Created in COMSOL Multiphysics 6.0

Analyzing Porous Structures on the Microscopic Scale

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 elementary volume (REV) whose properties are representative for the entire system.

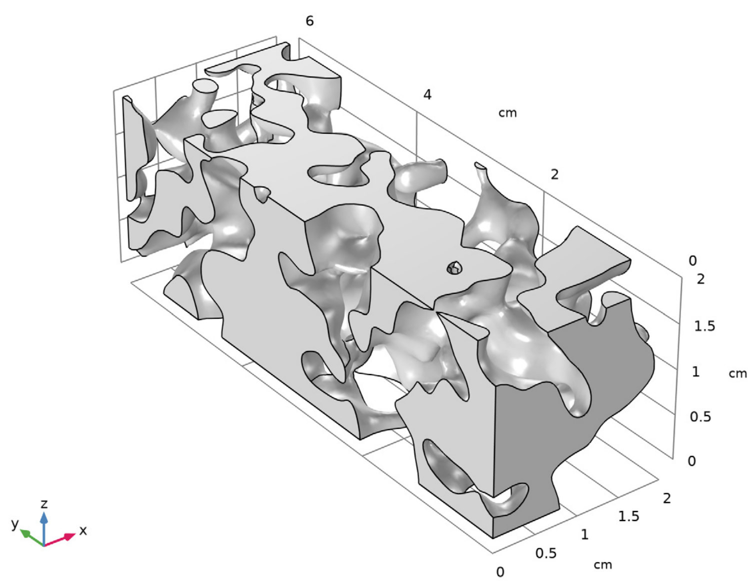


Figure 1: Geometry of the REV's pore volume.

Because only the area of the pore space is required for modeling, the porous matrix is not resolved explicitly. The REV has a quadratic cross section of 2 cm side length and a width of 6 cm. Water flows with a velocity of $u = 0.1$ 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 does not correspond to the actual situation, but for modeling an REV, 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.

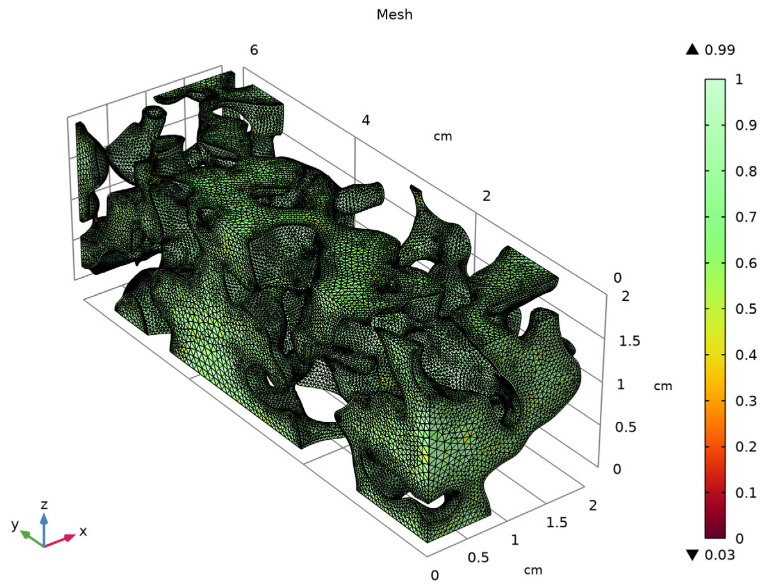


Figure 2: Mesh quality plot.

The velocity field in the REV 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.

