Mass Transfer from a Thin Domain

Introduction

This model 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**. For this purpose, the physics interfaces **Transport of Diluted Species** and **Laminar Flow** are used. The out-of-plane thickness, which is constant throughout the domain, is varied from 1 mm to 10 mm to investigate the accuracy of the approximation.

The **Out-of-Plane Flux** feature is useful when the concentration variation in the out-of-plane direction (along the thickness) is small, and when decreasing the computational time is important. As will be shown, by approximating the thin 3D component with the corresponding 2D component, solution time decreases significantly, without a significant decrease in accuracy.

Even though the geometry used in this example has a constant thickness throughout the domain, the **Out-of-Plane Flux** feature can be used for varying thicknesses. It is also possible to decrease a 3D or 2D domain to 1D.

Model Definition

The modeled domain has a square shape of side length 1 m with a constant thickness d_z. Three different thicknesses are solved for; 0.01 m, 0.005 m, and 0.001 m. Figure 1 illustrates the simplification made from 3D to 2D.
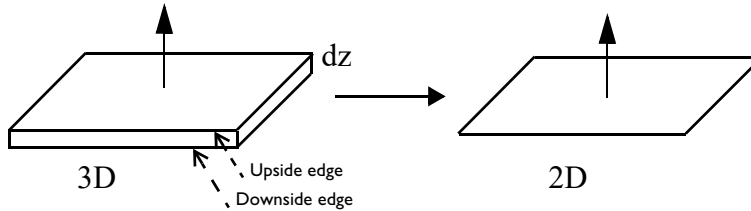

Figure 1: Model geometry reduction from 3D to 2D. The upward pointing arrows symbolize flux out from the domain. In this model there is only flux through the upper boundary. The upside and downside edges in 3D, for which concentration profiles are plotted in Figure 2 are indicated with dashed arrows.

The Single-Phase Flow interface solves for the velocity and pressure in a fluid as it flows through the thin domain. The fluid in turn transports a solute species whose concentration is solved for by the Transport of Diluted Species interface.

A **Concentration** feature (Transport of Diluted Species) as well as an **Inlet** feature (Laminar Flow) are added on the thin boundary where $x = 0$ (3D), and on the corresponding edge in 2D. The stationary mass transfer equation for the 2D problem is

$$\nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = \frac{J_{0,\mathrm{u},i} + J_{0,\mathrm{d},i}}{d_z},$$

where the left-hand side describes diffusion and convection, and the right-hand side is the out-of-plane source term, namely 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.

In this model example there is only flux through the upper boundary, giving

$$\nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = \frac{J_{0,\mathrm{u}}}{d_z}.$$

The parameters used in the model are found in the table below.

TABLE 1: PARAMETERS.

NAME	EXPRESSION	VALUE	DESCRIPTION
dz	10[mm]	0.01m	Out-of-plane thickness
L	1[m]	1 m	Side length of domain
u0	0.01[mm/s]	1e-5 m/s	Inlet fluid velocity
cb	3[mol/m^3]	3 mol/m^3	Parameter for flux expression
kc	8e-5[m/h]	2.2222e-8 m/s	Parameter for flux expression
conc	10[mol/m^3]	10 mol/m^3	Concentration for boundary condition
rho	1000[kg/m^3]	1000 kg/m^3	Fluid density
visc	1e-3[s*Pa]	0.001 Pa*s	Fluid dynamic viscosity

Results and Discussion

Figure 2 shows the concentration on an edge along the x-axis for all three thicknesses solved for, and for both the 2D and the 3D component. For the 3D component, the concentration along both the upside and the downside edges are plotted (see Figure 1 for

an illustration of these edges). The concentration profiles are significantly different for the three thickness used, something that is captured well by the 2D approximation.
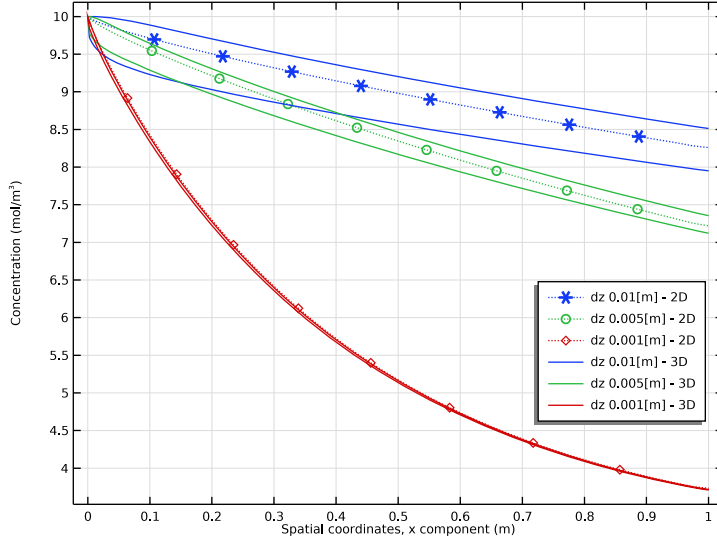

Figure 2: Concentration profiles along edge in 2D and 3D, for all the three thicknesses d_z solved for.

