



Model created in COMSOL Multiphysics 6.4

Fine Chemical Production in a Plate Reactor

Introduction

Plate reactors operating under continuous conditions have potential to replace batch reactors, primarily in fine chemicals and pharmaceuticals production. An advantage 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 improve energy-efficiency at small scales.

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.

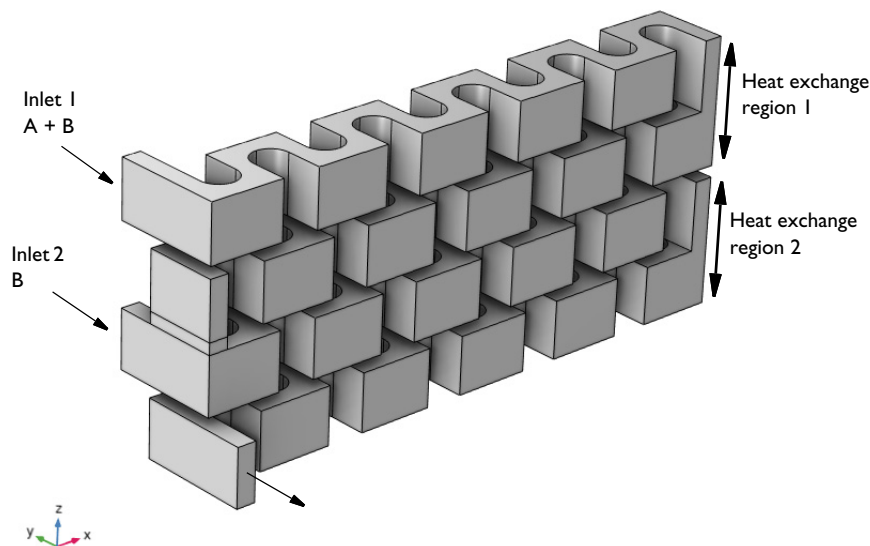
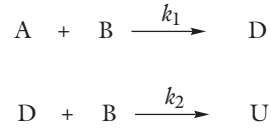


Figure 1: 3D geometry of a reactor plate. Two inlet streams are indicated as are the two heat exchange zones.

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.



The reaction rates ($\text{mol}/(\text{m}^3 \cdot \text{s})$) are given by:

$$r_1 = k_1 c_A c_B$$

$$r_2 = k_2 c_D c_B$$

where the rate constants for reaction j are temperature dependent according to the Arrhenius equation as follows:

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

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

$$Q_j = r_j H_j \quad (2)$$

The Arrhenius parameters and heat of reactions are summarized in [Table 1](#).

TABLE 1: ARRHENIUS PARAMETERS AND HEATS OF REACTIONS.

REACTION	FREQUENCY FACTOR	ACTIVATION ENERGY	HEAT OF REACTION
1	$1 \cdot 10^4 (\text{m}^3/\text{mol}\cdot\text{s})$	$4 \cdot 10^4 (\text{J}/\text{mol})$	$-1.1 \cdot 10^5 (\text{J}/\text{mol})$
2	$1 \cdot 10^7 (\text{m}^3/\text{mol}\cdot\text{s})$	$6 \cdot 10^4 (\text{J}/\text{mol})$	$-1 \cdot 10^6 (\text{J}/\text{mol})$

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 2](#).

TABLE 2: 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.

