(m^3·s)) are given by:

$$r_1 = kc_Ac_B$$

$$r_2 = kc_Dc_B$$

where rate constants are temperature dependent according to the Arrhenius equation:

$$k = A\exp\left(-\frac{E}{R_g T}\right) \tag{1}$$

Both reactions are exothermic, and the rate of energy expelled is given by:

$$Q_j = r_j H_j \tag{2}$$

The Arrhenius parameters and heat of reaction are given below:

REACTION	FREQUENCY FACTOR	ACTIVATION ENERGY	HEAT OF REACTION
1	$1\cdot10^4$(m^3/mol/s)	$4\cdot10^4$ (J/mol)	$-1.1\cdot10^5$ (J/mol)
2	$1\cdot10^7$(m^3/mol/s)	$6\cdot10^4$ (J/mol)	$-1\cdot10^6$ (J/mol)

The higher activation energy of reaction 2 makes the reaction rate more temperature sensitive compared to reaction 1. As both reactions are exothermic there is a risk that elevated temperatures will make the second reaction dominant, producing the unwanted product U. From this point of view, it is important to dissipate the heat of the reaction in such a way that the temperature allows for reaction 1 to proceed at a reasonable rate while reaction 2 is inhibited. In the present model, the second half of the reactor exchanges heat with a cooling medium that is at a lower temperature compared to the first half.

MOMENTUM-, ENERGY-, AND MASS TRANSPORT

The model accounts for coupled momentum- , energy- , and mass transport within the plate reactor:

- The fluid flow (momentum transport) is described by the Navier-Stokes equations at steady state. This is set up with the Laminar Flow interface.
- The energy balance equation applied to the reactor domain considers heat transport through convection and conduction. This is modeled with the Heat Transfer in Fluids interface.
- The mass transfer in the reactor domain accounts for convection and diffusion. This is done with the Transport of Diluted Species interface.

The boundary conditions utilized in the three interfaces are listed in Table 1.

TABLE 1: BOUNDARY CONDITIONS FOR THE INTERFACES.

LOCATION	LAMINAR FLOW	HEAT TRANSFER IN FLUIDS	TRANSPORT OF DILUTED SPECIES
Inlet	Normal velocity, u_0	Temperature, T_0	Concentration, $c_{i,0}$
Outlet	Pressure, p_0	Outflow (only convective transport)	Outflow (only convective transport)
Walls	No slip	Heat exchange $-k\nabla T\cdot\mathbf{n} = h(T_x - T)$	No Flux

Results and Discussion

Figure 2 shows the streamlines of the fluid flow in the reactor plate. The color scale indicates the concentration of reactant A.

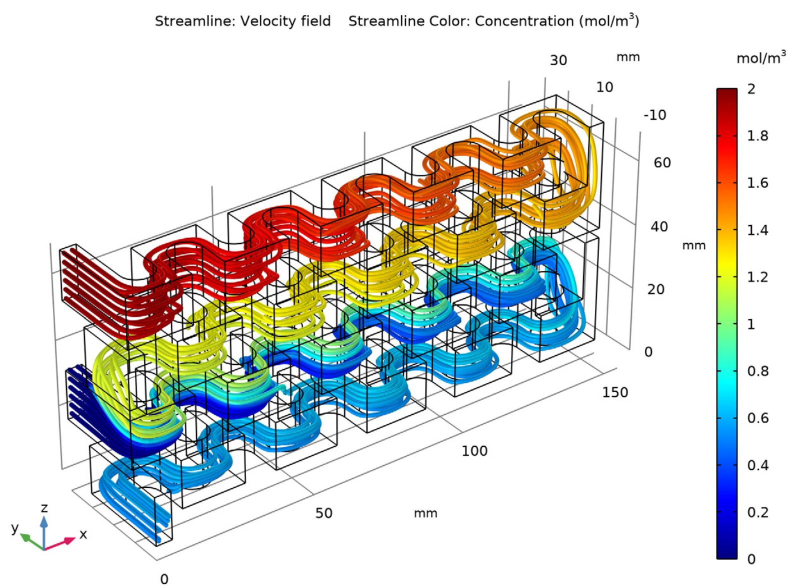

Figure 2: Streamlines of the fluid flow with the concentration of reactant A indicated by the color scale.

