Model created in COMSOL Multiphysics 6.4

Estimating Permeability from Microscale Porous Structures

Introduction

This tutorial model demonstrates how to compute porosity and permeability of a sphere packing from a fully resolved microscopic model. These values are then used to model the sphere packing on the macroscopic scale using Darcy's Law.

Model Definition

The geometry used to calculate the permeability in the microscopic scale is shown in the figure below.

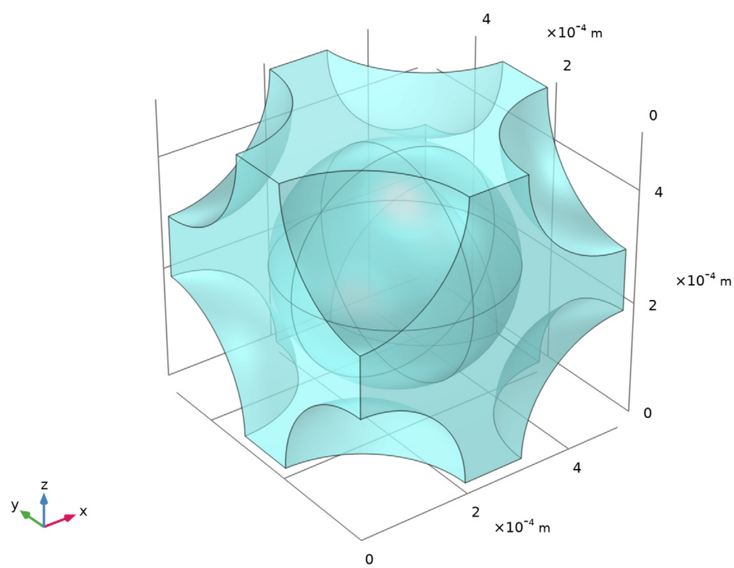


Figure 1: Geometry of the unit cell of a sphere packing.

A body-centered cubic (BCC) lattice is used. The flow around the spheres is described using the Creeping Flow interface. A pressure difference of 1 Pa is applied. The boundaries that correspond to the solid-fluid interface are defined as walls and the remaining boundaries are symmetry boundaries.

From this set up the porosity and permeability can be calculated. 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 (m^2) the following relationship is used

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

whereas the pressure gradient ∇p is replaced by the pressure drop across the unit divided by the size of the unit cell L and the velocity vector $\mathbf{u}$ is replaced by the normal velocity u_{out} in flow direction (z direction), hence

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

The computation is carried out for a range of porosities, and the resulting permeability values are used to determine a power-law relationship using the Least-Squares Fit method. The power law takes the form:

$$\kappa = b\varepsilon_{\mathrm{p}}^{n} \tag{1}$$

with the coefficients b and n to be computed from the fit.
To verify that a macroscopic approach using homogenization by deploying Darcy's Law gives accurate values, the model compares the mass flow per unit area (L^2).

Results and Discussion

The velocity field in the unit cell is shown in Figure 2.

