Model created in COMSOL Multiphysics 6.4

Analyzing Porous Structures on the Microscopic Scale

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Introduction

Modeling flow through realistic porous structures is difficult due to the complexity of the structure itself. Resolving the flow field in detail is not feasible in real-life applications. Therefore, macroscopic approaches utilizing averaged quantities of the porous structure, such as porosity and permeability, are used. This example analyzes the flow field at the pore scale in detail. The results are used to validate and adapt the macroscopic description, which in turn are used to model large-scale porous geometries.

Model Definition

The modeled geometry shown in Figure 1 is a representative volume element (RVE) whose properties are representative for the entire system.

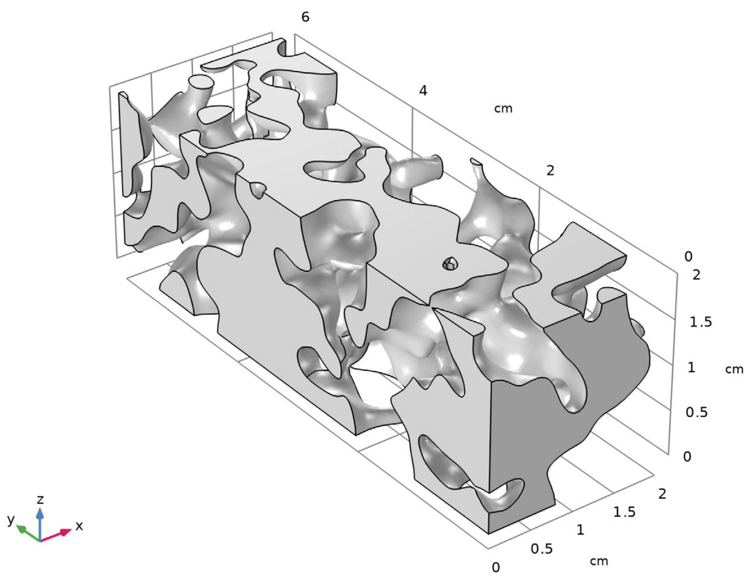


Figure 1: Geometry of the RVE's pore volume.

Because only the area of the pore space is required for modeling, the porous matrix is not resolved explicitly. The RVE has a quadratic cross section of 2 cm side length and a width of 6 cm. Water flows with a velocity of $u = 0.1\ \mathrm{mm/s}$ and can flow out freely in the normal direction at the other end. The other boundaries are assumed to be symmetry boundaries.

This condition does not correspond to the actual situation, but for modeling an RVE, symmetry boundary conditions are very well suited.

To characterize the flow inside the porous structure one can estimate the Reynolds number according to

$$\mathrm{Re} = \frac{\rho u L}{\mu}$$

with the water density $\rho = 1000\ \mathrm{kg/m^3}$ and viscosity $\mu = 10^{-3}\ \mathrm{Pa{\cdot}s}$. The cross-section side length serves as the characteristic length scale, L. This results in $\mathrm{Re} = 2$ and the Stokes equation can be used to describe the flow where inertia terms are neglected.

Finally, the goal of the model is to obtain the averaged values for porosity and permeability to describe a macroscopic model with, for example, Darcy's law or the Brinkman equation. The porosity is defined as the fraction of pore space volume V_{fluid} to total volume V_{tot}:

$$\varepsilon = \frac{V_{\mathrm{fluid}}}{V_{\mathrm{tot}}}.$$

To calculate the permeability κ ($\mathrm{m^2}$) the following relationship is used:

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p$$

Approximating the pressure gradient ∇p by the pressure difference between the inlet and the outlet, Δp, divided by the side length L, and replacing the velocity vector $\mathbf{u}$ by the outlet velocity u_{out} in the flow direction gives the expression

$$\kappa = u_{\mathrm{out}}\mu\frac{L}{\Delta p}.$$

Results and Discussion

First of all it is interesting to have a look at the mesh, or rather the mesh quality. Although the mesh quality in itself says nothing about the quality of the results, a good mesh quality is beneficial for convergence. The overall mesh quality as shown in Figure 2 is very good.