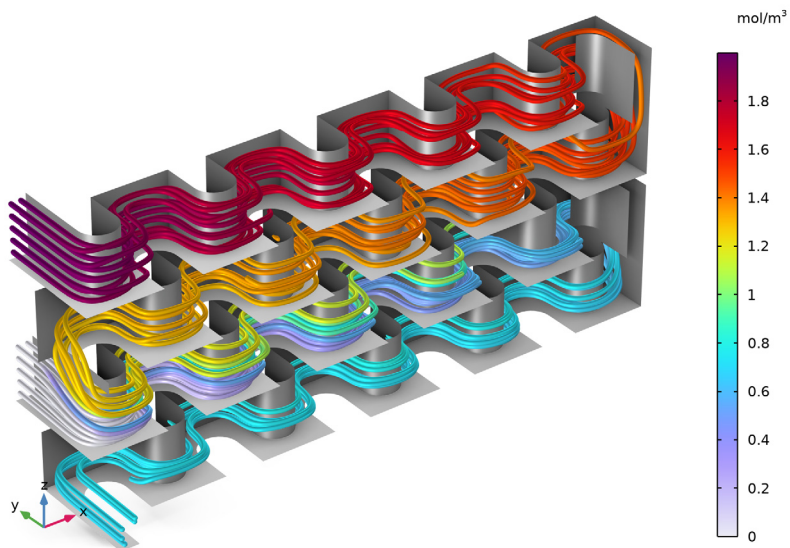


Figure 2: Streamlines of the fluid flow with the concentration of reactant A indicated by the color scale.

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.

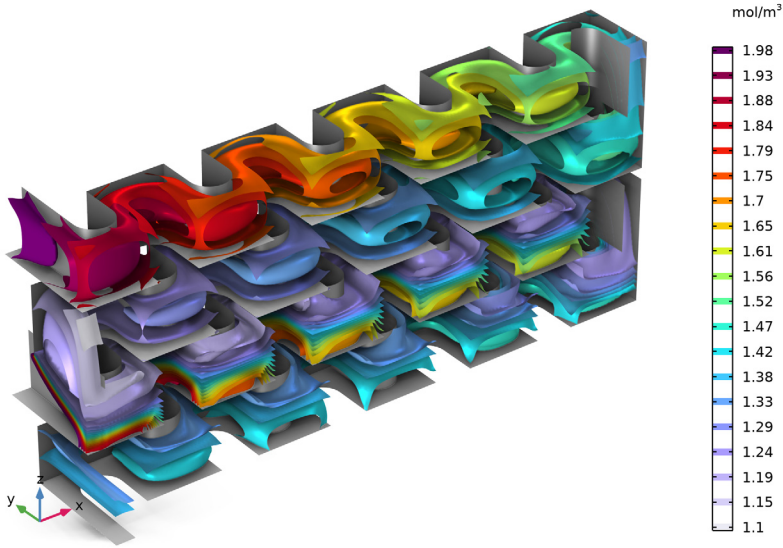


Figure 3: The concentration of reactant B (mol/m³) across the reactor volume.

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

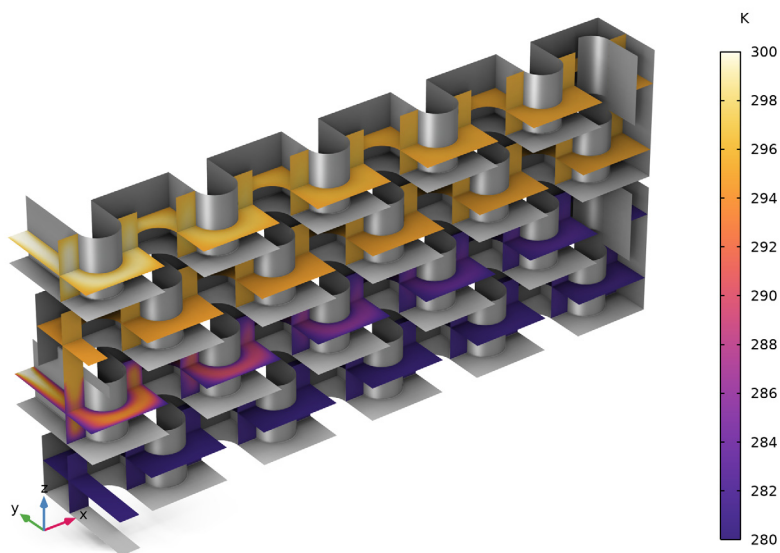


Figure 4: Temperature distribution in the reactor plate.