The difference between the 2D and 3D solutions decreases as the thickness decreases, but even for the largest thickness the difference is quite small.

The quantitative difference between the concentration profiles in 2D and 3D with d_z = 0.01 is seen in Figure 3.
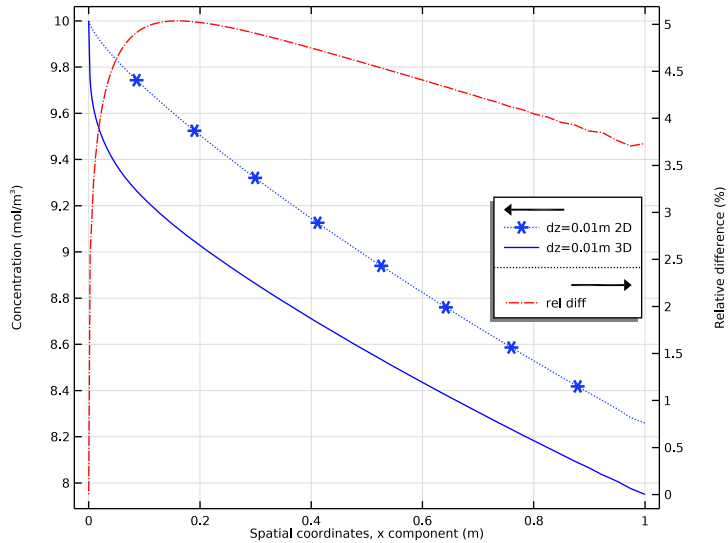
Figure 3: Concentration profiles in 2D and 3D (downside edge), and their relative difference for $d_z = 0.01$ m. Using the concentration along the downside edge gives the largest relative difference.

For this system, the relative difference is just above 5%, but the computation time for the parametric sweep decreased from more than 2 minutes in 3D to a few seconds in 2D.

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

I In the **Model Wizard** window, click ⚛ **2D**.

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

3 Click **Add**.

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

5 Click **Add**.

6 Click → **Study**.

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

8 Click ☑ **Done**.

GEOMETRY 1

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 parameter L.

GEOMETRY 1

Square 1 (sq1)

1 In the **Geometry** toolbar, click ▢ **Square**.

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

3 In the **Side length** text field, type L.

4 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**.

Set up the mass transfer physics.

TRANSPORT OF DILUTED SPECIES (TDS)

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

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

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

Tips: 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.

Transport Properties 1

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

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

3 From the **u** list, choose **Velocity field (spf)**.

Here we use the velocity field from the laminar flow interface.

Almost done with setting up the diluted species interface. The last two things to do is adding the concentration boundary condition, as well as the out-of-plane flux feature.

Concentration 1

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

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

3 Select the **Species c** check box.

4 In the $c_{0,c}$ text field, type conc, one of the parameters in **Global Definitions**.

Now choose the boundary for the concentration boundary condition just defined.

5 Select Boundary 1 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.

Out-of-Plane Flux 1

1 In the **Physics** toolbar, click ⬤ **Domains** and choose **Out-of-Plane Flux**.

2 Select Domain 1 only.

Keep the **Flux type** as is. Remember that in this example there is only flux out from the upside of the domain.

3 In the **Settings** window for **Out-of-Plane Flux**, locate the **Upside Inward Flux** section.

4 Select the **Species c** check box.

5 In the $J_{0,c,u}$ text field, type `-kc*(c-cb)`.

The negative sign is needed to assign an outward flux.

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 Select the **Use shallow channel approximation** check box.

4 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 ρ list, choose **User defined**. In the associated text field, type `rho`.

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

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 Specify the **u** vector as

u0	x
0	y

Now for the last two steps for this physics; add an **Inlet** and an **Outlet** feature.

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.

MESH 1

Having set up the physics interfaces, now build a mesh.

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, i.e. 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 70.

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

7 Select the **Reverse direction** check box.

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 **Symmetric distribution** check box.

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** check box.

