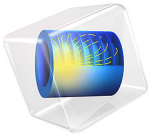


Effective Diffusivity in Porous Materials

This example introduces the concept of effective diffusivity in porous media by comparing the transport through an artificial porous structure described in a detailed model with a simplified homogeneous porous media approach using effective transport properties.

The exercise consists of two parts. The first part describes how to create the model with a detailed geometry. The second part shows how to define a homogeneous model for porous media using an effective diffusivity calculated using the detailed model from the first part.

Introduction

Transport through porous structures is usually treated using simplified homogeneous models with effective transport properties. This is in most cases a necessity, since the typical dimensions of the pores and particles making up the porous structure are several orders of magnitude smaller than the size of the domain that is to be modeled.

However, it might be interesting to investigate the assumptions and simplifications done when homogenizing a porous structure by comparing a homogeneous model with a model defined using the detailed structure.

The artificial porous structure used in this example is shown in Figure 1 below.

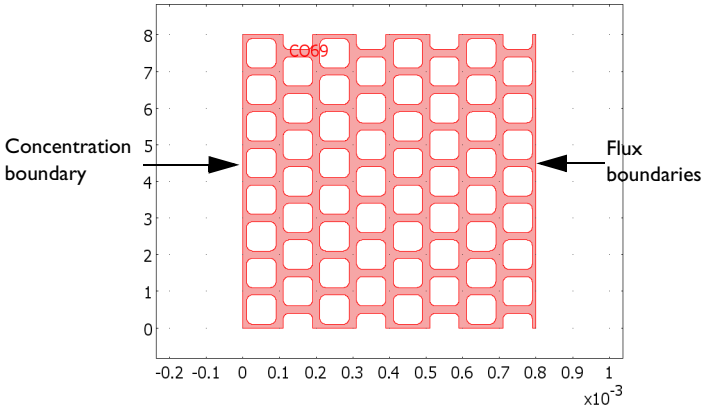


Figure 1: Artificial porous structure. The domain colored in red is accessible for diffusion.

Model Definition

The model equation in the modeled domain shown in Figure 1 is the time-dependent equation

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = 0$$

where c denotes concentration (mol/m^3 using SI units) and D the diffusion coefficient (m^2/s) of the solute.

The boundary conditions are of three different types. A concentration boundary condition applies at the left vertical boundary in Figure 1. It is expressed as

$$c = c_0$$

where c_0 is a given concentration.

The right vertical boundary in Figure 1 is set according to

$$(-D\nabla c) \cdot \mathbf{n} = k_m(c - c_1)$$

where k_m is the mass transfer coefficient (m/s), and c_1 is the concentration in a bulk solution outside of the porous structure.

All other boundaries are insulating boundaries according to

$$(-D\nabla c) \cdot \mathbf{n} = 0$$

The initial condition is given by a bell-shaped profile along the x-axis with its maximum at $x = 0$ and a corresponding value of $c = c_0$:

$$c(t_0) = c_0 \exp(-ax^2)$$

Assume a gaseous solution with a solute content of 3 mol/m^3 at the concentration boundary. The diffusion coefficient is set to $1{\cdot}10^{-5}$ m^2/s.

The second part of this exercise uses a homogenized 1D model geometry with effective transport properties and an average porosity. The model equation then becomes:

$$\varepsilon\frac{\partial c}{\partial t} + \nabla \cdot (-D^{\text{eff}}\nabla c) = 0$$

where ε denotes the average porosity and D^{eff} is the effective diffusivity. These properties are calculated from the results of the detailed structure; see the next section. At the boundaries, the concentration and flux conditions described above apply.

The simulations are run for t = 0 to 0.1 s, when the simulation reaches steady state. Figure 2 below shows the concentration profile after 0.05 s in the porous structure. Already at this stage the concentration has almost reached steady state, which is visible by the nearly linear concentration profile across the structure.