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 (mol/m³)** table, enter the following settings:


<u> </u>
cA
<u> </u>
cB
<u> </u>
cD
<u> </u>
cU

- 12 Click  **Study**.
- 13 In the **Select Study** tree, select **General Studies > Stationary**.
- 14 Click  **Done**.

GLOBAL DEFINITIONS


Load the model parameters from a text file.

Parameters I

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


GEOMETRY I

Insert the geometry sequence.

- 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 `plate_reactor_geom_sequence.mph`.
 - 3 In the **Geometry** toolbar, click  **Build All**.
Disable the analysis of the geometry as the remaining small geometric details can be kept.
 - 4 In the **Model Builder** window, click **Geometry I**.
 - 5 In the **Settings** window for **Geometry**, locate the **Cleanup** section.
 - 6 Clear the **Automatic detection of small details** checkbox.
- Add a selection which will be used later for visualizing the results.

DEFINITIONS

Cylinder 1

- 1 In the **Definitions** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, locate the **Geometric Entity Level** section.
- 3 From the **Level** list, choose **Boundary**.
- 4 Locate the **Size and Shape** section. In the **Outer radius** text field, type 3.
- 5 In the **Bottom distance** text field, type 0.1.
- 6 In the **Start angle** text field, type 90.
- 7 In the **End angle** text field, type 270.
- 8 Locate the **Position** section. In the **y** text field, type 20.
- 9 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.
- 10 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity intersects cylinder**.

Cylinder 2

- 1 Right-click **Cylinder 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Cylinder**, locate the **Position** section.
- 3 In the **z** text field, type 18.

Cylinder 3

- 1 Right-click **Cylinder 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Cylinder**, locate the **Position** section.
- 3 In the **x** text field, type 6.

4 In the **z** text field, type $18*2$.


Cylinder 4

- 1 Right-click **Cylinder 3** and choose **Duplicate**.
- 2 In the **Settings** window for **Cylinder**, locate the **Position** section.
- 3 In the **z** text field, type $18*3$.



Cylinder 5

- 1 Right-click **Cylinder 4** and choose **Duplicate**.
- 2 In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
- 3 In the **Outer radius** text field, type 0.5.
- 4 In the **Top distance** text field, type 10.
- 5 In the **Start angle** text field, type 1.
- 6 In the **End angle** text field, type 360.
- 7 Locate the **Position** section. In the **x** text field, type 1.
- 8 In the **z** text field, type $18*2-1$.

Explicit 1


- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundaries 29, 31–33, 47, 50, 52, 53, 68, 71–73, 87, 90, 92, 93, 108, 111–113, 127, 130, 132, 133, 148, 151–153, 167, 170, 172, 173, 188, 191–193, 207, and 210 only.

Wall selection

- 1 In the **Definitions** toolbar, click  **Union**.
- 2 In the **Settings** window for **Union**, type Wall selection in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Input Entities** section. Under **Selections to add**, click  **Add**.
- 5 In the **Add** dialog, in the **Selections to add** list, choose **Cylinder 1**, **Cylinder 2**, **Cylinder 3**, **Cylinder 4**, **Cylinder 5**, and **Explicit 1**.
- 6 Click **OK**.

ADD MATERIAL


- 1 In the **Materials** 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 the **Add to Component** button in the window toolbar.
- 5 In the **Materials** toolbar, click  **Add Material** to close the **Add Material** window.


LAMINAR FLOW (SPF)

Since the operating fluid is aqueous, the flow is assumed to be incompressible.


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.

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** checkbox.

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** checkbox.
- 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 $H1$.

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 Mn_A .


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 Mn_B .

Species: D

- 1 In the **Model Builder** window, click **Species: D**.
- 2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.
- 3 In the M text field, type Mn_D .

