Model created in COMSOL Multiphysics 6.4

Cross-Flow Mass Transfer in a Thin Domain

Introduction

This application shows how mass transfer out from a thin 3D domain can be approximated using a 2D component with the domain feature Out-of-Plane Flux. This feature is useful when the concentration gradient in the out-of-plane direction (along the thickness) is small, and decreasing the computational time is important.

In this example, the Transport of Concentrated Species and Laminar Flow physics interfaces are used to solve for the mass transfer and fluid flow. The Reacting Flow multiphysics coupling feature is used to couple the physical properties. The out-of-plane thickness, which is constant throughout the domain, is varied from 1 mm to 5 mm. As will be shown, by approximating the thin 3D component with a corresponding 2D component, the solution time decreases without a significant decrease in accuracy.

Model Definition

The geometry has a base rectangular shape with a side length 10 cm and width 5 cm. A symmetry feature is introduced to simplify the geometry and only model half of the channel width. The parametric sweep node solves for three different thicknesses, d_z, as follows: 1 mm, 2 mm, and 5 mm. Figure 1 below shows the geometry reduction from 3D to 2D.

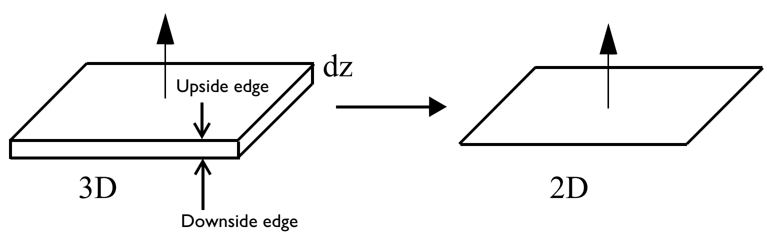

Figure 1: Model geometry reduction from 3D to 2D. The upward pointing arrows symbolize the normal of the flux from the domain. In this model there is only flux from the upper boundary into the domain. The upside and downside edges in 3D, for which concentration profiles are plotted in Figure 5 are indicated.

The Laminar Flow interface solves for the velocity and pressure within a gas as it flows through the thin domain. The flow inlet is defined on the thin boundary where $x = 0$ (3D), and on the corresponding edge in 2D. The gas is compose of three species A, B, and C, whose concentrations are solved for by the Transport of Concentrated Species interface. The total inward flux of species A is defined on the upside boundary of the thickness where

$z = d_z$ (3D), and on the entire domain in 2D. The stationary mass transfer equation for the 2D problem is defined as follows:

$$\nabla \cdot \mathbf{j}_i + \rho(\mathbf{u} \cdot \nabla)\omega_i = \frac{j_{0,\mathrm{u},i} + j_{0,\mathrm{d},i}}{d_\mathrm{z}},$$

where the left-hand side describes diffusion and convection, and the right-hand side is the out-of-plane source term, defined as the sum of the out-of-plane molar flux on the upside, $j_{0,\mathrm{u}}$, and on the downside, $j_{0,\mathrm{d}}$, divided by the out-of-plane thickness d_z. Since there is only flux through the upper boundary in this example, the 2D mass transfer equation simplifies as follows:

$$\nabla \cdot \mathbf{j}_i + \rho(\mathbf{u} \cdot \nabla)\omega_i = \frac{j_{0,\mathrm{u},i}}{d_z}.$$

Figure 2 and Figure 3 below show the concentrations of species A, B, and C for the 2D and 3D geometries respectively for a thickness of 2 mm.

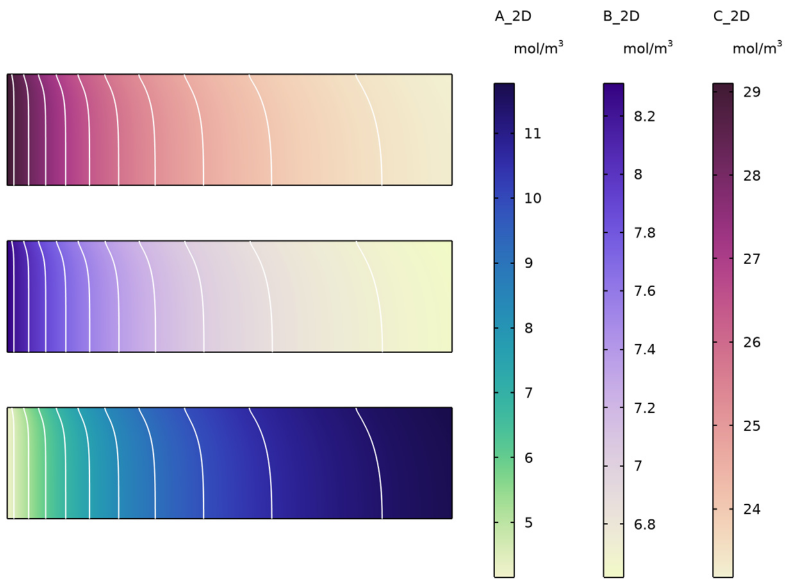

Figure 2: Concentration profiles (bottom to top: A, B, C) for 2D geometry for d_z *= 2 mm. Lines represent the contour plot.*

Figure 2 shows that the concentration of species A increases due to the incoming flux which therefore dilutes the concentrations of species B and C. The variation in the concentration close to the outer wall is due to the no-slip condition from the fluid flow.