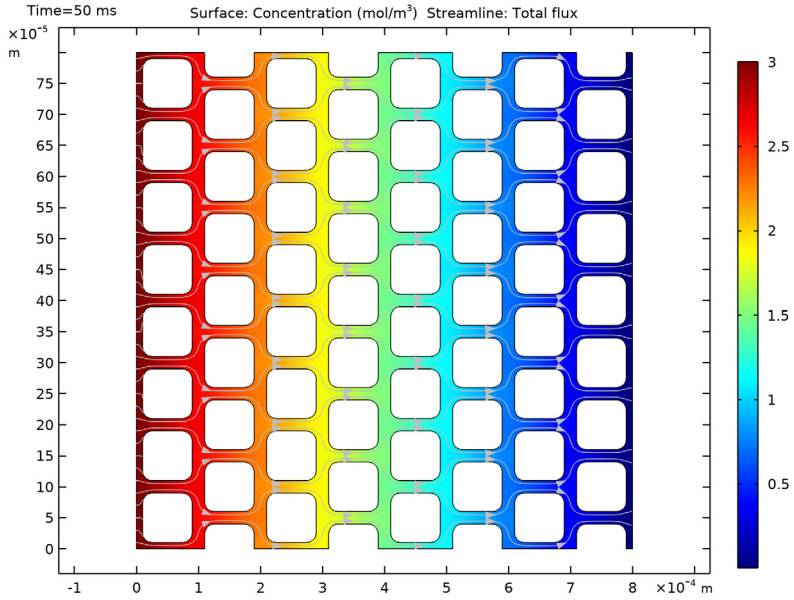


Figure 2: Concentration profile in the modeled artificial porous structure at t = 0.05 s.

When modeling porous media, the exact concentration in the pore structure is not the most important issue because the description of the structure is homogenized and not detailed as in Figure 2. The most interesting issue is then the description of the flux. To calculate the average flux, integrate over the flux boundary and divide by its length, L_0, which yields the following expression:

$$N_{\text{average}} = \frac{1}{L_0}\int_0^{L_0} k_m(c - c_1)\,dS$$

Figure 3 shows the value of this integral as a function of time. If you let the process reach steady-state, the average flux becomes $8.051 \cdot 10^{-3}$ mol/(m^2/s). Considering the almost linear profile across the structure, it is natural to replace the porous structure with a 1D

homogenized structure along the x-axis. It is then possible to calculate the effective diffusivity according to the following:

$$D^{\text{eff}}\frac{(c_0 - c_{\text{out}})}{L_1} = N_{\text{average}}$$

where c_{out} is the average concentration (mol/m^3) at the flux boundary, and L_1 is the length of the geometry along the x-axis. The average concentration is obtained by integrating according to the expression below:

$$c_{\text{out}} = \frac{1}{L_0}\int_0^{L_0} c\,dy$$

This gives an average concentration $c_{\text{out}} = 1.63 \cdot 10^{-3}$ mol/m^3. Using $L_1 = 8 \cdot 10^{-4}$ m, the effective diffusivity is:

$$D^{\text{eff}} = \frac{8.051 \cdot 10^{-3} \times 8.0 \cdot 10^{-4}}{(3 - 1.63 \cdot 10^{-3})}$$

which yields a value for the effective diffusivity of $2.15 \cdot 10^{-6}$ m^2/s compared to the "free" diffusivity of $1 \cdot 10^{-5}$ m^2/s. The effective and "free" diffusivities are usually related according to the equation

$$D^{\text{eff}} = D\frac{\varepsilon}{\tau}$$

where ε is the porosity of the structure and τ is the tortuosity, which is a measure of the actual length per unit effective length a molecule has to diffuse in a porous structure. To calculate the porosity of the modeled structure, you integrate the value 1 over the structure and then divide this by the length and width of the structure:

$$\varepsilon = \frac{1}{L_0 L_1}\int_0^{L_1}\int_0^{L_0} 1\,dx\,dy$$

resulting in a value of 0.383. The value of τ can then be calculated to 1.62. In addition, the tortuosity is usually expressed as a power of the porosity, resulting in an expression for the effective diffusivity according to

$$D^{\text{eff}} = D\varepsilon^p$$

If you use the calculated values for porosity and effective diffusivity, the value for p is 1.60. The experimental values for p for porous structures used for transport in catalysts, soils, and other porous structures is usually in the range 1.5–2.

Using the value of the effective diffusivity, a simple homogenized 1D model provides the possibility to compare the value of the flux using a homogenized model to the value using the detailed 2D structure. Figure 3 shows that there is an excellent agreement between the model using a detailed geometry and the homogenized model. The difference in the time-dependent flux is hardly visible between the two cases in the graph.