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** checkbox.
- 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: U

As for B, U does not correspond to uranium, but to the unwanted product. Therefore, it is necessary to clear the box in **Enable formula**.

- 1 In the **Model Builder** window, click **Species: U**.
- 2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.
- 3 Clear the **Enable formula** checkbox.
- 4 In the M text field, type Mn_U.

Species I

- 1 In the **Physics** toolbar, click  **Domains** and choose **Species**.
- 2 In the **Settings** window for **Species**, locate the **Name** section.
- 3 In the text field, type H2O.

Since H2O corresponds to water, the function **Enable formula** can be used, which provides you with the correct density and molecular weight for water.

- 4 Locate the **Chemical Formula** section. Select the **Enable formula** checkbox.
- 5 In the **Model Builder** window, click **Chemistry (chem)**.
- 6 In the **Settings** window for **Chemistry**, locate the **Species Matching** section.
- 7 Find the **Bulk species** subsection. From the **Species solved for** list, choose **Transport of Diluted Species**.
- 8 In the table, enter the following settings:

Species	Type	Molar concentration	Value (mol/m ³)
A	Variable	cA	Solved for
B	Variable	cB	Solved for
D	Variable	cD	Solved for
H2O	Free species	User defined	csolv
U	Variable	cU	Solved for

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


HEAT TRANSFER IN FLUIDS (HT)

Initial Values I


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

- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the T text field, type T_0 .

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 of reactions (chem)**.
- 4 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.


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 **Upstream Properties** section. In the T_{ustr} text field, type T_0 .


Inflow 2

- 1 Right-click **Inflow 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inlet 2**.


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. From the **Flux type** list, choose **Convective heat flux**.
- 5 In the h text field, type hx .
- 6 In the T_{ext} text field, type $T_0 - 5 [K]$.

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. From the **Flux type** list, choose **Convective heat flux**.
- 5 In the h text field, type hx .
- 6 In the T_{ext} text field, type $T0-20[\text{K}]$.

TRANSPORT OF DILUTED SPECIES (TDS)


Fluid 1

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Transport of Diluted Species (tds)** click **Fluid 1**.
- 2 In the **Settings** window for **Fluid**, 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 $c_{0,cA}$ text field, type $cA1$.
- 5 In the $c_{0,cB}$ 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 $c_{0,cB}$ 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  **More Generators** 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


Step 2: Stationary 2

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

Stationary - Laminar Flow


- 1 In the **Model Builder** window, click **Step 1: Stationary**.
- 2 In the **Settings** window for **Stationary**, type Stationary - Laminar Flow in the **Label** text field.
- 3 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkboxes for **Chemistry (chem)**, **Heat Transfer in Fluids (ht)**, and **Transport of Diluted Species (tds)**.
- 4 In the **Solve for** column of the table, under **Component 1 (comp1) > Multiphysics**, clear the checkbox for **Reacting Flow, Diluted Species 1 (rfd1)**.

Stationary - Heat and Mass Transfer


- 1 In the **Model Builder** window, under **Study 1** click **Step 2: Stationary 2**.
- 2 In the **Settings** window for **Stationary**, type Stationary - Heat and Mass Transfer in the **Label** text field.
- 3 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Laminar Flow (spf)**.
- 4 In the **Study** toolbar, click  **Compute**.

RESULTS

Velocity field

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type *Velocity* field in the **Label** text field.
- 3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.
- 4 Locate the **Color Legend** section. Select the **Show units** checkbox.

Streamline I

- 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 I

- 1 Right-click **Streamline I** 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 I (comp I) > Transport of Diluted Species > Species cA > cA - Molar concentration, cA - mol/m³**.
- 3 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prism**.

Velocity field

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

Surface I

- 1 In the **Settings** window for **Surface**, click to expand the **Title** section.
- 2 From the **Title type** list, choose **None**.




Material Appearance I

- 1 Right-click **Surface I** 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)**.