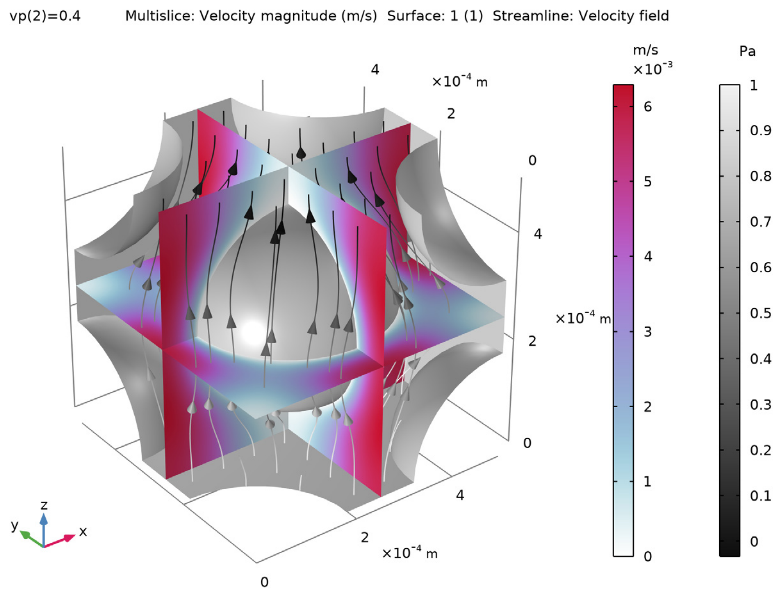


Figure 2: Velocity in the unit cell.

The Least-Squares Fit (Figure 3) results in b = 7.3e-9 and n = 4.2.

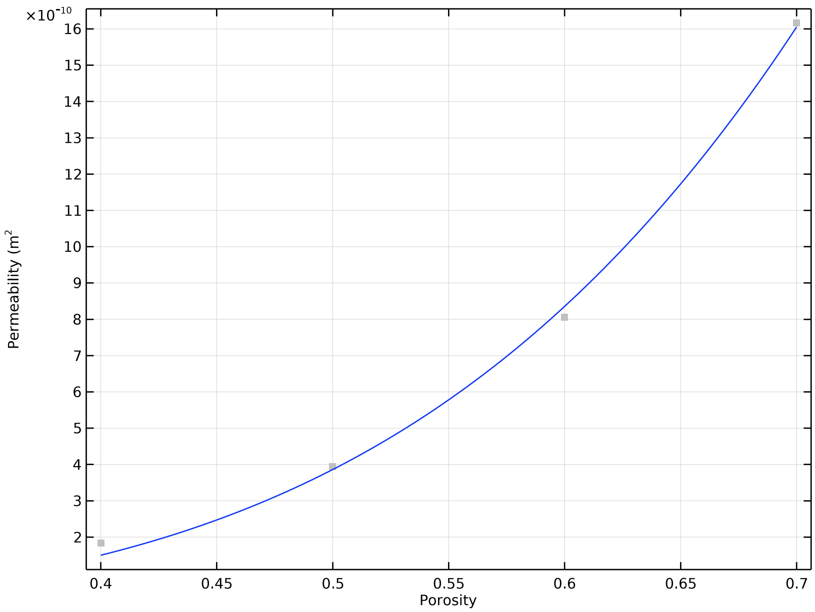


Figure 3: Computed results (gray squares) and fitted function (blue line).

[Figure 4](#) shows the pressure distribution in the macroscopic model.

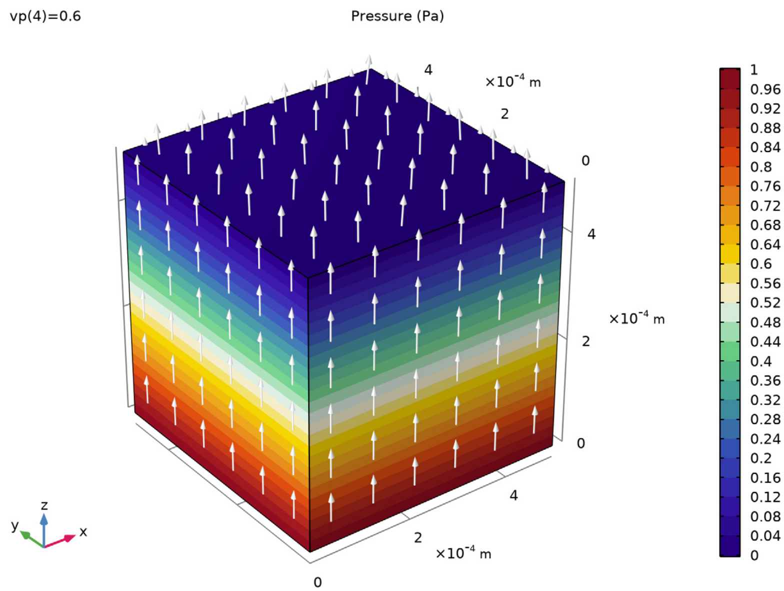


Figure 4: Pressure field for the macroscopic model.