The isosurfaces for the concentration of reactant B are shown in Figure 3. The chemical reactions clearly consume the reactant along the entire reactor volume. The injection stream at the second inlet port mixes with the main stream, in effect making the distribution of B more uniform in the second part of the reactor.

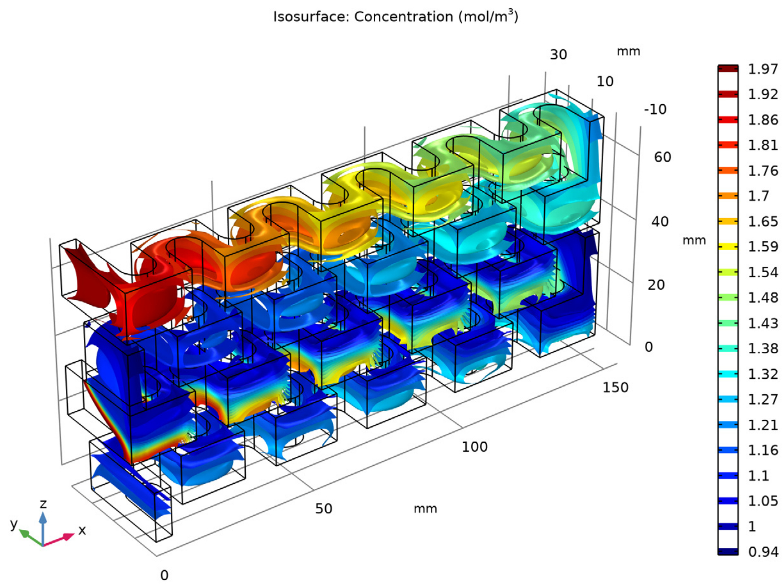

Figure 3: The concentration of reactant B (mol/m^3) across the reactor volume.

Figure 4 shows the temperature distribution, represented by horizontal and vertical cut planes.

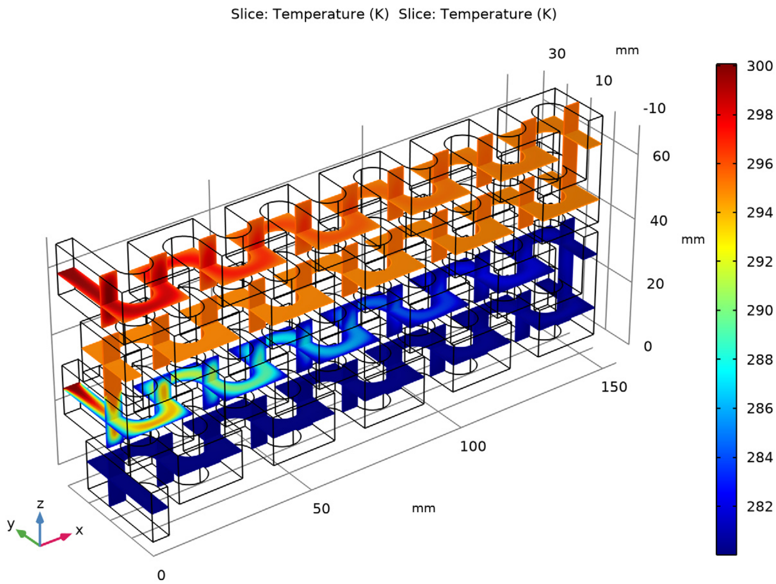

Figure 4: Temperature distribution in the reactor plate.