Surface 1

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

Selection 1

- 1 In the **Velocity field** toolbar, click  **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Wall selection**.
- 4 In the **Velocity field** toolbar, click  **Plot**.
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Temperature

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Temperature in the **Label** text field.
- 3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.
- 4 Locate the **Color Legend** section. Select the **Show units** checkbox.

Slice 1

- 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 **xy-planes**.
- 4 In the **Planes** text field, type 4.
- 5 Click to expand the **Range** section. Select the **Manual color range** checkbox.
- 6 In the **Minimum** text field, type 280.
- 7 In the **Maximum** text field, type 300.
- 8 Locate the **Coloring and Style** section. From the **Color table** list, choose **HeatCameraLight**.

Slice 2

- 1 In the **Model Builder** window, right-click **Temperature** and choose **Slice**.
- 2 In the **Settings** window for **Slice**, click to expand the **Title** section.
- 3 From the **Title type** list, choose **None**.
- 4 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**.
- 5 Locate the **Plane Data** section. From the **Plane** list, choose **zx-planes**.

- 6 In the **Planes** text field, type 1.
- 7 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Slice 1**.


Temperature

In the **Temperature** toolbar, click  **Surface**.

Surface 1

- 1 In the **Settings** window for **Surface**, click to expand the **Title** section.
- 2 From the **Title type** list, choose **None**.




Material Appearance 1

- 1 In the **Temperature** toolbar, click  **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)**.


Surface 1

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

Selection 1

- 1 In the **Temperature** toolbar, click  **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Wall selection**.
- 4 In the **Temperature** toolbar, click  **Plot**.
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Concentration B


- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Concentration B in the **Label** text field.
- 3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.
- 4 Locate the **Color Legend** section. Select the **Show units** checkbox.

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 - Molar concentration, cB - mol/m³**.
- 3 Locate the **Levels** section. In the **Total levels** text field, type 20.

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


Concentration B

In the **Concentration B** toolbar, click  **Surface**.

Surface 1

- 1 In the **Settings** window for **Surface**, click to expand the **Title** section.
- 2 From the **Title type** list, choose **None**.




Material Appearance 1

- 1 In the **Concentration B** toolbar, click  **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)**.

Surface 1

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

Selection 1

- 1 In the **Concentration B** toolbar, click  **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Wall selection**.
- 4 In the **Concentration B** toolbar, click  **Plot**.
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Improve the concentration surface plots.

Concentration, A, Surface (tds)

- 1 In the **Model Builder** window, under **Results** click **Concentration, A, Surface (tds)**.
- 2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.
- 3 Clear the **Plot dataset edges** checkbox.



Surface 1

- 1 In the **Model Builder** window, expand the **Concentration, A, Surface (tds)** node, then click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **Prism**.

Process the surface plots for species B, D, and U in the same manner.


Check the mass conservation using **Results Templates** for the mole balances.

RESULT TEMPLATES


- 1 In the **Results** toolbar, click  **Result Templates** to open the **Result Templates** window.
- 2 Go to the **Result Templates** window.
- 3 In the tree, select **Study 1/Solution 1 (sol1) > Transport of Diluted Species > Mole Balance, A (tds)**, **Study 1/Solution 1 (sol1) > Transport of Diluted Species > Mole Balance, B (tds)**, **Study 1/Solution 1 (sol1) > Transport of Diluted Species > Mole Balance, D (tds)**, and **Study 1/Solution 1 (sol1) > Transport of Diluted Species > Mole Balance, U (tds)**.
- 4 Click the **Add Result Template** button in the window toolbar.
- 5 In the **Results** toolbar, click  **Result Templates** to close the **Result Templates** window.

RESULTS


Mole Balance, A (tds)

- 1 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.
- 2 In the **Expression** text field, type $(-int4+int3)/int1$.
- 3 In the **Column header** text field, type Mole balance, relative error.
- 4 In the **Mole Balance, A (tds)** toolbar, click  **Evaluate**.