To compare the accuracy of the power law model with the pore-scale model, the normal mass flow is computed and compared. The results are in good agreement (Figure 5).

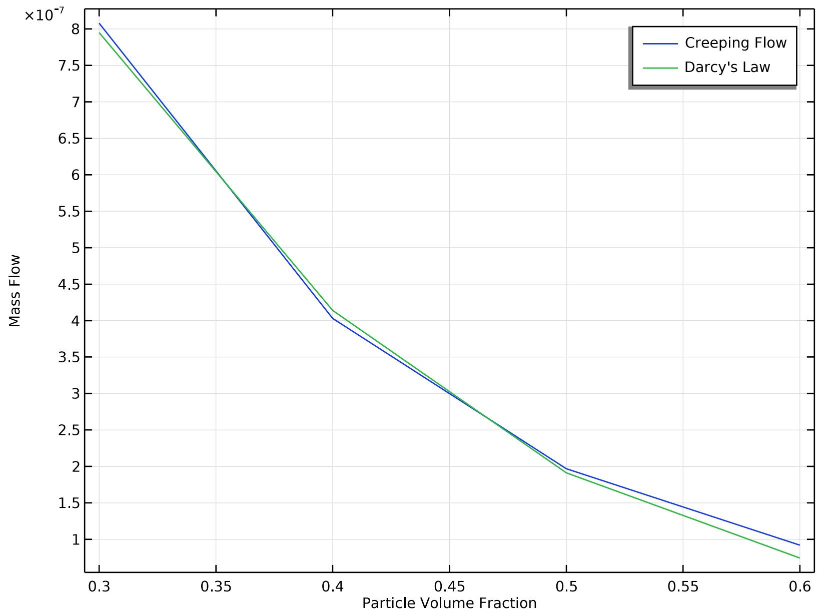


Figure 5: Normal mass flow (outflow) for different porosities compared.

Notes About the COMSOL Implementation

To generate the geometry of the unit cell of a sphere packing the COMSOL Multiphysics Part Libraries can be used. They contain sets of common parts or components that can simplify and streamline the construction of more complex geometries. The part library **Representative Volume Elements** offers several geometry parts for 2D and 3D geometries to choose from.

Application Library path: `Porous_Media_Flow_Module/Fluid_Flow/permeability_estimation`

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**.

Start setting up the model by defining some geometry parameters as the particle diameter, particle distance, and side length of the unit cell.

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
vp	0.5	0.5	Particle volume fraction
sp	1	1	Ratio of corner particle to center particle diameter
L	5e-4[m]	5E-4 m	Side length of unit cell
dp	((vp)*L^3/(1/6*pi*(1+sp^3)))^(1/3)	3.908E-4 m	Particle diameter
por	1-vp	0.5	Porosity

GEOMETRY 1

Now choose a representative volume element from the COMSOL Multiphysics part libraries and adjust it as desired.

PART LIBRARIES

1 From the **Windows** menu, choose **Part Libraries**.

2 In the **Part Libraries** window, select **COMSOL Multiphysics > Unit Cells and RVEs > Particulate Composites > particulate_body_centered_cubic** in the tree.

3 Click **Add to Geometry**.

4 In the **Select Part Variant** dialog, select **Specify particle volume fraction** in the **Select part variant** list.

5 Click **OK**.

GEOMETRY 1

Particulate Composite, Body-Centered Cubic 1 (pi1)

1 In the **Model Builder** window, expand the **Geometry 1** node, then click **Particulate Composite, Body-Centered Cubic 1 (pi1)**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
vp	vp	0.5	Particle volume fraction
sp	sp	1	Ratio of corner particle diameter to center particle diameter
wm	L	5E-4 m	Cell width
dm	L	5E-4 m	Cell depth
hm	L	5E-4 m	Cell height

The part comes with predefined selections. Only keep the selections that are used for the physics setup. This is optional.