Additionally, conservation of mass is calculated from the difference between the total flux across the boundary and the total flux across the surface. The absolute difference in mass is normalized with the inlet flux to calculate the relative error, which is below 0.35% for species A and 0.080% for species B. Only the conservation of species A and B are checked since the concentration of species C is not directly solved for and is instead obtained from a mass constraint specification.

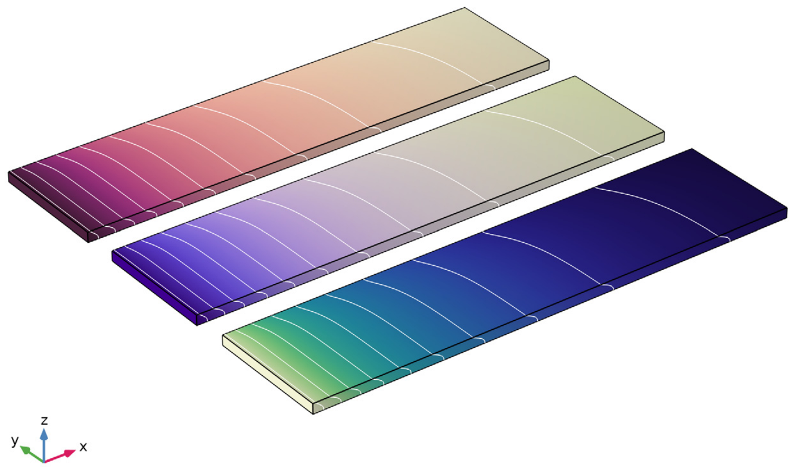

Figure 3: Concentration profiles (right to left: A, B, C) for 3D geometry for d_z = 2 mm. Lines represent the contour plot. Refer to Figure 2 *for the legend.*

Figure 3 shows the concentration profiles for the 3D component which are similar to the corresponding 2D profiles from Figure 2. In the 3D geometry there is variation in the z-direction concentration profile which can be seen for all three thicknesses for species A in Figure 4 below.

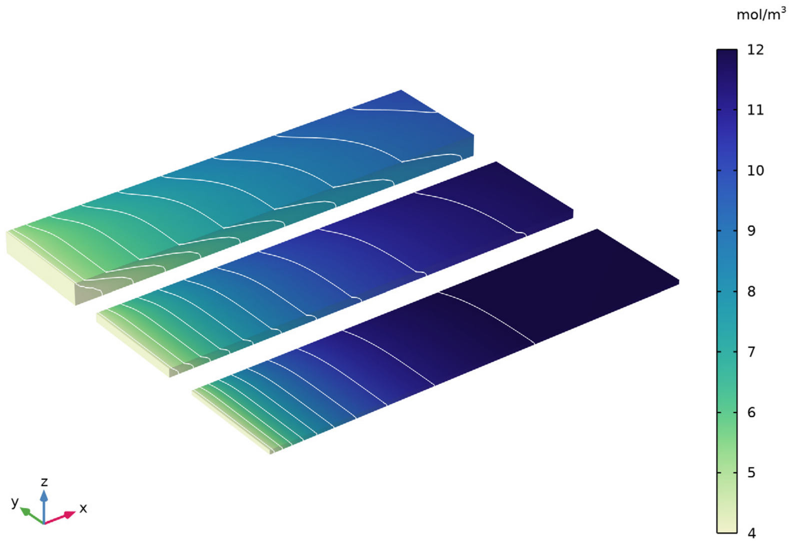

Figure 4: Concentration profile for species A for each thickness solved for (left to right: 5 mm, 2 mm, 1 mm). Lines represent the concentration contour plot.

Figure 4 shows that as the thickness increases, there is more variation in the concentration of species A between the upside and downside edges of the 3D component. This variation will affect the accuracy of the 2D approximation as seen in Figure 5, which shows the concentration profile of species A along the center of the channel for all thicknesses and dimensions. For the 3D component, the concentration along both the upside and the downside edges are plotted. The concentration profiles of the 2D approximation is consistent with the 3D results and is most accurate for the smallest thickness, where there is little variation between the upside and downside edge concentration profiles.

The computation time for the parametric sweep decreased from over 2 minutes to just seconds from the 3D to 2D components and the maximum relative error is just above 5% for the largest thickness. Therefore, this approximation is appropriate when the geometric and flow parameters ensure there is little variation in the concentration profile across the thickness and when saving computational time is important.