Mole Balance, B (tds)


- 1 In the **Model Builder** window, click **Mole Balance, B (tds)**.
- 2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.
- 3 In the **Expression** text field, type $(-int4+int3)/int1$.
- 4 In the **Column header** text field, type Mole balance, relative error.
- 5 In the **Mole Balance, B (tds)** toolbar, click  **Evaluate**.

Mole Balance, D (tds)

- 1 In the **Model Builder** window, click **Mole Balance, D (tds)**.
- 2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.
- 3 In the **Expression** text field, type $(-int4+int3)/int2$.
- 4 In the **Column header** text field, type Mole balance, relative error.
- 5 In the **Mole Balance, D (tds)** toolbar, click  **Evaluate**.

Mole Balance, U (tds)


- 1 In the **Model Builder** window, click **Mole Balance, U (tds)**.
- 2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.
- 3 In the **Expression** text field, type $(-int4+int3)/int2$.

- 4 In the **Column header** text field, type Mole balance, relative error.
- 5 In the **Mole Balance, U (tds)** toolbar, click  **Evaluate**.

Appendix — Geometry Modeling Instructions

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

NEW

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


ADD COMPONENT

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


GEOMETRY 1

- 1 In the **Settings** window for **Geometry**, locate the **Units** section.
- 2 From the **Length unit** list, choose **mm**.


Block 1 (blk1)

- 1 In the **Geometry** toolbar, click  **Block**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type 155.
- 4 In the **Depth** text field, type 20.
- 5 In the **Height** text field, type 15.

Block 2 (blk2)


- 1 In the **Geometry** toolbar, click  **Block**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type 10.
- 4 In the **Depth** text field, type 10.
- 5 In the **Height** text field, type 15.
- 6 Locate the **Position** section. In the **x** text field, type 5.

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 5.

- 4 In the **Height** text field, type 15.
- 5 Locate the **Position** section. In the **x** text field, type 10.
- 6 In the **y** text field, type 10.


Array 1 (arr1)

- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Array**.
- 2 Select the objects **blk2** and **cyll** only.
- 3 In the **Settings** window for **Array**, locate the **Size** section.
- 4 In the **x size** text field, type 5.
- 5 Locate the **Displacement** section. In the **x** text field, type 30.
- 6 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. Click **New**.
- 7 In the **New Cumulative Selection** dialog, type **Object to subtract** in the **Name** text field.
- 8 Click **OK**.

Mirror 1 (mir1)

- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Mirror**.
- 2 In the **Settings** window for **Mirror**, locate the **Input** section.
- 3 From the **Input objects** list, choose **Object to subtract**.
- 4 Select the **Keep input objects** checkbox.
- 5 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.
- 6 Locate the **Point on Plane of Reflection** section. In the **y** text field, type 10.
- 7 Locate the **Normal Vector to Plane of Reflection** section. In the **y** text field, type 1.
- 8 In the **z** text field, type 0.
- 9 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Object to subtract**.

Move 1 (mov1)

- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Move**.
- 2 In the **Settings** window for **Move**, locate the **Input** section.
- 3 From the **Input objects** list, choose **Mirror 1**.
- 4 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Object to subtract**.

5 Locate the **Displacement** section. In the **x** text field, type 15.

Difference 1 (dif1)

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

2 Select the object **blk1** only.

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

4 From the **Objects to subtract** list, choose **Object to subtract**.

Partition Domains 1 (pard1)

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

2 On the object **dif1**, select Domain 1 only.

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

4 From the **Partition with** list, choose **Extended faces**.

5 On the object **dif1**, select Boundaries 6 and 54 only.

6 In the tree, select **dif1**.

Block 3 (blk3)

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

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

3 In the **Width** text field, type 5.

4 In the **Depth** text field, type 20.

5 In the **Height** text field, type 3.

6 Locate the **Position** section. In the **x** text field, type 150.

7 In the **z** text field, type 15.

Array 2 (arr2)