4 Click to expand the **Boundary Selections** section. In the table, clear the **Keep** checkboxes for **Pair 1, Source**, **Pair 1, Destination**, **Pair 2, Source**, **Pair 2, Destination**, **Pair 3, Source**, **Pair 3, Destination**, **Pair 1**, **Pair 2**, and **Interior**.

Extract 1 (extract1)

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

2 In the **Settings** window for **Extract**, locate the **Entities or Objects to Extract** section.

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

4 From the **Input object handling** list, choose **Remove**.

5 On the object **pi1**, select Domain 2 only.

6 Click **Build All Objects**. Compare the geometry with Figure 1.

Create a selection for the symmetry boundaries.

Symmetry

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

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

3 From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Click the **Add** button for **Selections to add**.

5 In the **Add** dialog, select **Exterior (Particulate Composite, Body-Centered Cubic 1)** in the **Selections to add** list.

6 Click **OK**.

7 In the **Settings** window for **Difference Selection**, locate the **Input Entities** section.

8 Click the **Add** button for **Selections to subtract**.

9 In the **Add** dialog, select **Pair 3 (Particulate Composite, Body-Centered Cubic 1)** in the **Selections to subtract** list.

10 Click **OK**.

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

GLOBAL DEFINITIONS

Add some parameters to the **Parameters** list, that are used to set up the physics.

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
p0	1[Pa]	1 Pa	Pressure drop
rho_f	1000[kg/m^3]	1000 kg/m³	Fluid density
mu_f	1e-3[Pa*s]	0.001 Pa·s	Fluid viscosity

MATERIALS

Material 1 (mat1)

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

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)

Periodic Flow Condition 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Periodic Flow Condition**.
2. In the **Settings** window for **Periodic Flow Condition**, locate the **Boundary Selection** section.
3. From the **Selection** list, choose **Pair 3 (Particulate Composite, Body-Centered Cubic 1)**.
4. Locate the **Flow Condition** section. In the Δp text field, type `p0`.

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**.

   Currently, the system is underconstrained because only the pressure difference is known, not the absolute pressure. To obtain a unique solution, fix the pressure at one point.

Pressure Point Constraint 1

1. In the **Physics** toolbar, click **Points** and choose **Pressure Point Constraint**.
2. Select Point 28 only.

   Define an integration variable to calculate the normal velocity at the destination end of the periodic condition.

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 **Geometric entity level** list, choose **Boundary**.
4. Select Boundary 6 only.

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
`u_out`	`intop1(u*spf.nx+v*spf.ny+w*spf.nz)/L^2`	m/s	`Outlet velocity`
`k0`	`u_out*mu_f*L/p0`	m^2	`Permeability`

MESH 1

The physics-controlled mesh sets up a boundary layer mesh at the walls which ensures a good resolution of the steep velocity gradients in that region.

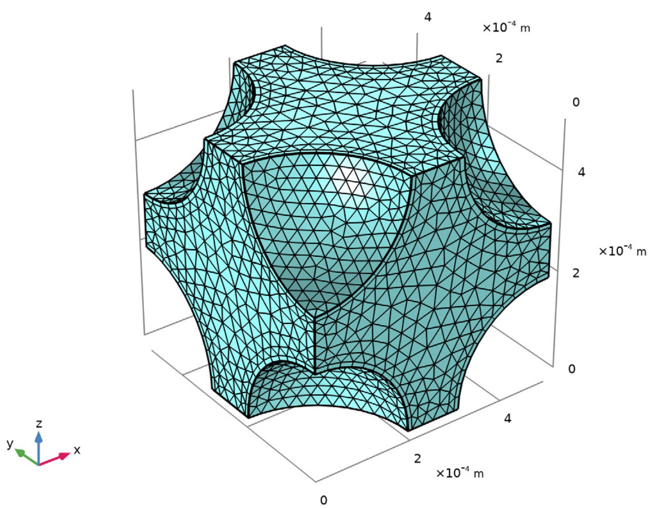
1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