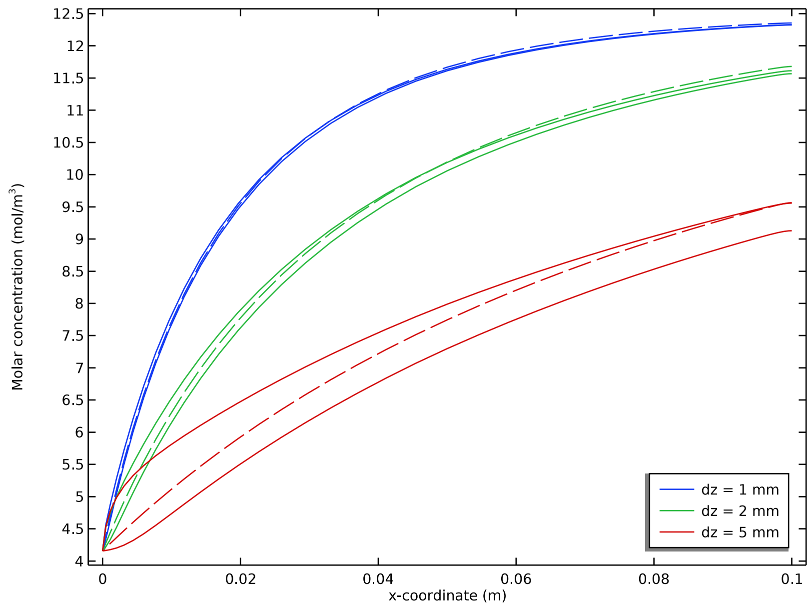

Figure 5: Concentration profiles of A along the center of channel in 2D and 3D, for all three thicknesses. Dashed lines represent the 2D approximation; Solid lines represent the 3D results along the upside and downside edges.

Application Library path: `Chemical_Reaction_Engineering_Module/Tutorials/thin_domain`

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 **2D**.

2 In the **Select Physics** tree, select **Chemical Species Transport** > **Transport of Concentrated Species (tcs)**.

3 Click **Add**.

4 In the **Number of species** text field, type 3.

5 In the **Mass fractions (1)** table, enter the following settings:

wA_2D
wB_2D
wC_2D

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

7 Click **Add**.

8 Click **Study**.

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

10 Click **Done**.

Start by adding some global parameters.

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 `thin_domain_parameters.txt`.

Build the geometry for the 2D component by using the added global parameters L and W. Since there is symmetry in the x direction, only half of the channel domain will be modeled and a symmetry feature will be introduced to save computational time.

GEOMETRY 1

Rectangle 1 (r1)

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

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

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

4 In the **Height** text field, type W/2.

5 Click **Build Selected**.

Either the ribbon or the context menu in the **Model Builder** can be used when setting up a model. To access the context menu, right-click the node that you want to modify in the **Model Builder**.

Next, set up the mass-transfer physics.

TRANSPORT OF CONCENTRATED SPECIES (TCS)

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

2 In the **Settings** window for **Transport of Concentrated Species**, locate the **Out-of-Plane Thickness** section.

3 In the d_z text field, type `dz`, one of the parameters in **Global Definitions**.

Tip: To access the list of global parameters (or other useful things), place the cursor in the text field, press Ctrl+Space, localize the parameter by expanding relevant nodes, and choose the parameter by double-clicking.

4 Locate the **Species** section. From the **From mass constraint** list, choose **wC_2D**.

Species Molar Masses 1

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

2 In the **Settings** window for **Species Molar Masses**, locate the **Molar Mass** section.

3 In the M_{wA2D} text field, type `MW`.

4 In the M_{wB2D} text field, type `MW`.

5 In the M_{wC2D} text field, type `MW`.

Next, introduce a symmetry feature to account for the reduced modeling domain.

Symmetry 1

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

2 Select Boundary 2 only.

Selecting boundaries can be done in several ways: either by clicking the boundary in the **Graphics** window or by using **Paste Selection**, located in the **Boundary Selection** section. A third way is to define an **Explicit** node (right-click **Definitions** in the Model Builder and choose **Explicit** under **Selections**), and select the explicit selection in the **Selection** list in the **Boundary Selection** section found in the **Concentration** settings window.

Inflow 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.
2. In the **Settings** window for **Inflow**, locate the **Inflow** section.
3. In the $\omega_{0,\mathrm{wA2D}}$ text field, type `wA_in`.
4. In the $\omega_{0,\mathrm{wB2D}}$ text field, type `wB_in`.
5. Select Boundary 1 only.

Outflow 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.
2. Select Boundary 4 only.

Out-of-Plane Flux 1

1. In the **Physics** toolbar, click **Domains** and choose **Out-of-Plane Flux**.
2. In the **Settings** window for **Out-of-Plane Flux**, locate the **Upside Inward Flux** section.
3. Select the **Species wA_2D** checkbox.
4. In the $j_{0,\mathrm{u},wA2D}$ text field, type `kcw*(wA_wall-wA_2D)`.
5. Select Domain 1 only.

Now set up the laminar flow interface with a **Use shallow channel approximation**; to account for out-of-plane thickness. Previously it was checked (not included in these modeling instructions) that the flow has a sufficiently low Reynolds number to be considered laminar for all three thicknesses that will be modeled.

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 **Compressible flow (Ma<0.3)**.
4. Select the **Use shallow channel approximation** checkbox.
5. In the d_z text field, type `dz`.

Fluid Properties 1

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Laminar Flow (spf)** click **Fluid Properties 1**.
2. In the **Settings** window for **Fluid Properties**, locate the **Fluid Properties** section.