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

2 Select the object **pard1** only.

3 In the **Settings** window for **Array**, locate the **Size** section.

4 In the **z size** text field, type 4.

5 Locate the **Displacement** section. In the **z** text field, type 18.


Mirror 2 (mir2)

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


2 Select the objects **arr2(1,1,2)** and **arr2(1,1,4)** only.

- 3 In the **Settings** window for **Mirror**, locate the **Point on Plane of Reflection** section.
- 4 In the **x** text field, type 77.5.
- 5 Locate the **Normal Vector to Plane of Reflection** section. In the **x** text field, type 1.
- 6 In the **z** text field, type 0.


Block 4 (blk4)

- 1 In the **Geometry** toolbar, click  **Block**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type 5.
- 4 In the **Depth** text field, type 20.
- 5 In the **Height** text field, type 3.
- 6 Locate the **Position** section. In the **x** text field, type 150.
- 7 In the **z** text field, type 51.

Block 5 (blk5)

- 1 In the **Geometry** toolbar, click  **Block**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type 5.
- 4 In the **Depth** text field, type 20.
- 5 In the **Height** text field, type 3.
- 6 Locate the **Position** section. In the **z** text field, type 33.

Extrude 1 (ext1)


- 1 In the **Geometry** toolbar, click  **Extrude**.
- 2 On the object **mir2(1)**, select Boundary 63 only.
- 3 On the object **mir2(2)**, select Boundary 63 only.
- 4 In the **Settings** window for **Extrude**, locate the **Distances** section.
- 5 In the table, enter the following settings:

Distances (mm)
10


- 6 Click  **Build Selected**.

Extrude 2 (ext2)


- 1 Right-click **Extrude 1 (ext1)** and choose **Duplicate**.

- 2 On the object **arr2(1,1,1)**, select Boundary 2 only.
- 3 In the **Settings** window for **Extrude**, 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**.


Inlet 1

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Explicit Selection**.
- 2 In the **Settings** window for **Explicit Selection**, type Inlet in the **Label** text field.
- 3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 On the object **fin**, select Boundary 35 only.
- 5 In the **Label** text field, type Inlet 1.


Inlet 2

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Explicit Selection**.
- 2 In the **Settings** window for **Explicit Selection**, type Inlet 2 in the **Label** text field.
- 3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 On the object **fin**, select Boundary 34 only.


Outlet

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Explicit Selection**.
- 2 In the **Settings** window for **Explicit Selection**, type Outlet in the **Label** text field.
- 3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 On the object **fin**, select Boundary 2 only.


Box Selection - Heat Exchanger 1

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Box Selection**.
- 2 In the **Settings** window for **Box Selection**, type Box Selection - Heat Exchanger 1 in the **Label** text field.
- 3 Locate the **Box Limits** section. In the **z minimum** text field, type 33.1.
- 4 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside box**.


Box Selection - Heat Exchanger 2

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Box Selection**.
- 2 In the **Settings** window for **Box Selection**, type Box Selection - Heat Exchanger 2 in the **Label** text field.
- 3 Locate the **Box Limits** section. In the **z maximum** text field, type 33.
- 4 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside box**.


Box Selection - Heat Exchanger Connection

- 1 Right-click **Box Selection - Heat Exchanger 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Box Selection**, type Box Selection - Heat Exchanger Connection in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Box Limits** section. In the **z minimum** text field, type 34.
- 5 In the **z maximum** text field, type 35.
- 6 Click  **Build Selected**.
- 7 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity intersects box**.


Adjacent Selection - Heat Exchanger 1

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Adjacent Selection**.
- 2 In the **Settings** window for **Adjacent Selection**, type Adjacent Selection - Heat Exchanger 1 in the **Label** text field.
- 3 Locate the **Input Entities** section. Click **+ Add**.
- 4 In the **Add** dialog, select **Box Selection - Heat Exchanger 1** in the **Input selections** list.
- 5 Click **OK**.