4 Click 🔳 **Build Selected**.

And that was the last step in the mesh build. Time to solve the model.

STUDY 1

Use 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)	`0.01, 0.005, 0.001`	m

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

RESULTS

Pressure (spf)

Clicking through the default plots gives a picture of the solved system. The concentration decreases from the initial value down to the parameter value for cb, just as expected. The velocity plot shows very thin gradients along the walls parallel to the x-axis. Since the flow setting Fully developed flow was used, there are no changes in the incoming flow.

Now plot the concentration along the edge where y = 0.

Concentration profiles

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

2 In the **Settings** window for **1D Plot Group**, type Concentration profiles in the **Label** text field.

2D

1 Right-click **Concentration profiles** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type 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 **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 **Dotted**.

8 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

9 Click to expand the **Legends** section. Select the **Show legends** check box.

10 From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
dz 0.01[m] - 2D

12 In the **Concentration profiles** toolbar, click ⬛ **Plot**.

13 In the table, enter the following settings:

Legends
dz 0.01[m] - 2D
dz 0.005[m] - 2D
dz 0.001[m] - 2D

Move the legend so that none of the curves are hidden.

Concentration profiles

1 In the **Model Builder** window, click **Concentration profiles**.

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

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

4 In the **y-position** text field, type 0.2.

From the plot just created it is seen that the out-of-plane thickness influences the resulting concentration profiles significantly. Now, set up the 3D component and compare the resulting concentration plots for the two 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 L.

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 ![icon] **Build Selected**.

COMPONENT 2 (COMP2)

In the **Home** toolbar, click ![icon] **Windows** and choose **Add Physics**.

ADD PHYSICS

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

2 In the tree, select **Recently Used>Transport of Diluted Species (tds)**.

3 Click **Add to Component 2** in the window toolbar.

4 In the tree, select **Recently Used>Laminar Flow (spf)**.

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

TRANSPORT OF DILUTED SPECIES 2 (TDS2)

Transport Properties 1

1 In the **Model Builder** window, under **Component 2 (comp2)> Transport of Diluted Species 2 (tds2)** click **Transport Properties 1**.

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

3 From the **u** list, choose **Velocity field (spf2)**.

Concentration 1

1 In the **Physics** toolbar, click ![icon] **Boundaries** and choose **Concentration**.

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

3 Select the **Species c2** check box.

4 In the $c_{0,c2}$ text field, type conc.

5 Select Boundary 1 only.

Flux 1

1 In the **Physics** toolbar, click ![icon] **Boundaries** and choose **Flux**.

2 In the **Settings** window for **Flux**, locate the **Inward Flux** section.

3 Select the **Species c2** check box.

4 In the $J_{0,c2}$ text field, type -kc*(c2-cb).

5 Select Boundary 4 only.

LAMINAR FLOW 2 (SPF2)

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 ρ list, choose **User defined**. In the associated text field, type rho.

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

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 Specify the **u** vector as

u0	x
0	y
0	z

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** check box.

4 Select Boundary 6 only.

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

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

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

Mapped 1

1 In the **Mesh** toolbar, click △ **Boundary** 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 70.

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

7 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 Select the **Symmetric distribution** check box.

6 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 10.

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

6 Select the **Symmetric distribution** check box.

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 [icon] **Clear Selection**.

4 Select Boundaries 2 and 5 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** check box.

4 Click [icon] **Build All**.

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

ROOT

In the **Home** toolbar, click [icon] **Windows** and choose **Add Study**.

ADD STUDY

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

2 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check boxes
   for **Transport of Diluted Species (tds)** and **Laminar Flow (spf)**.

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

4 Click **Add Study** in the window toolbar.

In the **Model Builder** window, click **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)	0.01,0.005,0.001	m

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

RESULTS

Concentration, Streamline (tds2)
Looking at the default plots for the 3D component, it is clear that they are quite similar to the corresponding 2D plots. Continue by adding the 3D component data to the 1D Plot Group set up earlier.

3D

1 In the **Model Builder** window, right-click **2D** and choose **Duplicate**.

Plot the concentration profile for the edge on the upside boundary, as well as for the edge on the downside boundary.