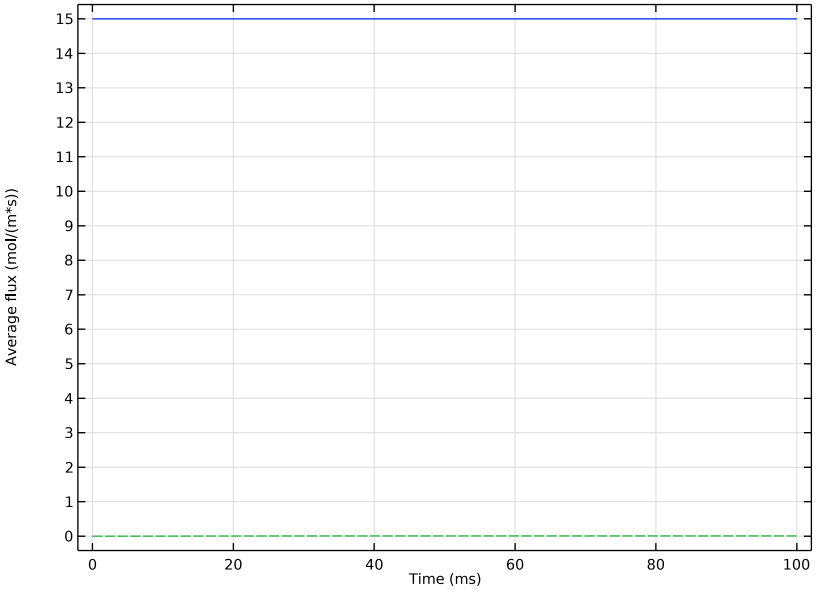


Figure 3: Average flux at the flux boundary in the detailed 2D model (solid blue line) and the 1D homogenized approximation (dashed green line).

Notes About the COMSOL Implementation

Both models described above are straightforward to define in COMSOL Multiphysics. One feature that is of great use in this example is the ability to define integration coupling operators to generate the values of the integrals needed to evaluate the results. The definition of these integrals is described in detail in the step-by-step instructions below.

Application Library path: `COMSOL_Multiphysics/Diffusion/effective_diffusivity`

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 Diluted Species (tds)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

6 Click **Done**.

Insert the geometry sequence to focus on the simulation. If you want to know how to build the geometry, you find instructions in the appendix.

GEOMETRY 1

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

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

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

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 In the table, enter the following settings:

Name	Expression	Value	Description
D2	1e-5[m^2/s]	1E-5 m²/s	Diffusion coefficient
c_max	3[mol/m^3]	3 mol/m³	Peak initial concentration
k_f	5[m/s]	5 m/s	Mass transfer coefficient
a	1000	1000	Dimensionless constant

Variables 1

1 In the **Home** toolbar, click a= **Variables** and choose **Global Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
c0	c_max*exp(a*(-(x/0.4[mm])^2))	mol/m³	Initial concentration

The geometry sequence contains several selections. They are useful when defining the boundary conditions and a nonlocal integration coupling, and also during postprocessing.

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 **Transport Mechanisms** section.

3 Clear the **Convection** check box.

This setting gives a pure diffusion interface.

Transport Properties 1

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

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

3 In the D_c text field, type D2.

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 In the *c* text field, type `c0`.

Concentration 1

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

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

3 From the **Selection** list, choose **Left boundary**.

4 Locate the **Concentration** section. Select the **Species c** check box.

5 In the $c_{0,c}$ text field, type `c_max`.

Flux 1

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

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

3 From the **Selection** list, choose **Right boundary**.

4 Locate the **Inward Flux** section. From the **Flux type** list, choose **External convection**.

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

6 In the $k_{c,c}$ text field, type `k_f`.

DEFINITIONS

Proceed to define a variable for the average flux through the porous structure. Begin by defining a nonlocal average coupling on the rightmost boundary.

Average 1 (aveop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Average**.

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

3 From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Left boundary**.

Variables 2

1 In the **Definitions** toolbar, click **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`flux_avg`	`aveop1(k_f*c)`	mol/(m²·s)	`Average flux`

MESH 1

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Build All**.

STUDY 1

Step 1: Time Dependent

1. In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.
2. In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
3. From the **Time unit** list, choose **ms**.
4. In the **Output times** text field, type `range(0,2,100)`.
5. In the **Home** toolbar, click **Compute**.

RESULTS

Concentration (tds)

The first default plot shows concentration and flux stream lines.

