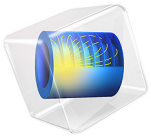


Model created in COMSOL Multiphysics 6.4

Large Swelling in Polymer Hydrogels

Introduction

Polymer hydrogels consist of a crosslinked network of long-chained polymers and a large number of imbibed solvent molecules. A wide range of hydrogels can be produced by controlling the chemistry of the polymer network, its crosslinking, and the type of solvent. This class of materials is therefore used in a wide range of applications, such as medical devices, targeted drug delivery, design of tissue-like materials, and in stimuli-sensitive actuators (Ref. 1).

Polymer gels can undergo large deformations as a result of mechanical loads as well as changes in the chemical potential of the surrounding solvent. At time scales much shorter than that typical of diffusion of the solvent molecules, the mechanical response is isochoric, allowing only changes in gel shape. At longer time scales, however, the solvent molecules have sufficient time to rearrange and the gel can thus undergo large changes in both shape and volume.

This example model demonstrates how to implement a coupled nonlinear field theory of large deformation and solvent diffusion for polymer hydrogels in COMSOL Multiphysics® based on the work in Ref. 1. The implementation is validated by a comparison with two benchmark problems: inhomogeneous swelling of a gel bonded to a rigid substrate (Ref. 2) and uniaxial consolidation under creep loading (Ref. 1).

Theoretical Background

The gel is considered as a homogenized, continuous, single-phase material. The presence of the solvent is described by the molar concentration $c(\mathbf{X}, t)$, which denotes the number of moles of solvent per unit reference volume of the polymer gel at position $\mathbf{X}$ and time t. As is common, the reference configuration is taken to be the dry polymer network (that is, $c(\mathbf{X}, 0) = 0$). The gel is regarded as an open system since it can exchange solvent molecules with the environment. The concentration c must therefore obey the local form of the volume balance

$$\dot{c} + \nabla \cdot \overline{\mathbf{Q}} = 0 \tag{1}$$

Herein, $\overline{\mathbf{Q}} = \mathbf{Q}/V_{\mathrm{m}}$ denotes the molar flux of solvent (SI unit: mol/(m^2·s)), $\mathbf{Q}$ is the volumetric flux, and V_{m} is the molar volume (SI unit: m^3/mol) of the solvent. When inertia is neglected, the local momentum balance takes the form

$$\nabla \cdot \mathrm{P} + (\rho_{\mathrm{S}} + M_{\mathrm{m}} c)\mathbf{B} = \mathbf{0} \tag{2}$$

with $\mathbf{P}$ being the first Piola–Kirchhoff stress in the gel, ρ_S the mass density of the polymer network, M_m the molar mass of the solvent, and $\mathbf{B}$ the mass-specific body force. In the following, body forces are neglected.

The free energy density of polymer gels is often split additively into two contributions (Ref. 1): one related to stretching of the polymer chains and one related to the mixing between the polymers and the solvent molecules, that is,

$$\psi(\mathbf{F}, c) = \psi_s(\mathbf{F}) + \psi_{mix}(c) \tag{3}$$

Herein, the free energy of stretching is given as

$$\psi_s(\mathbf{F}) = \frac{G}{2}(I_1 - 3 - 2\log J) \tag{4}$$

and the free energy of mixing takes the form

$$\psi_{mix}(c) = -K_{mix}\left[V_m c \log\left(1 + \frac{1}{V_m c}\right) + \frac{\chi}{1 + V_m c}\right] \tag{5}$$

In these expressions, G is the initial shear modulus of the polymer network, I_1 is the first invariant of the right Cauchy–Green deformation tensor $\mathbf{C} = \mathbf{F}^T\mathbf{F}$, $J = \det(\mathbf{F})$ is the volume ratio, K_{mix} is the bulk stiffness of mixing, and χ is a dimensionless constant related to the enthalpy of mixing. Note that the free energy density is expressed per unit reference volume and is written as a function of the deformation gradient $\mathbf{F}$ and the solvent concentration c.