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

There is no need to define the density now since it will be directly defined from the **Transport of Concentrated Species** physics interface when the **Multiphysics Coupling** is added.

Symmetry 1

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

2 Select Boundary 2 only.

Inlet 1

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

2 Select Boundary 1 only.

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

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

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `u0`.

Outlet 1

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

2 Select Boundary 4 only.

Just as a reminder, save the model from time to time.

MULTIPHYSICS

Reacting Flow 1 (nirf1)

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

Having set up the physics interfaces and coupled the relevant interacting physical properties together, now build a mesh.

MESH 1

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

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Modify the **User-controlled mesh**; by deleting three of the default nodes, and adding a **Mapped** node instead.

Corner Refinement 1, Free Triangular 1, Size 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1**, Ctrl-click to select **Size 1**, **Corner Refinement 1**, and **Free Triangular 1**.

2 Right-click and choose **Delete**.

Mapped 1

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

The order of the nodes is of importance so the Mapped node needs to be placed above the Boundary Layers node.

2 Drag and drop below **Size**.

Distribution 1

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

2 Select Boundaries 2 and 3 only, the two boundaries parallel to the x-axis, that is, in the direction of the incoming flow.

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

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

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

6 In the **Element ratio** text field, type 10.

7 Select the **Symmetric distribution** checkbox.

8 Click **Build Selected**.

Distribution 2

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

2 Select Boundaries 1 and 4 only, the two boundaries parallel to the y-axis.

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

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

5 In the **Number of elements** text field, type 20.

6 In the **Element ratio** text field, type 5.

7 Select the **Reverse direction** checkbox.

8 Click **Build Selected**.

Boundary Layer Properties 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Mesh 1** > **Boundary Layers 1** node, then click **Boundary Layer Properties 1**.

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

3 In the **Number of layers** text field, type 12.

4 In the **Thickness adjustment factor** text field, type 1.

Boundary Layers 1

1 In the **Model Builder** window, click **Boundary Layers 1**.

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

In this model the transition to the interior mesh is handled explicitly by using a mapped mesh. Disable the automatic functionality for producing a smooth transition between the boundary layer mesh and the interior mesh.

3 Clear the **Smooth transition to interior mesh** checkbox.

4 Click **Build Selected**.

The mesh setup is now complete. It is time to solve the model.

STUDY 1

Use a Parametric Sweep to solve for three different thicknesses dz.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
dz (Out-of-plane thickness)	1, 2, 5	mm

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

RESULTS

Clicking through the default plots gives a picture of the solved system. The velocity profile shows small gradients along the wall parallel to the x-axis due to the no slip boundary condition. The velocity increases slightly along the x-axis since due to the flux of species A. The concentration of species A increases along the x-axis as expected due to the inward flux which also results in a decreasing concentration of species B and C.

Follow the steps below to set up Figure 2 in the model documentation by replacing the default generated plots with another result template to show all three surfaces in the same graphic.

Concentration, A_2D (tcs), Concentration, B_2D (tcs), Concentration, C_2D (tcs)
Right-click and choose **Delete**.

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 Concentrated Species** > **Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)**.

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

Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)

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

2 From the **Parameter value (dz (mm))** list, choose **2**.

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

4 In the **Model Builder** window, expand the **Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)** node.

Total Flux, A_2D, Total Flux, B_2D, Total Flux, C_2D

1 In the **Model Builder** window, under **Results** > **Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)**, Ctrl-click to select **Total Flux, A_2D**, **Total Flux, B_2D**, and **Total Flux, C_2D**.

2 Right-click and choose **Delete**.

A_2D

Replace the default generated arrow lines with contours to better understand the variation in concentration on the surface.

Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)

In the **Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)** toolbar, click **Contour**.

A_2D Contour

1 In the **Settings** window for **Contour**, type `A_2D Contour` in the **Label** text field.

2 Locate the **Expression** section. In the **Expression** text field, type `tcs.c_wA_2D`.

3 Locate the **Levels** section. In the **Total levels** text field, type `10`.

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

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

6 Clear the **Color legend** checkbox.

7 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Repeat the same steps for species B and C.

Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)

In the **Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)** toolbar, click **Contour**.

B_2D Contour

1 In the **Settings** window for **Contour**, type `B_2D Contour` in the **Label** text field.

2 Locate the **Expression** section. In the **Expression** text field, type `tcs.c_wB_2D`.

3 Locate the **Levels** section. In the **Total levels** text field, type `10`.

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

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

6 Clear the **Color legend** checkbox.

7 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

8 In the **Index** text field, type `1`.

Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)

In the **Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)** toolbar, click **Contour**.

C_2D Contour

1 In the **Settings** window for **Contour**, type `C_2D Contour` in the **Label** text field.

2 Locate the **Expression** section. In the **Expression** text field, type `tcs.c_wC_2D`.

3 Locate the **Levels** section. In the **Total levels** text field, type `10`.

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

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

6 Clear the **Color legend** checkbox.

7 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

8 In the **Index** text field, type `2`.

Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)

1 In the **Model Builder** window, click **Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)**.

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

3 From the **Position** list, choose **Right**.

4 Click the **Show Grid** button in the **Graphics** toolbar.

5 In the **Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)** toolbar, click **Plot**.

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

A_2D, B_2D, C_2D

1 In the **Model Builder** window, under **Results > Plot array: Concentrations, A_2D, B_2D, C_2D (tcs)**, Ctrl-click to select **A_2D**, **B_2D**, and **C_2D**.