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

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

4 In the table, clear the **Use** checkbox for **Geometric Analysis, Detail Size**.

5 Click **Build All**.



STUDY 1

Perform a parametric sweep over the particle volume fraction to determine the power-law relationship between porosity and permeability

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.
2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.
3 Click **Add**.
4 In the table, click to select the cell at row number 1 and column number 2.
5 Click **Range**.
6 In the **Range** dialog, type `0.3` in the **Start** text field.
7 In the **Step** text field, type `0.1`.
8 In the **Stop** text field, type `0.6`.
9 Click **Replace**.
10 In the **Model Builder** window, click **Study 1**.
11 In the **Settings** window for **Study**, locate the **Study Settings** section.
12 Clear the **Generate default plots** checkbox, to disable the automatic generation of default plots. Instead, choose the relevant plots from the Result Templates after computation.
13 In the **Study** toolbar, click **Compute**.

RESULT TEMPLATES

Add and modify the velocity plot to obtain Figure 2.

1 In the **Results** toolbar, click **Result Templates** to open the **Result Templates** window.
2 Go to the **Result Templates** window.
3 In the tree, select **Study 1/Solution 1 (sol1)** > **Creeping Flow** > **Velocity (spf)**.
4 Click the **Add Result Template** button in the window toolbar.
5 In the **Results** toolbar, click **Result Templates** to close the **Result Templates** window.

RESULTS

Multislice 1

1 In the **Model Builder** window, expand the **Velocity (spf)** node, then click **Multislice 1**.
2 In the **Settings** window for **Multislice**, locate the **Coloring and Style** section.
3 From the **Color table** list, choose **Acanthaster**.

Surface 1

1 In the **Model Builder** window, right-click **Velocity (spf)** and choose **Surface**.
2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type 1.

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

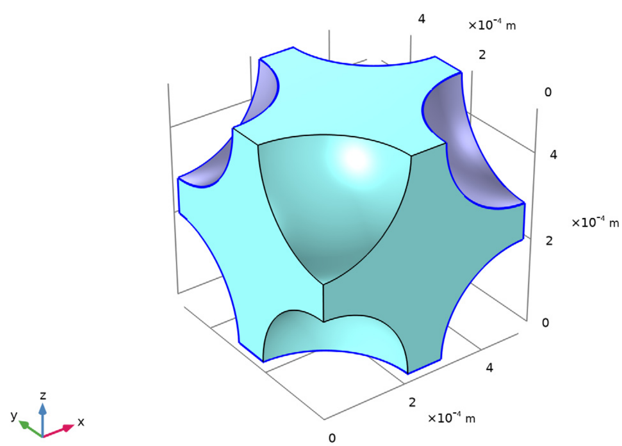
5 From the **Color** list, choose **Gray**.

Selection 1

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

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

3 From the **Selection** list, choose **All boundaries** and remove the top, bottom and front boundaries as shown below.



Streamline 1

1 In the **Model Builder** window, right-click **Velocity (spf)** and choose **Streamline**.

2 Select Boundary 5 only.

3 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

4 In the **Number** text field, type 40.

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

6 Select the **Number of arrows** checkbox. In the associated text field, type 80.

7 In the **Velocity (spf)** toolbar, click **Plot**.

Color Expression 1

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

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

3 In the **Expression** text field, type `p`.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **GrayPrint**.

Velocity (spf)

1 In the **Model Builder** window, under **Results** click **Velocity (spf)**.

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

3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

4 From the **Parameter value (vp)** list, choose **0.4**.

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

6 Locate the **Color Legend** section. Select the **Show units** checkbox.

7 In the **Velocity (spf)** toolbar, click **Plot**.

Compute the permeability for all parameters.