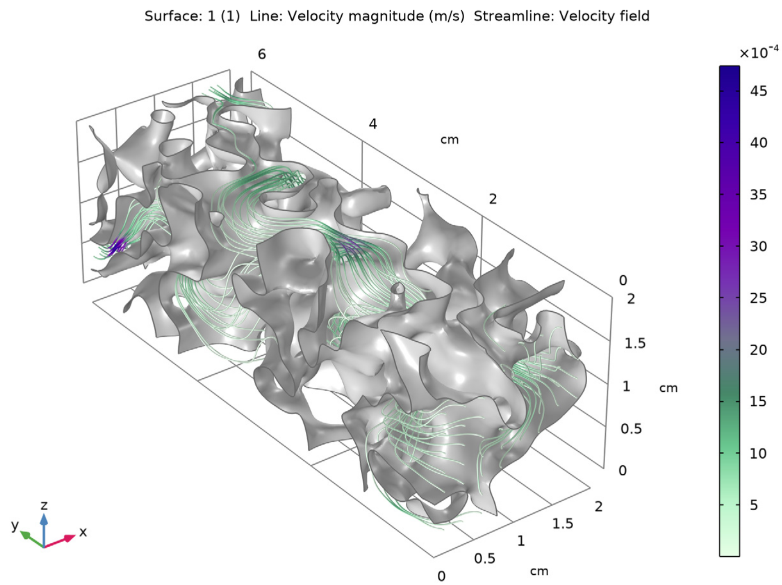


Figure 3: Velocity in the REV.

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 and remeshed directly in the meshing sequence. This means that the geometry sequence is kept empty. To resolve the velocity gradients at the boundaries of the porous matrix, add a boundary layer mesh.

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**.

   Import the STL file and remesh it directly in the meshing sequence. This means that the geometry sequence will be kept empty.

MESH 1

The meshing sequence will define the geometric model on which the physics is defined. The mesh is therefore set up completely before assigning material and physics.

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.

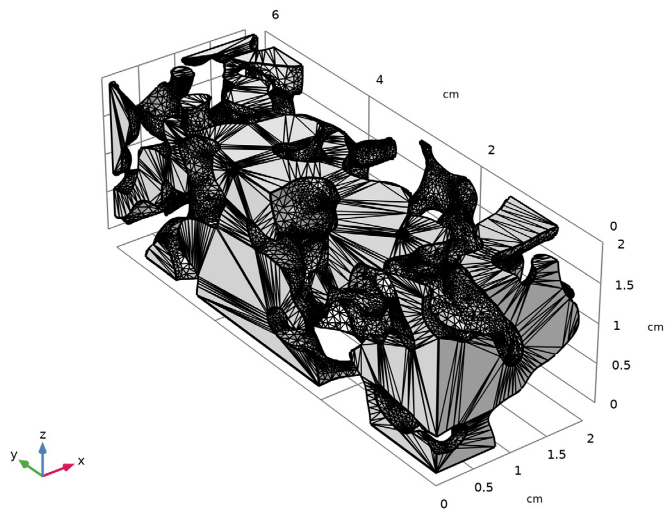
6 From the **Repair tolerance** list, choose **Absolute**.

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**.



Join Entities 1

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

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

Instead of clicking on boundaries in the **Graphics** window, paste the numbers from this document or type them in manually.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `14-20` in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Join Entities**, click **Build Selected**.

The imported STL file only contains a triangle mesh without domains. Use **Create Domains** to form the fluid domain in the enclosed volume.

Create Domains 1

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

2 In the **Settings** window for **Create Domains**, click **Build Selected**.

Take a look in the **Messages** log to confirm that the mesh now contains one domain and 37 boundaries.

Next, increase the quality of the triangle mesh by remeshing the faces using a **Free Triangular** operation. This will also result in triangles of more equal size.

Free Triangular 1

1 In the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.

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

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

Size

1 In the **Model Builder** window, expand the **Free Triangular 1** node, then click **Size**.

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

3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 From the **Predefined** list, choose **Fine**.

Free Triangular 1

Set an even finer mesh size on the free surface.

Size 1

1 In the **Model Builder** window, right-click **Free Triangular 1** and choose **Size**.

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

3 Click **Clear Selection**.

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `14 36 37` in the **Selection** text field.

6 Click **OK**.

7 In the **Settings** window for **Size**, locate the **Element Size** section.

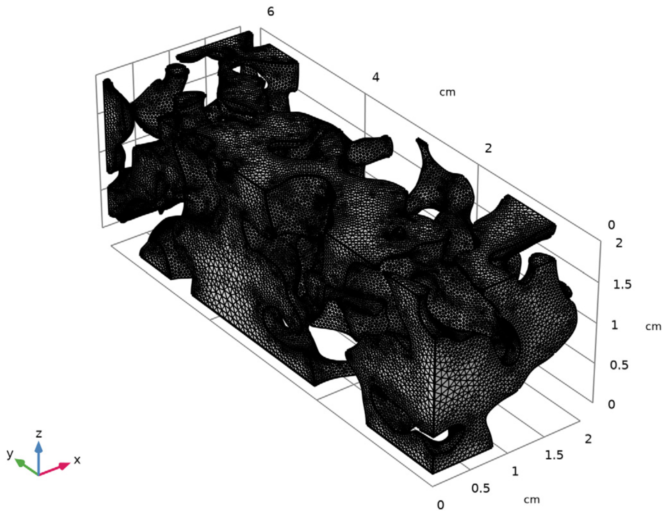
8 Click the **Custom** button.