Next, plot the concentrations of species A, B, and C along the center of the channel.

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

Concentrations Along Center

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

2 Locate the **Data** section. From the **Parameter selection (dz)** list, choose **From list**.

3 In the **Parameter values (dz (mm))** list box, select **2**.

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

5 Locate the **Grid** section. Clear the **Show grid** checkbox.

A_2D

1 In the **Concentrations Along Center** toolbar, click **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `A_2D` in the **Label** text field.

3 Select Boundary 2 only.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `tcs.c_wA_2D`.

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

6 In the **Expression** text field, type `x`.

7 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

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

9 Find the **Include** subsection. Clear the **Solution** checkbox.

10 Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `A`.

Repeat the same steps for species B and C.

Concentrations Along Center

In the **Concentrations Along Center** toolbar, click **Line Graph**.

B_2D

1 In the **Settings** window for **Line Graph**, type `B_2D` in the **Label** text field.

2 Select Boundary 2 only.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `tcs.c_wB_2D`.

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

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

6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

7 Locate the **Legends** section. Select the **Show legends** checkbox.

8 Find the **Include** subsection. Clear the **Solution** checkbox.

9 Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `B`.

Concentrations Along Center

In the **Concentrations Along Center** toolbar, click **Line Graph**.

C_2D

1 In the **Settings** window for **Line Graph**, type `C_2D` in the **Label** text field.

2 Select Boundary 2 only.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `tcs.c_wC_2D`.

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

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

6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

7 Locate the **Legends** section. Select the **Show legends** checkbox.

8 Find the **Include** subsection. Clear the **Solution** checkbox.

9 Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `C`.

10 In the **Concentrations Along Center** toolbar, click **Plot**.

Check that mass is conserved using an evaluation group result template. Only species A and B are checked since the concentration of species C is calculated from the mass constraint.

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 Concentrated Species** > **Mass Balance, A_2D (tcs)** and **Study 1/Solution 1 (sol1)** > **Transport of Concentrated Species** > **Mass Balance, B_2D (tcs)**.

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.

This evaluation group template calculates the absolute change in mass for each species which should be a value near zero. However, it is often also useful to calculate the relative error which is done by normalizing the absolute change in mass by the defined inflow.

RESULTS

Mass Balance, A_2D (tcs)

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 `Relative Error`.

4 In the **Mass Balance, A_2D (tcs)** toolbar, click **Evaluate**.

Mass Balance, B_2D (tcs)

1 In the **Model Builder** window, click **Mass Balance, B_2D (tcs)**.

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 `Relative Error`.

5 In the **Mass Balance, B_2D (tcs)** toolbar, click **Evaluate**.

Next, introduce a new 3D component and compare the resulting concentration plots for the different space dimensions.

ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component** > **3D**.

GEOMETRY 2

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 `L`.

4 In the **Depth** text field, type `W/2`.

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

6 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**.

ADD PHYSICS

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

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

3 In the tree, select **Chemical Species Transport** > **Transport of Concentrated Species (tcs)**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkbox for **Study 1**.

5 Click the **Add to Component 2** button in the window toolbar.

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

7 In the table, clear the **Solve** checkbox for **Study 1**.

8 Click the **Add to Component 2** button in the window toolbar.

9 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

TRANSPORT OF CONCENTRATED SPECIES 2 (TCS2)

1 In the **Settings** window for **Transport of Concentrated Species**, click to expand the **Dependent Variables** section.

2 In the **Number of species** text field, type 3.

3 In the **Mass fractions (1)** table, enter the following settings:

wA_3D
wB_3D
wC_3D

4 Locate the **Species** section. From the **From mass constraint** list, choose **wC_3D**.

Species Molar Masses 1

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Transport of Concentrated Species 2 (tcs2)** click **Species Molar Masses 1**.

2 In the **Settings** window for **Species Molar Masses**, locate the **Molar Mass** section.

3 In the M_{wA3D} text field, type MW.

4 In the M_{wB3D} text field, type MW.

5 In the M_{wC3D} text field, type MW.

Symmetry 1

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

2 Select Boundary 2 only.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.
2 In the **Settings** window for **Inflow**, locate the **Inflow** section.
3 In the $\omega_{0,\mathrm{wA3D}}$ text field, type `wA_in`.
4 In the $\omega_{0,\mathrm{wB3D}}$ text field, type `wB_in`.
5 Select Boundary 1 only.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.
2 Select Boundary 6 only.

Flux 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Flux**.
2 Select Boundary 4 only.
3 In the **Settings** window for **Flux**, locate the **Mass Transfer to Other Phases** section.
4 Select the **Account for Stefan velocity** checkbox.
5 Locate the **Inward Flux** section. Select the **Species wA_3D** checkbox.
6 In the $j_{0,\mathrm{wA3D}}$ text field, type `kcw*(wA_wall-wA_3D)`.