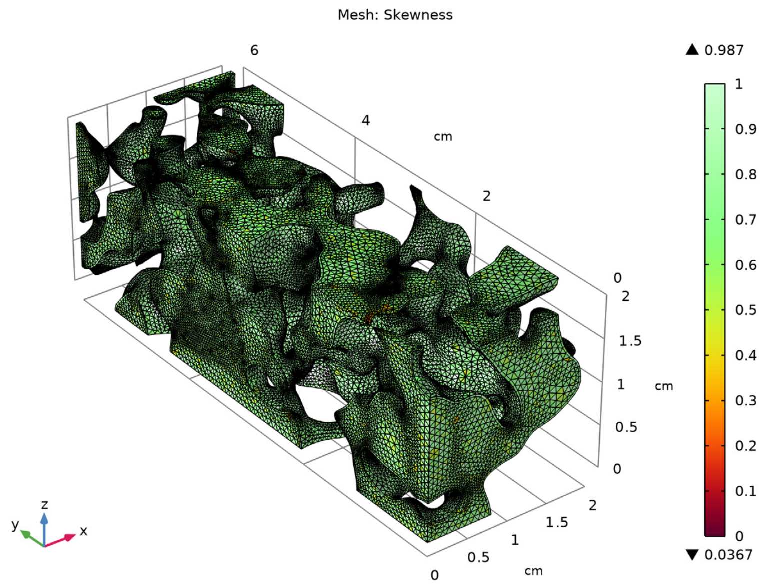


Figure 2: Mesh quality plot.

The velocity field in the RVE is shown in Figure 3. Characteristic for the flow in a porous material are areas with high and areas with low velocity. In some areas the flow also stagnates. This behavior is characterized by the permeability.

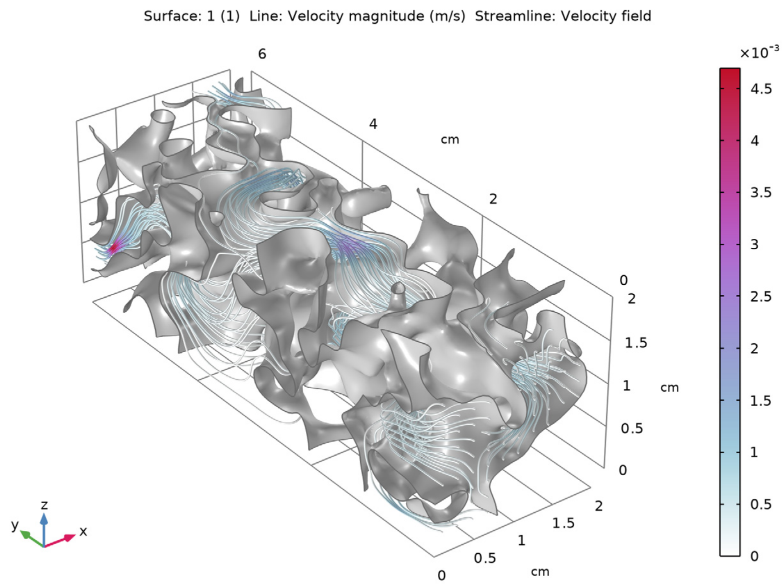


Figure 3: Velocity in the RVE.

From the simulation the values for the porosity and permeability are obtained, with $\varepsilon = 0.373$ and $\kappa \approx 3 \cdot 10^{-8} \mathrm{m}^2$.

Notes About the COMSOL Implementation

An STL file of the porous structure is imported in a mesh-based geometry sequence. This means that the geometry sequence is kept empty. The geometry is meshed with a physics-controlled mesh that adds a boundary layer mesh to resolve the velocity gradients at the boundaries of the porous matrix.

Application Library path: `Porous_Media_Flow_Module/Fluid_Flow/pore_scale_flow_3d`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

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

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GEOMETRY 1

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

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **cm**.

COMPONENT 1 (COMP1)

Create a mesh-based geometry and import the STL file. This means that the geometry sequence will be kept empty.

MESH-BASED GEOMETRY 1

In the **Mesh** toolbar, click **Add Mesh** and choose **Add Mesh-Based Geometry**.

Import 1

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

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

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `pore_scale_flow_3d.stl`.

5 From the **Boundary partitioning** list, choose **Detect boundaries**.

Increase the tolerance to collapse small and sliver mesh elements. This avoids the creation of small boundaries.