2 In the **Settings** window for **Line Graph**, type 3D in the **Label** text field.

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

4 Locate the **Selection** section. Click to select the ▭ **Activate Selection** toggle button.

5 Select Edges 3 and 5 only.

6 Locate the **y-Axis Data** section. In the **Expression** text field, type c2.

7 Locate the **Legends** section. In the table, enter the following settings:

Legends
dz 0.01[m] - 3D

Legends
dz 0.005[m] - 3D
dz 0.001[m] - 3D

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

9 Find the **Line markers** subsection. From the **Marker** list, choose **None**.

10 From the **Color** list, choose **Cycle (reset)**.

Concentration profiles

1 In the **Model Builder** window, click **Concentration profiles**.

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

3 Select the **y-axis label** check box.

4 In the associated text field, type Concentration (mol/m³).

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

6 In the **Concentration profiles** toolbar, click ⬛ **Plot**.

This is Figure 2. It is evident that the approximation using out-of-plane flux is very accurate for the smallest thickness. The accuracy of the approximation decrease with increased thickness. In the next plot it will be clear just how accurate the approximation is for the least accurate case.

Relative difference for dz=0.01

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

2 In the **Settings** window for **1D Plot Group**, type Relative difference for dz=0.01 in the **Label** text field.

By creating edge datasets and using the Join feature, it is possible to get the difference in concentration between the 2D and 3D components.

Edge 2D 1

1 In the **Results** toolbar, click ⬛ **More Datasets** and choose **Edge 2D**.

2 Select Boundary 2 only.

Edge 3D 2

1 In the **Model Builder** window, right-click **Datasets** and choose **Edge 3D**.

2 Select Edge 5 only.

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

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

Join 1

1 In the **Results** toolbar, click ▦ **More Datasets** and choose **Join**.

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

3 From the **Data** list, choose **Edge 2D 1**.

4 From the **Solutions** list, choose **One**.

5 From the **Parameter value (dz (m))** list, choose **0.01 m**.

6 Locate the **Data 2** section. From the **Data** list, choose **Edge 3D 2**.

7 From the **Solutions** list, choose **One**.

8 From the **Parameter value** list, choose **0.01**.

9 Locate the **Combination** section. From the **Method** list, choose **Explicit**.

Now, use this Join dataset in the plot group recently created.

Relative difference for dz=0.01

1 In the **Model Builder** window, under **Results** click **Relative difference for dz=0.01**.

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

3 From the **Dataset** list, choose **Join 1**.

c for edge 2D

1 Right-click **Relative difference for dz=0.01** and choose **Line Graph**.

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

3 Locate the **y-Axis Data** section. In the **Expression** text field, type data1(c).

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 **Dotted**.

7 Find the **Line markers** subsection. From the **Marker** list, choose **Asterisk**.

8 Locate the **Legends** section. Select the **Show legends** check box.

9 From the **Legends** list, choose **Manual**.

10 In the table, enter the following settings:

Legends
dz=0.01m 2D

11 In the **Relative difference for dz=0.01** toolbar, click ▣ **Plot**.

c2 for edge 3D

1 Right-click **c for edge 2D** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type c2 for edge 3D in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type data2(c2).

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

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

6 Find the **Line markers** subsection. From the **Marker** list, choose **None**.

7 Locate the **Legends** section. In the table, enter the following settings:

Legends
dz=0.01m 3D

8 In the **Relative difference for dz=0.01** toolbar, click ⊙ **Plot**.

The concentration curve for the edge in 3D has a reverse pointing x-axis. Go back to the Edge 3D dataset and fix that.

Edge 3D 2

1 In the **Model Builder** window, under **Results>Datasets** click **Edge 3D 2**.

2 In the **Settings** window for **Edge 3D**, click to expand the **Advanced** section.

3 Select the **Reverse direction** check box.

Relative difference for dz=0.01

Now plot the relative difference between the two curves. Do this on a second y-axis.

relative difference in concentration

1 In the **Model Builder** window, right-click **c2 for edge 3D** and choose **Duplicate**.

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

3 Locate the **y-Axis Data** section. In the **Expression** text field, type (data1(c)-data2(c2))/data1(c)*100.

4 Select the **Description** check box.

5 In the associated text field, type Relative difference (%).

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

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

8 Locate the **Legends** section. In the table, enter the following settings:

Legends
rel diff

Relative difference for dz=0.01

1 In the **Model Builder** window, click **Relative difference for dz=0.01**.

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

3 Select the **Two y-axes** check box.

4 Select the **y-axis label** check box.

5 In the associated text field, type Concentration (mol/m^3).

6 Select the **Secondary y-axis label** check box.

7 In the associated text field, type Relative difference (%).

8 In the table, select the **Plot on secondary y-axis** check box for **relative difference in concentration**.

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

10 In the **Relative difference for dz=0.01** toolbar, click ⬛ **Plot**.

11 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

This is Figure 3. From this figure it is seen that the largest relative difference in concentration, resulting from approximating the 3D component with a 2D component, is just above 5%.