Adjacent Selection - Heat Exchanger 2

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Adjacent Selection**.
- 2 In the **Settings** window for **Adjacent Selection**, type Adjacent Selection - Heat Exchanger 2 in the **Label** text field.
- 3 Locate the **Input Entities** section. Click **+ Add**.
- 4 In the **Add** dialog, select **Box Selection - Heat Exchanger 2** in the **Input selections** list.
- 5 Click **OK**.


Heat Exchanger 1

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Difference Selection**.
- 2 In the **Settings** window for **Difference Selection**, type Heat Exchanger 1 in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Input Entities** section. Click the **+ Add** button for **Selections to add**.
- 5 In the **Add** dialog, select **Adjacent Selection - Heat Exchanger 1** in the **Selections to add** list.
- 6 Click **OK**.
- 7 In the **Settings** window for **Difference Selection**, locate the **Input Entities** section.
- 8 Click the **+ Add** button for **Selections to subtract**.
- 9 In the **Add** dialog, select **Inlet 1** in the **Selections to subtract** list.
- 10 Click **OK**.

Heat Exchanger 2

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Difference Selection**.
- 2 In the **Settings** window for **Difference Selection**, type Heat Exchanger 2 in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Input Entities** section. Click the **+ Add** button for **Selections to add**.
- 5 In the **Add** dialog, select **Adjacent Selection - Heat Exchanger 2** in the **Selections to add** list.
- 6 Click **OK**.
- 7 In the **Settings** window for **Difference Selection**, locate the **Input Entities** section.
- 8 Click the **+ Add** button for **Selections to subtract**.
- 9 In the **Add** dialog, in the **Selections to subtract** list, choose **Inlet 2** and **Outlet**.
- 10 Click **OK**.

Exterior Walls

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Union Selection**.
- 2 In the **Settings** window for **Union Selection**, type Exterior Walls in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Input Entities** section. Click **+ Add**.


5 In the **Add** dialog, in the **Selections to add** list, choose **Box Selection - Heat Exchanger Connection, Heat Exchanger 1**, and **Heat Exchanger 2**.

6 Click **OK**.

Interior boundaries Heat Exchanger 1

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

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

3 Click  **Add**.

4 In the **Add** dialog, select **Box Selection - Heat Exchanger 1** in the **Input selections** list.

5 Click **OK**.

6 In the **Settings** window for **Adjacent Selection**, locate the **Output Entities** section.

7 From the **Exterior boundaries** list, choose **None**.

8 Select the **Interior boundaries** checkbox.

9 In the **Label** text field, type Interior boundaries Heat Exchanger 1.

10 Click  **Build Selected**.

Interior boundaries Heat Exchanger 2

1 Right-click **Interior boundaries Heat Exchanger 1** and choose **Duplicate**.

2 In the **Settings** window for **Adjacent Selection**, type Interior boundaries Heat Exchanger 2 in the **Label** text field.

3 Locate the **Input Entities** section. In the **Input selections** list box, select **Box Selection - Heat Exchanger 1**.

4 Click  **Delete**.

5 Click  **Add**.

6 In the **Add** dialog, select **Box Selection - Heat Exchanger 2** in the **Input selections** list.

7 Click **OK**.

8 In the **Settings** window for **Adjacent Selection**, click  **Build Selected**.

All interior boundaries

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

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

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


4 In the **Label** text field, type All interior boundaries.

5 Locate the **Input Entities** section. Click  **Add**.

6 In the **Add** dialog, in the **Selections to add** list, choose **Interior boundaries Heat Exchanger 1** and **Interior boundaries Heat Exchanger 2**.

7 Click **OK**.

Mesh Control Faces 1 (mcf1)

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

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

3 From the **Faces to include** list, choose **All interior boundaries**.

4 Click  **Build Selected**.