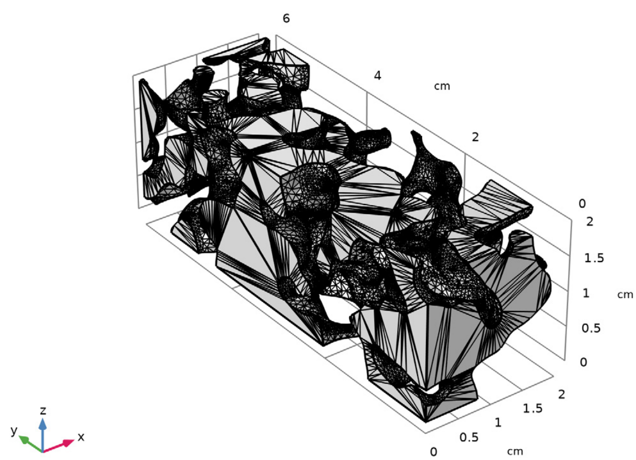
6 From the **Repair tolerance** list, choose **Absolute**.

7 In the **Absolute tolerance** text field, type `1e-5`.

An increased **Maximum neighbor angle** will aid the algorithm in forming as few boundaries as possible while still recognizing the planar faces.

8 Locate the **Detect Faces** section. In the **Maximum neighbor angle** text field, type `62`.

9 Locate the **Import** section. Click **Import**.



Inlet

Create selections to use them throughout the model set up.

1 In the **Mesh** toolbar, click **Selections** and choose **Box Selection**.

2 In the **Settings** window for **Box Selection**, type `Inlet` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Box Limits** section. In the **y maximum** text field, type `0.01`.

5 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside box**.

6 Click **Build Selected**.

Outlet

1 In the **Mesh** toolbar, click **Selections** and choose **Box Selection**.

2 In the **Settings** window for **Box Selection**, type `Outlet` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Box Limits** section. In the **y minimum** text field, type `5.99`.

5 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside box**.

Wall

1 In the **Mesh** toolbar, click **Selections** and choose **Box Selection**.

2 In the **Settings** window for **Box Selection**, type `Wall` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Box Limits** section. In the **x minimum** text field, type `0.01`.

5 In the **x maximum** text field, type `1.99`.

6 In the **y minimum** text field, type `0.01`.

7 In the **y maximum** text field, type `5.99`.

8 In the **z minimum** text field, type `0.01`.

9 In the **z maximum** text field, type `1.99`.

Symmetry

1 In the **Mesh** toolbar, click **Selections** and choose **Complement Selection**.

2 In the **Settings** window for **Complement Selection**, type `Symmetry` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Click + **Add**.

5 In the **Add** dialog, in the **Selections to invert** list, choose **Inlet**, **Outlet**, and **Wall**.

6 Click **OK**.

Join Entities 1

Join all the boundaries of the free surface to one boundary.

1 In the **Mesh** toolbar, click **Entities** and choose **Join Entities**.

2 In the **Settings** window for **Join Entities**, locate the **Geometric Entity Selection** section.

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

4 From the **Selection** list, choose **Wall**.

5 Click **Build Selected**.

Finalize

1 In the **Model Builder** window, right-click **Finalize** and choose **Build Selected**.

Take a look at the **Information** section of **Join Entities 1** or in the **Messages** log to confirm that the mesh now contains one domain and 37 boundaries.

GLOBAL DEFINITIONS

Add some parameters that are used to set up the model.

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
rho_f	1000[kg/m^3]	1000 kg/m³	Fluid density
mu_f	1e-3[Pa*s]	0.001 Pa·s	Fluid viscosity
u_in	1e-4[m/s]	1E-4 m/s	Inlet velocity
width	2[cm]	0.02 m	REV width
length	6[cm]	0.06 m	REV length
V_tot	width^2*length	2.4E-5 m³	Total REV volume

MATERIALS

Material Link 1 (matlnk1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **More Materials** > **Material Link**.

2 In the **Settings** window for **Material Link**, locate the **Link Settings** section.

3 Click **Blank Material**.

GLOBAL DEFINITIONS

Material 1 (mat1)

1 In the **Model Builder** window, under **Global Definitions** > **Materials** click **Material 1 (mat1)**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	rho_f	kg/m³	Basic
Dynamic viscosity	mu	mu_f	Pa·s	Basic

CREEPING FLOW (SPF)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Creeping Flow (spf)**.