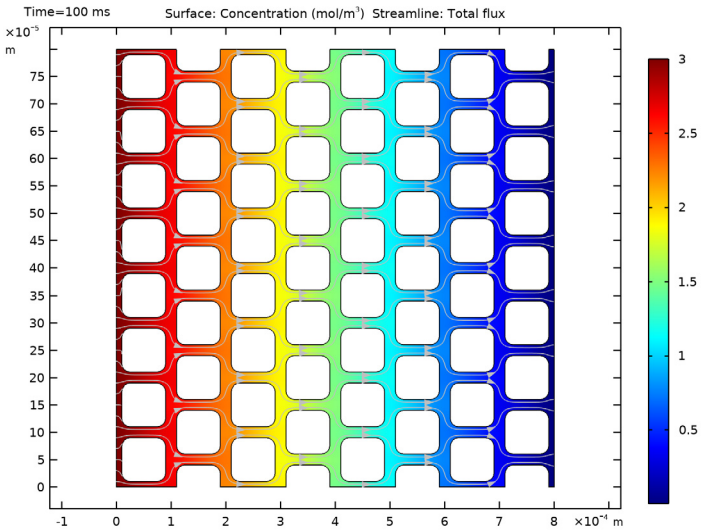
Streamline 1

1. In the **Model Builder** window, expand the **Concentration (tds)** node, then click **Streamline 1**.
2. In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
3. From the **Positioning** list, choose **On selected boundaries**.
4. Locate the **Selection** section. Select the **Activate Selection** toggle button.
5. Select Boundary 1 only.
6. Locate the **Streamline Positioning** section. In the **Number** text field, type 40.
7. In the **Concentration (tds)** toolbar, click **Plot**.

Concentration (tds)

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

The plot shows the concentration at the end time, that is, 0.1 seconds.



You can also plot the concentration at different time steps.

2 In the **Model Builder** window, click **Concentration (tds)**.

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

4 From the **Time (ms)** list, choose **50**.

5 In the **Concentration (tds)** toolbar, click **Plot**.

Compare this plot to the one shown in Figure 2.

1D Plot Group 2

Now, plot the average flux.

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

Point Graph 1

1 Right-click **1D Plot Group 2** and choose **Point Graph**.

2 In the **Settings** window for **Point Graph**, locate the **Selection** section.

3 From the **Selection** list, choose **Top-right vertex**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>flux_avg - Average flux - mol/(m²·s)**.

Molar fluxes

1 In the **Model Builder** window, click **1D Plot Group 2**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

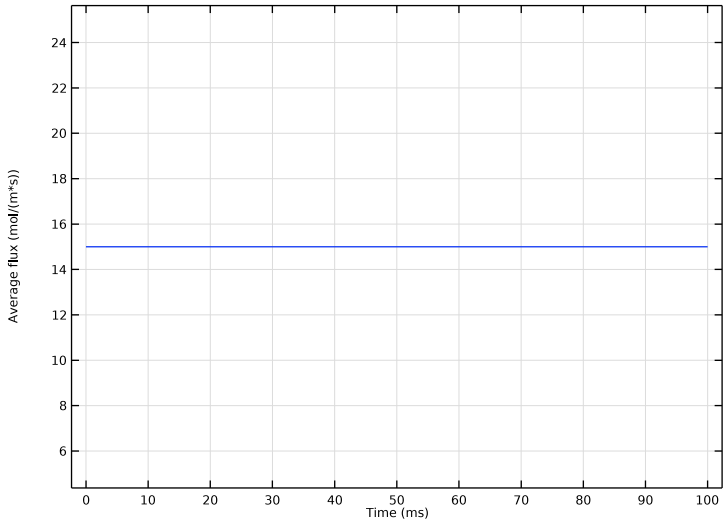
3 In the **Label** text field, type `Molar fluxes`.

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

5 Locate the **Plot Settings** section. Select the **y-axis label** check box.

6 In the associated text field, type `Average flux (mol/(m*s))`.

7 In the **Molar fluxes** toolbar, click **Plot**.



To get the porosity of the domain for the 1D model, perform a surface integration.

Surface Integration 1

1 In the **Results** toolbar, click **More Derived Values** and choose **Integration> Surface Integration**.

2 In the **Settings** window for **Surface Integration**, locate the **Selection** section.

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

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit
1/(0.8[mm])^2	1

The denominator in this expression represents the product of the length and the width of the 2D model structure.

5 Click **Evaluate**.

TABLE

1 Go to the **Table** window.

The evaluated value of the integral should be close to 0.383.

ROOT

Now turn to the 1D model.

ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component>1D**.

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 Diluted Species (tds)**.

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

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

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

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** check box for **Transport of Diluted Species (tds)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Time Dependent**.

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

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

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

GEOMETRY 2

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 2 (comp2)** right-click **Geometry 2** and choose **Interval**.