LAMINAR FLOW 2 (SPF2)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Laminar Flow 2 (spf2)**.
2 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.
3 From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

Fluid Properties 1

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Laminar Flow 2 (spf2)** click **Fluid Properties 1**.
2 In the **Settings** window for **Fluid Properties**, locate the **Fluid Properties** section.
3 From the μ list, choose **User defined**. In the associated text field, type `visc`.

Symmetry 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Symmetry**.
2 Select Boundary 2 only.

Inlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.
2 In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.

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

4 Locate the **Fully Developed Flow** section. In the U_{av} text field, type u0.

5 Select Boundary 1 only.

Outlet 1

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

2 In the **Settings** window for **Outlet**, locate the **Pressure Conditions** section.

3 Select the **Normal flow** checkbox.

4 Select Boundary 6 only.

ADD PHYSICS

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

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

3 In the **Physics** toolbar, click **Add Physics** to close the **Add Physics** window.

Reacting Flow 2 (nirf2)

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

Continue by setting up the mesh. Use the same procedure as for the 2D component.

MESH 2

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

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Corner Refinement 1, Free Tetrahedral 1, Size 1, Size 2

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Mesh 2**, Ctrl-click to select **Size 1**, **Size 2**, **Corner Refinement 1**, and **Free Tetrahedral 1**.

2 Right-click and choose **Delete**.

Mapped 1

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

2 Drag and drop below **Size**.

Distribution 1

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

2 Select Edges 5 and 8 only.

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

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

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

6 In the **Element ratio** text field, type 10.

7 Select the **Symmetric distribution** checkbox.

8 Click **Build Selected**.

Mapped 1

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

2 Select Boundary 4 only.

Distribution 2

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Mesh 2** > **Mapped 1** right-click **Distribution 1** and choose **Duplicate**.

2 Select Edges 4 and 11 only.

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

4 In the **Number of elements** text field, type 20.

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

6 Clear the **Symmetric distribution** checkbox.

7 Click **Build Selected**.

Now add a swept mesh to mesh the thickness of the domain.

Swept 1

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

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 6.

5 In the **Element ratio** text field, type 2.

6 Select the **Symmetric distribution** checkbox.

Boundary Layers 1

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Mesh 2** click **Boundary Layers 1**.

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

3 From the **Geometric entity level** list, choose **Entire geometry**.

Boundary Layer Properties 1

1 In the **Model Builder** window, expand the **Boundary Layers 1** node, then click **Boundary Layer Properties 1**.

2 In the **Settings** window for **Boundary Layer Properties**, locate the **Geometric Entity Selection** section.

3 Click **Clear Selection**.

4 Select Boundary 2 only.

Boundary Layers 1

1 In the **Model Builder** window, click **Boundary Layers 1**.

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

3 Clear the **Smooth transition to interior mesh** checkbox.

4 Click **Build All**.

The physics interfaces and the mesh are all done for the 3D component. Now add a study and solve the model.

ADD STUDY

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

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

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkboxes for **Transport of Concentrated Species (tcs)** and **Laminar Flow (spf)**.

4 Find the **Multiphysics couplings in study** subsection. In the table, clear the **Solve** checkbox for **Reacting Flow 1 (nirf1)**.

5 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies** > **Stationary**.

6 Click the **Add Study** button in the window toolbar.

7 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
dz (Out-of-plane thickness)	`1, 2, 5`	`mm`

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

RESULTS

Looking at the default plots for the 3D component, it is clear that they are quite similar to the corresponding 2D plots. Optionally, edit the default plots.

Surface

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

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

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

4 From the **Color table transformation** list, choose **Reverse**.

Surface 1

1 In the **Model Builder** window, expand the **Results** > **Pressure (spf)** 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 **Agama**.

Multislice 1

1 In the **Model Builder** window, expand the **Velocity (spf2)** node, then click **Multislice 1**.

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

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

4 From the **Color table transformation** list, choose **Reverse**.

Surface

1 In the **Model Builder** window, expand the **Pressure (spf2)** node, then click **Surface**.

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

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

Follow the steps below to set up Figure 3 in the model documentation.

Concentration, A_3D, Streamline (tcs2), Concentration, A_3D, Surface (tcs2), Concentration, B_3D, Streamline (tcs2), Concentration, B_3D, Surface (tcs2), Concentration, C_3D, Streamline (tcs2), Concentration, C_3D, Surface (tcs2)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Concentration, A_3D, Streamline (tcs2)**, **Concentration, A_3D, Surface (tcs2)**, **Concentration, B_3D, Streamline (tcs2)**, **Concentration, B_3D, Surface (tcs2)**, **Concentration, C_3D, Streamline (tcs2)**, and **Concentration, C_3D, Surface (tcs2)**.

2 Right-click and choose **Delete**.

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 2/Parametric Solutions 1 (5) (sol3)** > **Transport of Concentrated Species 2** > **Plot array: Concentrations, A_3D, B_3D, C_3D (tcs2)**.