For most hydrogels, it is natural to assume that volume changes are exclusively due to changes in solvent content, whereas the polymers and the solvent themselves are incompressible. This constraint establishes a direct link between the solvent concentration and the volume ratio, that is,

$$J = 1 + V_m c \tag{6}$$

Because of this constraint, it is convenient to introduce another form of the free energy density by a Legendre transform, see Ref. 2. Let

$$\Psi(\mathbf{F}, \bar{\mu}) = \psi(\mathbf{F}, c) - \bar{\mu} c \tag{7}$$

with $\bar{\mu}$ denoting the chemical potential of the solvent in units of J/mol. By invoking thermodynamic restrictions, the expression for the first Piola–Kirchhoff stress, the solvent concentration, and the solvent flux read

$$P = \frac{\partial \Psi}{\partial \mathbf{F}}, \quad c = -\frac{\partial \Psi}{\partial \bar{\mu}}, \quad \mathbf{Q} = -\mathbf{M}\nabla\mu \tag{8}$$

where the second-order tensor $\mathbf{M}$ (SI unit: $\mathrm{m}^4/(\mathrm{N\,s})$) is called the mobility tensor, which is required to be symmetric and positive definite. For convenience, we have also introduced the chemical potential in units of pressure, $\mu = \bar{\mu}/V_\mathrm{m}$. Note that the constitutive law for the solvent flux is analogous to Darcy's law in porous media; in fact, we can identify the material permeability tensor $\kappa = \mu_\mathrm{f}\mathbf{M}$ (SI unit: m^2) given the solvent viscosity μ_f. In Ref. 1, an expression for the spatial solvent mobility tensor is derived based on the solvent diffusivity D, which is assumed to be isotropic in the current configuration. After converting the units, applying a pull-back operation to the material frame, and using the molecular incompressibility constraint, the material mobility tensor analogous to Equation (30) in Ref. 1 reads

$$\mathbf{M} = J\mathbf{F}^{-1}\left(V_\mathrm{m}\frac{cV_\mathrm{m}}{J}\frac{D}{N_\mathrm{A}k_\mathrm{B}T}\mathbf{I}\right)\mathbf{F}^{-\mathrm{T}} = (J-1)\frac{V_\mathrm{m}D}{N_\mathrm{A}k_\mathrm{B}T}\mathbf{C}^{-1} \tag{9}$$

Here, N_A and k_B denote the Avogadro number and the Boltzmann constant, respectively. The free energy density (Equation 7) and the local form of the volume balance (Equation 1) can now be expressed entirely in terms of the new dependent variables. By using the molecular incompressibility constraint, we obtain the free energy density

$$\Psi(\mathbf{F},\mu) = \frac{G}{2}(I_1 - 3 - 2\log J) - K_\mathrm{mix}\left[(J-1)\log\left(\frac{J}{J-1}\right) + \frac{\chi}{J}\right] - \mu(J-1) \tag{10}$$

Furthermore, inserting the constitutive equation for the solvent flux (Equation 8_3) into the local volume balance (Equation 1) and making use of the molecular incompressibility constraint yields

$$\dot{J} = \nabla\cdot(\mathbf{M}\nabla\mu) \tag{11}$$

Finally, the first Piola–Kirchhoff stress follows by inserting Equation 10 into Equation 8_1

$$\mathbf{P} = G(\mathbf{F} - \mathbf{F}^{-\mathrm{T}}) + K_\mathrm{mix}\left[J\log\left(1-\frac{1}{J}\right) + 1 + \frac{\chi}{J}\right]\mathbf{F}^{-\mathrm{T}} - J\mu\mathbf{F}^{-\mathrm{T}} \tag{12}$$

Thus, all equations have been formulated in terms of $\mathbf{F}$ and μ as dependent variables instead of $\mathbf{F}$ and c. This is the natural choice of dependent variables in terms of boundary conditions because the chemical potential is continuous across boundaries, whereas the solvent concentration is not. Instead, once the boundary value problem is solved, c can be computed from the volume ratio J using Equation 6.