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

3 In the table, enter the following settings:

Coordinates (m)
0
8e-4

4 Click **Build Selected**.

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

GLOBAL DEFINITIONS

Parameters 1

Add the following parameters to those you already defined.

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
epsilon	0.383	0.383	Porosity
D1	2.15e-6[m^2/s]	2.15E-6 m²/s	Diffusion coefficient, 1D

TRANSPORT OF DILUTED SPECIES 2 (TDS2)

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

2 In the **Settings** window for **Transport of Diluted Species**, locate the **Transport Mechanisms** section.

3 Clear the **Convection** check box.

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 **Diffusion** section.

3 In the D_{c2} text field, type `D1/epsilon`.

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 In the $c2$ text field, type `c0`.

Concentration 1

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

2 Select Boundary 1 only.

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

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

5 In the $c_{0,c2}$ text field, type `c_max`.

Flux 1

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

2 Select Boundary 2 only.

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

4 From the **Flux type** list, choose **External convection**.

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

6 In the $k_{c,c2}$ text field, type `k_f/epsilon`.

DEFINITIONS (COMP2)

Create a variable for the flux in the homogenized 1D model.

Variables 3

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

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`flux_hom`	`k_f*c2`	mol/(m²·s)	`Flux, 1D model`

MESH 2

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

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Extra fine**.

4 Click **Build All**.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 From the **Time unit** list, choose **ms**.

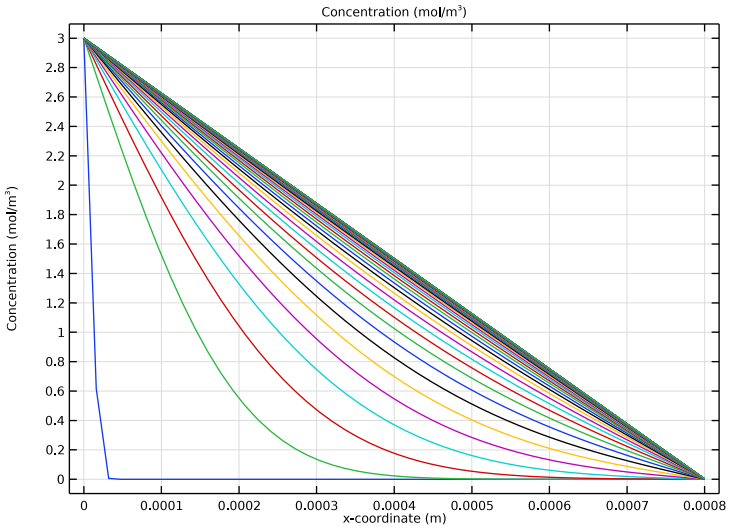
4 In the **Output times** text field, type `range(0,2,100)`.

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

RESULTS

Concentration (tds2)

The default plot for the 1D model shows the concentration for all time steps.



Finally, plot the result for the flux at the flux boundary in the homogenized 1D model in the same plot as the 2D result for comparison.

Point Graph 2

1 In the **Model Builder** window, right-click **Molar fluxes** and choose **Point Graph**.

2 In the **Settings** window for **Point Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 2 (3) (sol2)**.

4 Select Boundary 2 only.

5 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 2 (comp2)>Definitions>Variables>flux_hom - Flux, 1D model - mol/(m²·s)**.

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

7 In the **Molar fluxes** toolbar, click **Plot**.

Compare the result with that shown in Figure 3.

Appendix — Geometry Modeling Instructions

This section describes the individual steps for building the geometry sequence.

These steps replace the **Insert Sequence** step in the previous instruction

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 `0.08[mm]`.

4 Locate the **Position** section. In the **x** text field, type `0.01[mm]`.

5 In the **y** text field, type `0.01[mm]`.

6 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

7 From the **Show in physics** list, choose **Off**.

With the last step, the square can be used as an input object for various geometry operations.