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

Plot array: Concentrations, A_3D, B_3D, C_3D (tcs2)

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

2 From the **Parameter value (dz (mm))** list, choose **2**.

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

4 Locate the **Color Legend** section. From the **Position** list, choose **Right**.

5 Click to expand the **Plot Array** section. From the **Array axis** list, choose **y**.

6 In the **Relative padding** text field, type `0.3`.

A_3D Contour

1 In the **Plot array: Concentrations, A_3D, B_3D, C_3D (tcs2)** toolbar, click **Contour**.

2 In the **Settings** window for **Contour**, type `A_3D Contour` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `tcs2.c_wA_3D`.

4 Locate the **Levels** section. In the **Total levels** text field, type `10`.

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

6 From the **Color** list, choose **White**.

7 Clear the **Color legend** checkbox.

8 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

9 In the **Index** text field, type `2`.

Plot array: Concentrations, A_3D, B_3D, C_3D (tcs2)

In the **Plot array: Concentrations, A_3D, B_3D, C_3D (tcs2)** toolbar, click **Contour**.

B_3D Contour

1 In the **Settings** window for **Contour**, type `B_3D Contour` in the **Label** text field.

2 Locate the **Expression** section. In the **Expression** text field, type `tcs2.c_wB_3D`.

3 Locate the **Levels** section. In the **Total levels** text field, type `10`.

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

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

6 Clear the **Color legend** checkbox.

7 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

8 In the **Index** text field, type `1`.

Plot array: Concentrations, A_3D, B_3D, C_3D (tcs2)

In the **Plot array: Concentrations, A_3D, B_3D, C_3D (tcs2)** toolbar, click **Contour**.

C_3D Contour

1 In the **Settings** window for **Contour**, type `C_3D Contour` in the **Label** text field.

2 Locate the **Expression** section. In the **Expression** text field, type `tcs2.c_wC_3D`.

3 Locate the **Levels** section. In the **Total levels** text field, type `10`.

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

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

6 Clear the **Color legend** checkbox.

7 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

8 In the **Plot array: Concentrations, A_3D, B_3D, C_3D (tcs2)** toolbar, click **Plot**.

9 Click the **Show Grid** button in the **Graphics** toolbar.

Follow the steps below to set up Figure 4 in the model documentation.

Species A_3D

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

2 In the **Settings** window for **3D Plot Group**, type `Species A_3D` in the **Label** text field.

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

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

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

6 Locate the **Plot Array** section. Select the **Enable** checkbox.

7 From the **Array axis** list, choose **y**.

dz = 1 mm

1 In the **Species A_3D** toolbar, click **Volume**.

2 In the **Settings** window for **Volume**, type `dz = 1 mm` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2/ Parametric Solutions 1 (5) (sol3)**.

4 From the **Parameter value (dz (mm))** list, choose **1**.

5 Locate the **Expression** section. In the **Expression** text field, type `tcs2.c_wA_3D`.

To ensure all three volume plots have the same scale use the manual color range.

6 Click to expand the **Range** section. Select the **Manual color range** checkbox.

7 In the **Minimum** text field, type `4`.

8 In the **Maximum** text field, type `12`.

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

10 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Species A_3D

In the **Species A_3D** toolbar, click **Contour**.

dz = 1 mm Contour

1 In the **Settings** window for **Contour**, type `dz = 1 mm  Contour` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2/ Parametric Solutions 1 (5) (sol3)**.

3 From the **Parameter value (dz (mm))** list, choose **1**.

4 Locate the **Expression** section. In the **Expression** text field, type `tcs2.c_wA_3D`.

5 Locate the **Levels** section. In the **Total levels** text field, type `10`.

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

7 From the **Color** list, choose **White**.

8 Clear the **Color legend** checkbox.

9 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

Repeat the same steps for thicknesses 2 mm and 5 mm.

Species A_3D

In the **Species A_3D** toolbar, click **Volume**.

dz = 2 mm

1 In the **Settings** window for **Volume**, type `dz = 2 mm` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2/ Parametric Solutions 1 (5) (sol3)**.

3 From the **Parameter value (dz (mm))** list, choose **2**.

4 Locate the **Expression** section. In the **Expression** text field, type `tcs2.c_wA_3D`.

5 Locate the **Range** section. Select the **Manual color range** checkbox.

6 In the **Minimum** text field, type `4`.

7 In the **Maximum** text field, type `12`.

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

9 Clear the **Color legend** checkbox.

10 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

11 In the **Index** text field, type `1`.

Species A_3D

In the **Species A_3D** toolbar, click **Contour**.

dz = 2 mm Contour

1 In the **Settings** window for **Contour**, type `dz = 2 mm  Contour` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2/ Parametric Solutions 1 (5) (sol3)**.

3 From the **Parameter value (dz (mm))** list, choose **2**.

4 Locate the **Expression** section. In the **Expression** text field, type `tcs2.c_wA_3D`.

5 Locate the **Levels** section. In the **Total levels** text field, type `10`.

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

7 From the **Color** list, choose **White**.

8 Clear the **Color legend** checkbox.

9 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

10 In the **Index** text field, type `1`.

Species A_3D

In the **Species A_3D** toolbar, click **Volume**.

dz = 5 mm

1 In the **Settings** window for **Volume**, type `dz = 5 mm` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2/ Parametric Solutions 1 (5) (sol3)**.