Heat expelled by the reactions is seen to be quenched by the cooling in all parts of the reactor.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/plate_reactor`

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

2 In the **Select Physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Chemical Species Transport>Chemistry (chem)**.

5 Click **Add**.

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

7 Click **Add**.

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

9 Click **Add**.

10 In the **Number of species** text field, type `4`.

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

cA
cB
cD
cU

12 Click **Study**.

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

14 Click **Done**.

GEOMETRY 1

Insert the geometry sequence.

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

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

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

GLOBAL DEFINITIONS

Load the model parameters from a text file.

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 `plate_reactor_parameters.txt`.

DEFINITIONS

Variables 1

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

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
Q_exch1	(T0-5-T)*hx	W/m²	Heat exchange flux
Q_exch2	(T0-20-T)*hx	W/m²	Heat exchange flux

ADD MATERIAL

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

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

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

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

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

LAMINAR FLOW (SPF)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

2 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.

3 From the **Compressibility** list, choose **Weakly compressible flow**.

Inlet 1

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

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

3 From the **Selection** list, choose **Inlet 1**.

4 Locate the **Boundary Condition** section. From the list, choose **Fully developed flow**.

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `U1`.

Inlet 2

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

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

3 From the **Selection** list, choose **Inlet 2**.

4 Locate the **Boundary Condition** section. From the list, choose **Fully developed flow**.

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `U2`.

CHEMISTRY (CHEM)

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

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

3 From the T list, choose **Temperature (ht)**.

Reaction 1

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

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

3 In the **Formula** text field, type `A+B=>D`.

4 Click **Apply**.

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

6 In the A^f text field, type `Af1`.

7 In the E^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`.

Reaction 2

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

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

3 In the **Formula** text field, type `D+B=>U`.

4 Click **Apply**.

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

6 In the A^f text field, type `Af2`.

7 In the E^f text field, type `Ef2`.

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

9 In the H text field, type `H2`.

Species 1

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

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

3 In the text field, type `H2O`.

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

5 In the **Settings** window for **Chemistry**, locate the **Species Matching** section.

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

Species	Species concentration type	Molar concentration (mol/m^3)
H2O	Free species	csolv

7 Click to expand the **Mixture Properties** section. From the **Phase** list, choose **Liquid**.

Species: A

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

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

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

Species: B

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

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

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

Species: D

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

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

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

Species: U

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

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

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

Species: H2O

1 In the **Model Builder** window, click **Species: H2O**.

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

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

LAMINAR FLOW (SPF)

In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

Outlet 1

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

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

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

Activate normal flow to model that the channel is continuous after the outlet.

4 Locate the **Pressure Conditions** section. Select the **Normal flow** check box.

HEAT TRANSFER IN FLUIDS (HT)

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>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 `T0`.

Heat Source 1

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

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

3 From the Q_0 list, choose **Heat source of reactions (chem)**.

4 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

Temperature 1

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

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

3 From the **Selection** list, choose **Inlet 1**.

4 Locate the **Temperature** section. In the T_0 text field, type `T0`.

Temperature 2

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

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

3 From the **Selection** list, choose **Inlet 2**.

4 Locate the **Temperature** section. In the T_0 text field, type `T0`.

Outflow 1

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

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

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

Heat Flux 1

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

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

3 From the **Selection** list, choose **Heat Exchanger 1**.

4 Locate the **Heat Flux** section. In the q_0 text field, type `Q_exch1`.

Heat Flux 2

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

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

3 From the **Selection** list, choose **Heat Exchanger 2**.

4 Locate the **Heat Flux** section. In the q_0 text field, type `Q_exch2`.

TRANSPORT OF DILUTED SPECIES (TDS)

Transport Properties 1

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

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

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

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

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

6 In the D_{cU} text field, type `D`.

Reactions 1

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

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

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

4 Locate the **Reaction Rates** section. From the R_{cA} list, choose **Reaction rate for species A (chem)**.

5 From the R_{cB} list, choose **Reaction rate for species B (chem)**.

6 From the R_{cD} list, choose **Reaction rate for species D (chem)**.

7 From the R_{cU} list, choose **Reaction rate for species U (chem)**.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.
2 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.
3 From the **Selection** list, choose **Inlet 1**.
4 Locate the **Concentration** section. In the $c_{0,\mathrm{cA}}$ text field, type cA1.
5 In the $c_{0,\mathrm{cB}}$ text field, type cB1.