2 In the **Settings** window for **Creeping Flow**, click to expand the **Discretization** section.

3 From the **Discretization of fluids** list, choose **P1+P1**.

Linear elements reduce the number of degrees of freedom to be solved. Because the geometry already requires a fine mesh, using linear elements decreases computational time and memory requirements while maintaining sufficient accuracy.

Inlet 1

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

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

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Velocity** section. In the U_0 text field, type `u_in`.

Outlet 1

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

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

3 From the **Selection** list, choose **Outlet**.

4 Locate the **Pressure Conditions** section. Select the **Normal flow** checkbox.

Symmetry 1

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

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

3 From the **Selection** list, choose **Symmetry**.

MESH 1

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

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

3 From the **Element size** list, choose **Fine**.

4 Click **Build All**.

5 In the **Mesh** toolbar, click **Plot**.

RESULTS

Mesh 1

Compare with Figure 2. The overall mesh quality is very good. The amount of mesh elements with low quality (skewness) is low. Mesh quality is not an indication for the accuracy of the solution, but it affects the convergence behavior.

STUDY 1

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

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

3 Clear the **Generate default plots** checkbox.

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

RESULTS

Create the plot as shown in Figure 3.

In the **Model Builder** window, expand the **Results** node.

Surface 1

1 In the **Model Builder** window, expand the **Results > Datasets** node.

2 Right-click **Results > Datasets** and choose **Surface**.

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

4 From the **Selection** list, choose **Wall**.

Velocity

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

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

3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

Surface 1

1 Right-click **Velocity** and choose **Surface**.

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

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

4 Locate the **Expression** section. In the **Expression** text field, type `1`.

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

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

Line 1

1 In the **Model Builder** window, right-click **Velocity** and choose **Line**.

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

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

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

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

6 In the **Velocity** toolbar, click **Plot**.

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

8 On Windows, click the colored bar underneath, or — if you are running the cross-platform desktop — the **Color** button. Choose a darker shade of gray.

Streamline 1

1 Right-click **Velocity** and choose **Streamline**.

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

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Streamline Positioning** section. In the **Number** text field, type `60`.

5 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Tube**.

6 Select the **Radius scale factor** checkbox. In the associated text field, type `0.01`.

Color Expression 1

1 Right-click **Streamline 1** and choose **Color Expression**.

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

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

Next, determine the porosity and permeability for our REV in order to perform simulations at the macroscopic level.

DEFINITIONS

Integration 1 (intop1)

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

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

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

Average Inlet

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

2 In the **Settings** window for **Average**, type `Average Inlet` in the **Label** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Inlet**.

Average Outlet

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

2 In the **Settings** window for **Average**, type `Average Outlet` in the **Label** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Outlet**.

Variables 1

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
por	intop1(1)/V_tot		Porosity
dPdL	-(aveop2(p)-aveop1(p))/length	N/m^3	Pressure drop
u_out	spf.out1.massFlowRate/rho_f/width^2	m/s	Superficial outlet velocity
kappa	u_out*mu_f/dPdL	m^2	Permeability

Since you have introduced new variables, the solution needs to be updated. It is not necessary to compute the study again.

STUDY 1

In the **Study** toolbar, click **Update Solution**.

RESULTS

Global Evaluation 1

1 In the **Results** toolbar, click 8.5 **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, click **Add Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **por - Porosity - 1**.

3 Click **Add Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **kappa - Permeability - m²**.

4 Click **Evaluate**.

The results are shown in the **Table** window. The porosity is 0.373 and the permeability is about 3e-8m^2. These results can now be used for calculations of large scale models.

Streamline 1

To make the results even more descriptive, create an animation.

1 In the **Model Builder** window, under **Results** > **Velocity** click **Streamline 1**.

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

3 Find the **Point style** subsection. From the **Type** list, choose **Interactive arrow**.

4 In the **Extra release times** text field, type `2000`.

Animation 1

1 In the **Velocity** toolbar, click **Animation** and choose **Player**.

You can adjust the number of frames to obtain a smooth animation of the interactive arrows. This animation visualizes very nicely that there are regions in the porous medium with both very slow and very high velocity.