Global Evaluation 1

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

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

3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

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

Expression	Unit	Description
`por`		`Porosity`
`k0`	`m^2`	`Permeability`

5 Click **Evaluate**. The results are written to a table.

TABLE 1

1 Go to the **Table 1** window.

Compute the power-law parameters from the sweep results using a least-squares fit according to Equation 1.

GLOBAL DEFINITIONS

Least-Squares Fit 1 (lsq1_fun1)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Global** > **Least-Squares Fit**.

2 In the **Settings** window for **Least-Squares Fit**, locate the **Data** section.

3 From the **Data source** list, choose **Result table**.

4 Locate the **Data Column Settings** section. In the table, enter the following settings:

Columns	Type	Settings
vp	Ignored column	
Porosity	Argument	Name=x1
Permeability (m^2)	Function values	Name=lsq1_fun1, Expression=b*x1^n

5 In the **Expression** text field, type `b*x1^n`.

6 Locate the **Parameters** section. In the table, enter the following settings:

Parameter	Values	Scale	Lower bound	Upper bound
b	1e-9	1e-9		
n	2	1		

7 Click **Fit Parameters**.

Note, the results for `b` and `n` that appear in the **Parameters** section.

8 Click **Create Plot** and compare with Figure 3.

RESULTS

Power Law Permeability

1 In the **Settings** window for **1D Plot Group**, type `Power Law Permeability` in the **Label** text field.

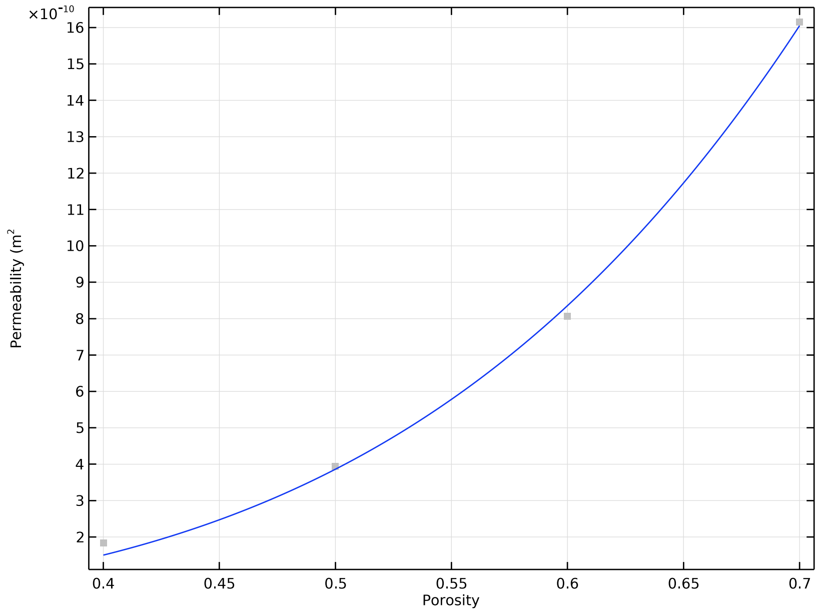
2 Locate the **Plot Settings** section.

3 Select the **x-axis label** checkbox. In the associated text field, type `Porosity`.

4 Select the **y-axis label** checkbox. In the associated text field, type `Permeability (m<sup>2</sup>`.

5 In the **Power Law Permeability** toolbar, click **Plot**.

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



ROOT

Now, add a new component to set up a Darcy's Law interface and use these values.

ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component** > **3D**.

GEOMETRY 2

Block 1 (blk1)

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

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Width** text field, type L.

4 In the **Depth** text field, type L.

5 In the **Height** text field, type L.

6 Click **Build All Objects**.

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 **Fluid Flow** > **Porous Media and Subsurface Flow** > **Darcy's Law (dl)**.

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

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

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

DARCY'S LAW (DL)

Fluid 1

1 In the **Settings** window for **Fluid**, locate the **Fluid Properties** section.

2 From the ρ list, choose **User defined**. In the associated text field, type `rho_f`.

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

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.

2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.