Fillet 1 (fil1)

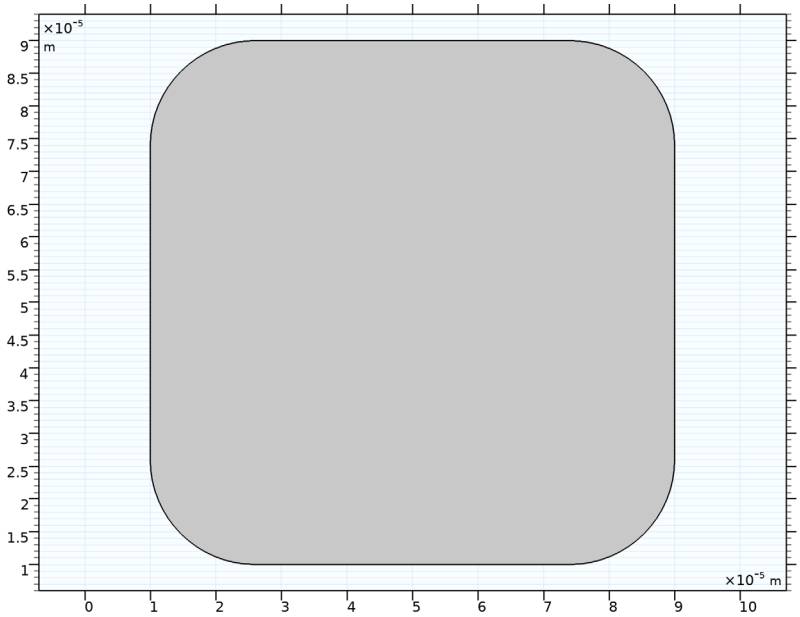
1 In the **Geometry** toolbar, click **Fillet**.

2 In the **Settings** window for **Fillet**, locate the **Points** section.

3 From the **Vertices to fillet** list, choose **Square 1**. This rounds all four corners.

4 Locate the **Radius** section. In the **Radius** text field, type `0.016[mm]`.

5 Click **Build Selected**.



Array 1 (arr1)

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

2 Select the object **fil1** only.

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

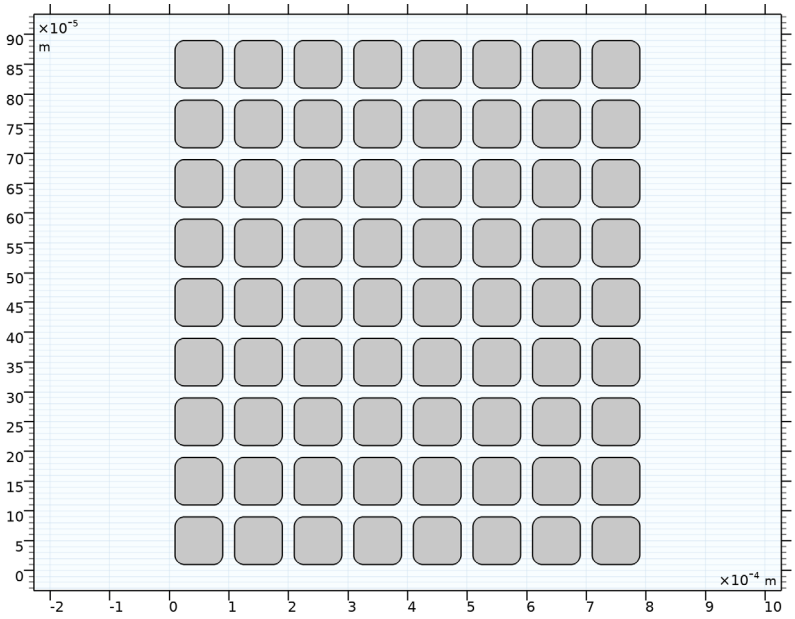
4 In the **x size** text field, type `8`.

5 In the **y size** text field, type `9`.

6 Locate the **Displacement** section. In the **x** text field, type `0.1[mm]`.

7 In the **y** text field, type `0.1[mm]`.

8 Click **Build Selected**.



There is an offset between the individual rows.

Move 1 (mov1)