9 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

10 In the associated text field, type `0.04[cm]`.

11 Click **Build Selected**.

The surface mesh is now of good quality.



Next, generate a tetrahedral mesh in the domain of the porous structure.

Free Tetrahedral 1

In the **Mesh** toolbar, click **Free Tetrahedral**.

Size

1 In the **Model Builder** window, expand the **Free Tetrahedral 1** node, then click **Size**.

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

3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 From the **Predefined** list, choose **Fine**.

5 Click **Build Selected**.

Boundary Layers 1

In order to resolve the large velocity gradients at the boundaries to the porous matrix properly, add a boundary layer mesh.

In the **Mesh** toolbar, click **Boundary Layers**.

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `14 36 37` in the **Selection** text field.

5 Click **OK**.

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

7 In the **Number of layers** text field, type `1`.

8 In the **Thickness adjustment factor** text field, type `10`.

9 Click **Build Selected**.

10 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.

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

Water

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

2 In the **Settings** window for **Material**, type `Water` in the **Label** text field.

3 Locate the **Material Contents** section. 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 Select Boundary 2 only.

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

4 In the U_0 text field, type `u_in`.

5 Locate the **Boundary Selection** section. Click **Create Selection**.

6 In the **Create Selection** dialog box, type `Inlet` in the **Selection name** text field.

7 Click **OK**.

Outlet 1

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

2 Select Boundaries 16 and 21 only.

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

4 Select the **Normal flow** check box.

5 Locate the **Boundary Selection** section. Click **Create Selection**.

6 In the **Create Selection** dialog box, type `Outlet` in the **Selection name** text field.

7 Click **OK**.

Create a few more selections to use them throughout the model set up.

DEFINITIONS

Wall

1. In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node.
2. Right-click **Definitions** and choose **Selections>Explicit**.
3. In the **Settings** window for **Explicit**, type `Wall` in the **Label** text field.
4. Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
5. Select Boundaries 4, 10, and 30 only.

   It might be easier to select the correct boundary by using the **Selection List** window. To open this window, in the **Home** toolbar click **Windows** and choose **Selection List**. (If you are running the cross-platform desktop, you find **Windows** in the main menu.)

   Note that the boundary numbering differs compared to the numbering in the meshing sequence. This is due to the associativity update that runs when the Finalize node is built.

All boundaries

1. In the **Definitions** toolbar, click **Explicit**.
2. In the **Settings** window for **Explicit**, locate the **Input Entities** section.
3. From the **Geometric entity level** list, choose **Boundary**.
4. Select the **All boundaries** check box.
5. In the **Label** text field, type `All boundaries`.

Symmetry

1. In the **Definitions** toolbar, click **Difference**.
2. In the **Settings** window for **Difference**, 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. Under **Selections to add**, click **Add**.
5. In the **Add** dialog box, select **All boundaries** in the **Selections to add** list.
6. Click **OK**.
7. In the **Settings** window for **Difference**, locate the **Input Entities** section.
8. Under **Selections to subtract**, click **Add**.
9. In the **Add** dialog box, in the **Selections to subtract** list, choose **Inlet**, **Outlet**, and **Wall**.

10 Click **OK**.

CREEPING FLOW (SPF)

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**.

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** check box.
4. In the **Home** toolbar, click **Compute**.

   Create the plot as shown in Figure 3.
5. In the **Results** toolbar, click **More Datasets** and choose **Surface**.

RESULTS

Surface 1

1. In the **Settings** window for **Surface**, locate the **Selection** section.
2. 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** check box.

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 `40`.

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

6 Select the **Radius scale factor** check box.

7 In the associated text field, type `0.0075`.

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 **AuroraBorealis**.

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 **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**.

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 0.371 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.