3 From the ε_p list, choose **User defined**. In the associated text field, type `por`.

4 From the **Permeability model** list, choose **Power law**.

5 In the b_{PL} text field, type `lsq1.b`.

6 In the n_{PL} text field, type `lsq1.n`.

Note, that `lsqq1.` refers to the **Least-Squares Fit** function.

Periodic Condition 1

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

2 Select Boundaries 3 and 4 only.

3 In the **Settings** window for **Periodic Condition**, locate the **Flow Condition** section.

4 In the Δp text field, type `p0`.

Again, the system is underconstrained. Darcy's Law does not include a predefined pressure constraint, but a general constraint can be applied just as easily.

5 Click the **Show More Options** button in the **Model Builder** toolbar.

6 In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics** > **Equation Contributions**.

7 Click **OK**.

Constraint 2

1 In the **Physics** toolbar, click **Points** and choose **Constraint**.

2 Select Point 6 only.

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

4 In the **Constraint expression** text field, type `p2`.

Note, that you need to type the variable to be constrained.

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

4 Disable the **Creeping Flow** interface for this study.

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

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

STUDY 2

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

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

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
vp (Particle volume fraction)	`range(0.3,0.1,0.6)`	

5 In the table, click to select the cell at row number 1 and column number 3.

6 In the **Model Builder** window, click **Study 2**.

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

8 Clear the **Generate default plots** checkbox, to disable the automatic generation of default plots. Instead, choose the relevant plots from the Result Templates after computation.

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

RESULT TEMPLATES

Add and modify the pressure plot to obtain Figure 4.

1 In the **Results** toolbar, click **Result Templates** to open the **Result Templates** window.

2 Go to the **Result Templates** window.

3 In the tree, select **Study 2/Parametric Solutions 2 (6) (sol8)** > **Darcy's Law** > **Pressure (dl)**.

4 Click the **Add Result Template** button in the window toolbar.

5 In the **Results** toolbar, click **Result Templates** to close the **Result Templates** window.

RESULTS

Arrow Surface 1

1 In the **Model Builder** window, right-click **Pressure (dl)** and choose **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

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

5 In the **Pressure (dl)** toolbar, click **Plot**.

Finally, compare the models using the normal mass flow.

Global Evaluation 2

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

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

3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

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

Expression	Unit	Description
u_out*L^2*rho_f	kg/s	Unit mass flow

5 Click next to **Evaluate**, then choose **New Table**.

Surface Integration 1

1 In the **Model Builder** window, right-click **Derived Values** and choose **Integration** > **Surface Integration**.

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

3 From the **Dataset** list, choose **Study 2/Parametric Solutions 2 (6) (sol8)**.

4 Select Boundary 4 only.

5 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 2 (comp2)** > **Darcy's Law** > **Boundary fluxes** > **dl.bndflux - Boundary flux - kg/(m²·s)**.

6 Click ▾ next to **Evaluate**, then choose **Table 2 - Global Evaluation 2**.

TABLE 2

1. Go to the **Table 2** window.
2. Click the **Table Graph** button in the window toolbar.

RESULTS

1D Plot Group 4

1. In the **Model Builder** window, under **Results** click **1D Plot Group 4**.
2. In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.
3. Select the **x-axis label** checkbox. In the associated text field, type `Particle Volume Fraction`.
4. Select the **y-axis label** checkbox. In the associated text field, type `Mass Flow`.

Table Graph 1

1. In the **Model Builder** window, click **Table Graph 1**.
2. In the **Settings** window for **Table Graph**, click to expand the **Legends** section.
3. Select the **Show legends** checkbox.
4. From the **Legends** list, choose **Manual**.
5. In the table, enter the following settings:

Legends
`Creeping Flow`
`Darcy's Law`

1D Plot Group 4

1. In the **Model Builder** window, click **1D Plot Group 4**.
2. In the **1D Plot Group 4** toolbar, click **Plot** and compare with Figure 5. The results are in good agreement.