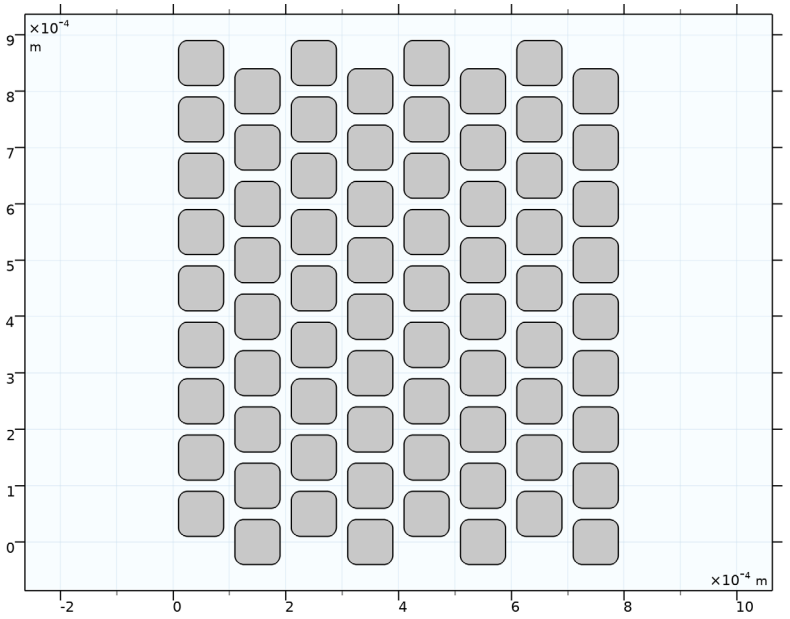
1 In the **Geometry** toolbar, click **Transforms** and choose **Move**.

2 In the **Settings** window for **Move**, locate the **Displacement** section.

3 In the **y** text field, type `-0.05[mm]`.

4 Select every second row of the array.

5 Click **Build Selected**.



The array of squares forms the holes in the geometry. Create the outer domain.

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 `0.8[mm]`.

4 In the **Height** text field, type `0.8[mm]`.

Difference 1 (dif1)

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

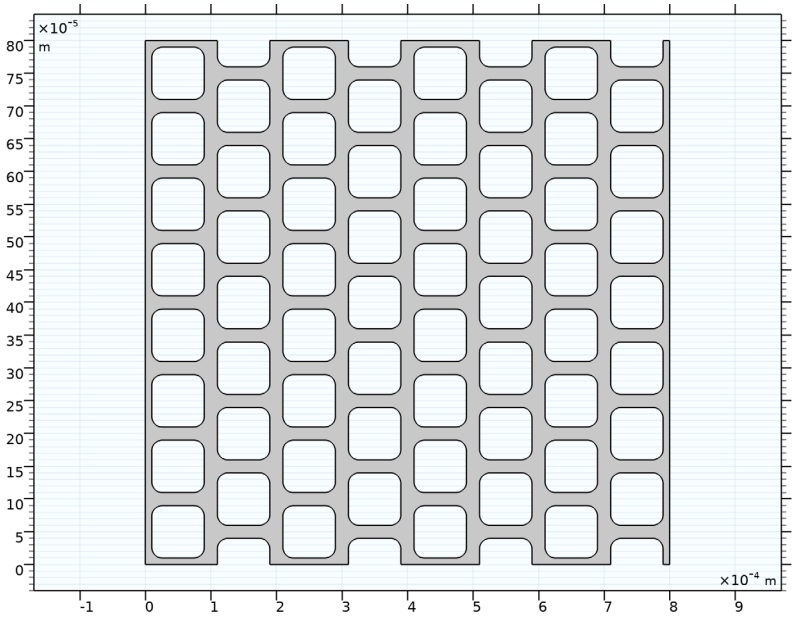
2 Select the object **r1** only.

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

4 Find the **Objects to subtract** subsection. Select the **Activate Selection** toggle button.

5 From the **Objects to subtract** list, choose **Square 1** since the first square creates a **Selection of Resulting Entities**, all squares are included in this selection.

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**.

Regarding physic settings and post processing it is helpful to define **Selections** on Point and Boundary level

Top-right vertex

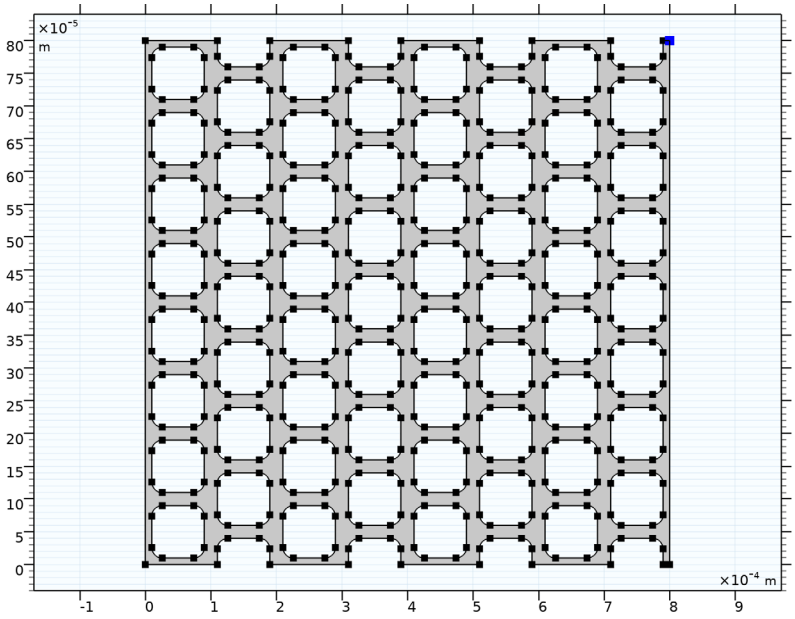
1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, locate the **Entities to Select** section.