Inflow 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.
2 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.
3 From the **Selection** list, choose **Inlet 2**.
4 Locate the **Concentration** section. In the $c_{0,\mathrm{cB}}$ text field, type cB2.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.
2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.
3 From the **Selection** list, choose **Outlet**.

MULTIPHYSICS

Couple all interfaces except the **Chemistry** node with the **Multiphysics** node.

Nonisothermal Flow 1 (nitf1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain>Nonisothermal Flow**.

Reacting Flow, Diluted Species 1 (rfd1)

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

MESH 1

Free Triangular 1

1 In the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.
2 Select Boundaries 10, 21, 219, and 242 only.

Size

1 In the **Model Builder** window, click **Size**.
2 In the **Settings** window for **Size**, locate the **Element Size** section.
3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `1`.

5 In the **Minimum element size** text field, type `0.5`.

6 In the **Resolution of narrow regions** text field, type `0.2`.

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 Domains 2, 3, 5, 6, 9–11, and 16–18 only.

5 Click **Build Selected**.

Free Triangular 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** right-click **Free Triangular 1** and choose **Duplicate**.

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

3 Click **Clear Selection**.

4 Select Boundaries 3, 17, 30, 217, 218, 224, 229, and 230 only.

5 Click **Build Selected**.

Swept 2

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

2 In the **Settings** window for **Swept**, click **Build All**.

STUDY 1

Stationary 2

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

Stationary 3

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

Step 1: Stationary

1 In the **Model Builder** window, 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 **Chemistry (chem)**, **Heat Transfer in Fluids (ht)**, and **Transport of Diluted Species (tds)**.

Step 2: Stationary 2

1 In the **Model Builder** window, click **Step 2: Stationary 2**.

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 **Laminar Flow (spf)** and **Heat Transfer in Fluids (ht)**.

Step 3: Stationary 3

1 In the **Model Builder** window, click **Step 3: Stationary 3**.

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 **Laminar Flow (spf)** and **Transport of Diluted Species (tds)**.

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

RESULTS

Velocity field

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 field` in the **Label** text field.

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

Streamline 1

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

2 Select Boundaries 23 and 24 only.

3 In the **Settings** window for **Streamline**, locate the **Coloring and Style** section.

4 Find the **Line style** subsection. From the **Type** list, choose **Tube**.

5 In the **Tube radius expression** text field, type `5e-4`.

6 Click the **Go to Default View** button in the **Graphics** toolbar.

Color Expression 1

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

2 In the **Settings** window for **Color Expression**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Transport of Diluted Species>Species cA>cA - Concentration - mol/m³**.

3 Click to expand the **Title** section. From the **Title type** list, choose **Automatic**.

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

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

3D Plot Group 14

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

Slice 1

1 Right-click **3D Plot Group 14** and choose **Slice**.

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

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

Temperature

1 In the **Model Builder** window, under **Results** click **3D Plot Group 14**.

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

Slice 2

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

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

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

As you can see, the two color legends are nearly aligned so a single legend is sufficient.

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

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

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

Concentration B

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 B` in the **Label** text field.

Isosurface 1

1 Right-click **Concentration B** 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 Diluted Species>Species cB>cB - Concentration - mol/m³**.

3 Locate the **Levels** section. In the **Total levels** text field, type `20`.

4 In the **Concentration B** toolbar, click **Plot**.

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