

# 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

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

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,  $J_{0,u}$ , and on the downside,  $J_{0,d}$ , divided by the out-of-plane thickness  $d_z$ .

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

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

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

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

TABLE I: PARAMETERS.

# 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 **Q** 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 I

Start by adding some global parameters.

## GLOBAL DEFINITIONS

#### Parameters 1

- I 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 thin\_domain\_parameters.txt.

Build the geometry for the 2D component, by using the added parameter L.

## GEOMETRY I

Square 1 (sq1)

- I 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)

- I In the Model Builder window, under Component I (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

- I In the Model Builder window, under Component I (compl)> Transport of Diluted Species (tds) click Transport Properties I.
- 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

- I 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

I 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)

- I In the Model Builder window, under Component I (compl) 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

- I In the Model Builder window, under Component I (compl)>Laminar Flow (spf) click Fluid Properties I.
- 2 In the Settings window for Fluid Properties, locate the Fluid Properties section.
- **3** From the  $\rho$  list, choose **User defined**. In the associated text field, type rho.
- **4** From the  $\mu$  list, choose **User defined**. In the associated text field, type visc.

Initial Values 1

- I In the Model Builder window, click Initial Values I.
- 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

I 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 I

- I 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 I

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

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 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 I, Free Triangular I, Size I

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

#### Mapped I

I 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 I

- I Right-click Mapped I 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 70.

- 6 In the Element ratio text field, type 10.
- 7 Select the **Reverse direction** check box.
- 8 Click 🖷 Build Selected.

#### Distribution 2

- I 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

- In the Model Builder window, expand the Component I (compl)>Mesh I> Boundary Layers I node, then click Boundary Layer Properties I.
- 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

- I In the Model Builder window, click Boundary Layers I.
- 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 I

Use Parametric Sweep to solve for three different thicknesses dz.

## Parametric Sweep

I 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

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Concentration profiles in the Label text field.

2D

- I 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 I/Solution I (soll).
- 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 From the Positioning list, choose Interpolated.
- 10 Click to expand the Legends section. Select the Show legends check box.
- II From the Legends list, choose Manual.

**12** In the table, enter the following settings:

Legends dz 0.01[m] - 2D

**I3** In the **Concentration profiles** toolbar, click **O Plot**.

**I4** 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

- I In the Model Builder window, click Concentration profiles.
- 2 In the Settings window for ID 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 I (blkI)

- I 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 틤 Build Selected.

Form Union (fin)

I In the Model Builder window, click Form Union (fin).

2 In the Settings window for Form Union/Assembly, click 📳 Build Selected.

## ADD PHYSICS

- I 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 Recently Used>Transport of Diluted Species (tds).
- 4 Click Add to Component 2 in the window toolbar.
- 5 In the tree, select Recently Used>Laminar Flow (spf).
- 6 Click Add to Component 2 in the window toolbar.
- 7 In the Home toolbar, click 🖄 Add Physics to close the Add Physics window.

#### TRANSPORT OF DILUTED SPECIES 2 (TDS2)

Transport Properties 1

- I In the Model Builder window, under Component 2 (comp2)> Transport of Diluted Species 2 (tds2) click Transport Properties I.
- 2 In the Settings window for Transport Properties, locate the Convection section.
- **3** From the **u** list, choose **Velocity field (spf2)**.

#### Concentration 1

- I In the Physics toolbar, click 🔚 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

- I In the Physics toolbar, click 🔚 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

- I In the Model Builder window, under Component 2 (comp2)>Laminar Flow 2 (spf2) click Fluid Properties I.
- 2 In the Settings window for Fluid Properties, locate the Fluid Properties section.
- **3** From the  $\rho$  list, choose **User defined**. In the associated text field, type rho.
- **4** From the  $\mu$  list, choose **User defined**. In the associated text field, type visc.

Initial Values 1

- I In the Model Builder window, click Initial Values I.
- 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 I

- I 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  $U_{\rm av}$  text field, type u0.
- **5** Select Boundary 1 only.

#### Outlet I

- I 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

- I 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 I, Free Tetrahedral I, Size I

- 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 I

- I In the Mesh toolbar, click A Boundary and choose Mapped.
- 2 Drag and drop below Size.

## Distribution I

- I Right-click Mapped I 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 I

- I In the Model Builder window, click Mapped I.
- **2** Select Boundary 4 only.

#### Distribution 2

- I In the Model Builder window, under Component 2 (comp2)>Mesh 2>Mapped I right-click Distribution I 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 A Swept.

## Distribution I

I Right-click Swept I 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

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

- I In the Model Builder window, expand the Boundary Layers I node, then click Boundary Layer Properties I.
- 2 In the Settings window for Boundary Layer Properties, locate the Geometric Entity Selection section.
- 3 Click Clear Selection.
- 4 Select Boundaries 2 and 5 only.

#### Boundary Layers 1

- I In the Model Builder window, click Boundary Layers I.
- 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 📗 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

- I In the Home toolbar, click 2 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** check boxes for **Transport of Diluted Species (tds)** and **Laminar Flow (spf)**.
- 4 Find the Studies subsection. In the Select Study tree, select General Studies>Stationary.
- 5 Click Add Study in the window toolbar.

6 In the Model Builder window, click the root node.

7 In the Home toolbar, click 2 Add Study to close the Add Study window.

## STUDY 2

Parametric Sweep

- I 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

I 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.

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

#### Concentration profiles

- I In the Model Builder window, click Concentration profiles.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- 3 Select the y-axis label check box. In the associated text field, type Concentration (mol/m<sup>3</sup>).
- 4 Click to expand the Title section. From the Title type list, choose None.
- **5** In the **Concentration profiles** toolbar, click **O 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

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID 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 I

- I In the **Results** toolbar, click **More Datasets** and choose **Edge 2D**.
- **2** Select Boundary 2 only.

## Edge 3D 2

- I 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 I (5) (sol3).

## Join I

- I In the **Results** toolbar, click **More Datasets** and choose **Join**.
- 2 In the Settings window for Join, locate the Data I section.
- 3 From the Data list, choose Edge 2D I.
- 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

- I In the Model Builder window, under Results click Relative difference for dz=0.01.
- 2 In the Settings window for ID Plot Group, locate the Data section.
- 3 From the Dataset list, choose Join I.

c for edge 2D

- I 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 From the **Positioning** list, choose **Interpolated**.
- 9 Locate the Legends section. Select the Show legends check box.
- **IO** From the Legends list, choose Manual.

II In the table, enter the following settings:

## Legends

dz=0.01m 2D

**12** In the **Relative difference for dz=0.01** toolbar, click **O** Plot.

c2 for edge 3D

- I 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

- I 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

- I 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. In the associated text field, type Relative difference (%).
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dash-dot.
- 6 From the Color list, choose Red.

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

#### Legends

#### rel diff

Relative difference for dz=0.01

- I In the Model Builder window, click Relative difference for dz=0.01.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- **3** Select the **Two y-axes** check box.
- 4 Select the y-axis label check box. In the associated text field, type Concentration (mol/m<sup>3</sup>).
- 5 Select the Secondary y-axis label check box. In the associated text field, type Relative difference (%).
- 6 In the table, select the Plot on secondary y-axis check box for relative difference in concentration.
- 7 Locate the Title section. From the Title type list, choose None.
- 8 In the Relative difference for dz=0.01 toolbar, click 💿 Plot.
- 9 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%.