3 From the **Geometric entity level** list, choose **Point**.

4 In the **Label** text field, type `Top-right vertex`.

5 On the object **fin**, select Point 532 only.



Left boundary

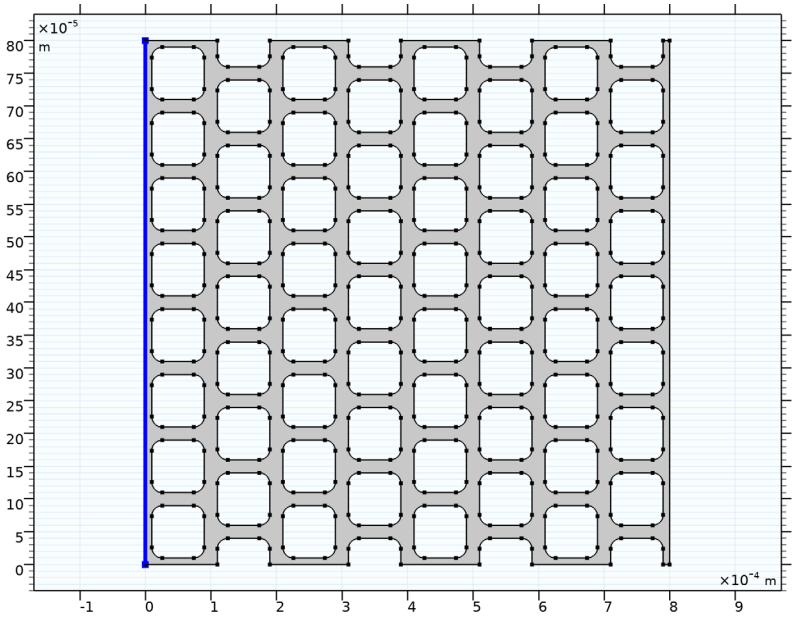
1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, locate the **Entities to Select** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 In the **Label** text field, type `Left boundary`.

5 On the object **fin**, select Boundary 1 only.



Right boundary

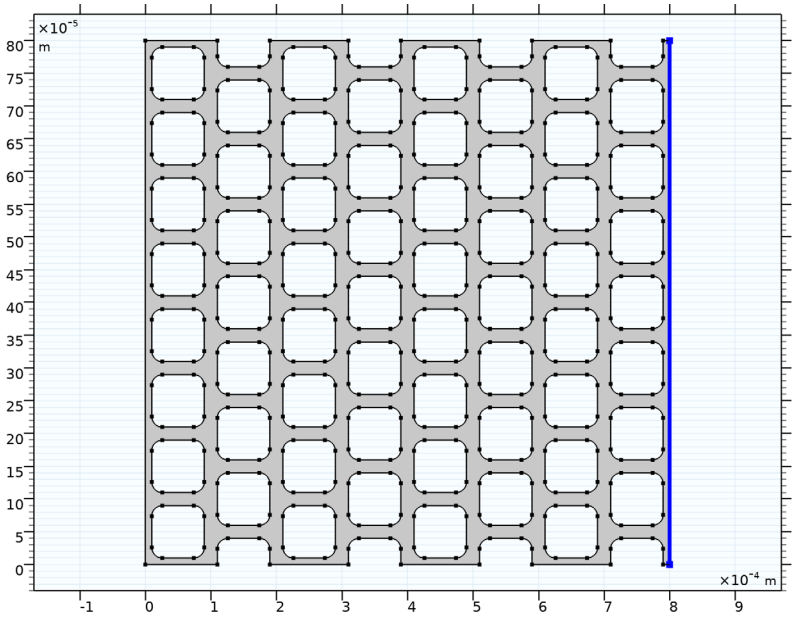
1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, locate the **Entities to Select** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 276 only.

5 In the **Label** text field, type `Right boundary`.



6 Click **Build Selected**.