3 Locate the **Expression** section. In the **Expression** text field, type `tcs2.c_wA_3D`.

4 Locate the **Range** section. Select the **Manual color range** checkbox.

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

6 In the **Maximum** text field, type `12`.

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

8 Clear the **Color legend** checkbox.

9 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

10 In the **Index** text field, type `2`.

Species A_3D

In the **Species A_3D** toolbar, click **Contour**.

dz = 5 mm Contour

1 In the **Settings** window for **Contour**, type `dz = 5 mm  Contour` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2/ Parametric Solutions 1 (5) (sol3)**.

3 Locate the **Expression** section. In the **Expression** text field, type `tcs2.c_wA_3D`.

4 Locate the **Levels** section. In the **Total levels** text field, type `10`.

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

6 From the **Color** list, choose **White**.

7 Clear the **Color legend** checkbox.

8 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

9 In the **Index** text field, type `2`.

10 In the **Species A_3D** toolbar, click **Plot**.

Next, add the 3D component results to the Concentration Along Center 1D Plot Group created earlier for the 2D geometry. Plot the concentration profile for the upside and downside edge boundaries.

Concentrations Along Center

In the **Model Builder** window, under **Results** click **Concentrations Along Center**.

A_3D

1 Right-click **Concentrations Along Center** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type A_3D in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2/ Parametric Solutions 1 (5) (sol3)**.

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

5 In the **Parameter values (dz (mm))** list box, select **2**.

6 Select Edges 3 and 5 only.

7 Locate the **y-Axis Data** section. In the **Expression** text field, type tcs2.c_wA_3D.

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

9 In the **Expression** text field, type x.

10 Locate the **Coloring and Style** section. From the **Color** list, choose **Cycle (reset)**.

Concentrations Along Center

In the **Concentrations Along Center** toolbar, click **Line Graph**.

B_3D

1 In the **Settings** window for **Line Graph**, type B_3D in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2/ Parametric Solutions 1 (5) (sol3)**.

3 From the **Parameter selection (dz)** list, choose **From list**.

4 In the **Parameter values (dz (mm))** list box, select **2**.

5 Select Edges 3 and 5 only.

6 Locate the **y-Axis Data** section. In the **Expression** text field, type tcs2.c_wB_3D.

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

8 In the **Expression** text field, type x.

Concentrations Along Center

In the **Concentrations Along Center** toolbar, click **Line Graph**.

C_3D

1 In the **Settings** window for **Line Graph**, type C_3D in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2/ Parametric Solutions 1 (5) (sol3)**.

3 From the **Parameter selection (dz)** list, choose **From list**.

4 In the **Parameter values (dz (mm))** list box, select **2**.

5 Select Edges 3 and 5 only.

6 Locate the **y-Axis Data** section. In the **Expression** text field, type `tcs2.c_wC_3D`.

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

8 In the **Expression** text field, type `x`.

9 In the **Concentrations Along Center** toolbar, click **Plot**.

Follow the steps below to set up Figure 5 in the model documentation.

Species A Concentration Along Center

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

2 In the **Settings** window for **1D Plot Group**, type `Species A Concentration Along Center` in the **Label** text field.

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

4 Locate the **Grid** section. Clear the **Show grid** checkbox.

A_2D

1 In the **Species A Concentration Along Center** toolbar, click **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `A_2D` in the **Label** text field.

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

4 Select Boundary 2 only.

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `tcs.c_wA_2D`.

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

7 In the **Expression** text field, type `x`.

8 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

Species A Concentration Along Center

In the **Species A Concentration Along Center** toolbar, click **Line Graph**.

A_3D

1 In the **Settings** window for **Line Graph**, type `A_3D` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Parametric Solutions 1 (5) (sol3)**.

3 Select Edges 3 and 5 only.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `tcs2.c_wA_3D`.

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

6 In the **Expression** text field, type `x`.

7 Locate the **Coloring and Style** section. From the **Color** list, choose **Cycle (reset)**.

8 Locate the **Legends** section. Select the **Show legends** checkbox.

9 Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `dz = `.

10 In the **Species A Concentration Along Center** toolbar, click **Plot**.

Species A Concentration Along Center

1 In the **Model Builder** window, click **Species A Concentration Along Center**.

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

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

4 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

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 2/Parametric Solutions 1 (5) (sol3)** > **Transport of Concentrated Species 2** > **Mass Balance, A_3D (tcs2)** and **Study 2/Parametric Solutions 1 (5) (sol3)** > **Transport of Concentrated Species 2** > **Mass Balance, B_3D (tcs2)**.

4 Click the **Add Result Template** button in the window toolbar.

Just like for the 2D mass conservation evaluation group, calculate the relative error.

RESULTS

Mass Balance, A_3D (tcs2)

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 `Relative Error`.

4 In the **Mass Balance, A_3D (tcs2)** toolbar, click **Evaluate**.

Mass Balance, B_3D (tcs2)

1 In the **Model Builder** window, click **Mass Balance, B_3D (tcs2)**.

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 `Relative Error`.

5 In the **Mass Balance, B_3D (tcs2)** toolbar, click **Evaluate**.