REFERENCE CONFIGURATION FOR THE FINITE ELEMENT IMPLEMENTATION

So far, the dry polymer network has been used as a reference configuration. In practice, however, hydrogels always contain a large amount of solvent. Moreover, the dry state is problematic in a numerical implementation because the free energy density of mixing is singular in the limit $J \to 1$. For these reasons, a new reference state is chosen where the gel is in a state of free swelling; that is, under no external forces and in equilibrium with a solvent of chemical potential μ_{ref}, see Ref. 2. Since the gel is homogeneous and isotropic, the free swelling is characterized by the deformation gradient $\mathbf{F}_0 = \lambda_0 \mathbf{I}$. The deformation gradient $\mathbf{F}$ can thus be multiplicatively decomposed as $\mathbf{F} = \mathbf{F}'\mathbf{F}_0$, with $\mathbf{F}'$ denoting the deformation gradient between the free swelling reference configuration and the current configuration. The stretch λ_0 can be computed by solving the free swelling boundary value problem, which reduces to a single algebraic equation,

$$G\left(\frac{1}{\lambda_0} - \frac{1}{\lambda_0^3}\right) + K_{\text{mix}}\left[\log\left(1 - \frac{1}{\lambda_0^3}\right) + \frac{1}{\lambda_0^3} + \frac{\chi}{\lambda_0^6}\right] - \mu_{\text{ref}} = 0 \tag{13}$$

With λ_0 determined, the free energy density and the mobility tensor in the new reference configuration follow by Piola transforms

$$\Psi'(\mathbf{F}', \mu) = \frac{1}{J_0}\Psi(\mathbf{F}'\mathbf{F}_0, \mu), \qquad \mathbf{M}' = \frac{1}{J_0}\mathbf{F}_0\mathbf{M}\mathbf{F}_0^{\mathrm{T}} \tag{14}$$

with $J_0 = \det(\mathbf{F}_0) = \lambda_0^3$. The expressions for Ψ' and $\mathbf{M}'$ that are needed for the COMSOL Multiphysics implementation are therefore given by

$$\Psi'_{\text{s}} = \frac{G}{2J_0}(\lambda_0^2 I'_1 - 3 - 2\log(J_0 J')) \tag{15}$$

for the free energy of stretching,

$$\Psi'_{\text{mix}} = -K_{\text{mix}}\left[\left(J' - \frac{1}{J_0}\right)\log\left(\frac{J_0 J'}{J_0 J' - 1}\right) + \frac{\chi}{J_0^2 J'}\right] \tag{16}$$

for the free energy of mixing, and

$$\mathbf{M}' = \left(J' - \frac{1}{J_0}\right)\frac{V_{\text{m}} D}{N_{\text{A}} k_{\text{B}} T}(\mathbf{C}')^{-1} \tag{17}$$

for the mobility tensor with respect to the swollen reference configuration. Note that the variables $J' = \det(\mathbf{F}')$, $\mathbf{C}' = \mathbf{F}'^{\mathrm{T}}\mathbf{F}'$, and $I'_1 = \operatorname{tr}(\mathbf{C}')$ are functions of the deformation gradient $\mathbf{F}'$ that maps material line elements from the swollen reference configuration to the current

configuration, which is the deformation that we solve for. In the absence of intrinsic inelastic processes, these variables are available in the Solid Mechanics interface as `solid.Jel`, `solid.Cel`, and `solid.I1Cel`, respectively.

BENCHMARK PROBLEMS

To validate the model implementation, two axisymmetric benchmark problems are studied. First, the long-term, stationary solution to the swelling of a cylindrical gel that is immersed in a pure solvent and bonded to a rigid substrate is computed and compared with results reported in Ref. 2. The aspect ratio of the gel is varied in a parametric sweep, and the results are compared to semi-analytical calculations of homogeneous free and uniaxial swelling in the limiting cases of pillar-like and disk-like gel geometries, respectively. For wide and short (that is, disk-like) gels, the lateral edge of the gel deforms severely and comes in contact with the rigid surface. Although only the long-term, stationary solution is of interest in this benchmark, a time-dependent study is used to demonstrate how contact-dependent boundary conditions for the solvent flux can be implemented.

The second benchmark problem concerns the time-dependent uniaxial consolidation of a cylindrical gel under creep compression, see Ref. 1. A cylindrical gel is constrained radially, and a load is applied at the top while the bottom boundary is fixed. Free fluid flow is allowed through a porous filter at the top. The coupled problem is solved in a 2D axisymmetric geometry, and the results are compared with those computed in Ref. 1 where the consolidation problem is reduced to a one-dimensional diffusion-like differential equation.

MODEL PARAMETERS

The model parameters used for the two benchmark problems are given in the following table.

TABLE 1: MODEL PARAMETERS FOR THE TWO BENCHMARK PROBLEMS.

Parameter	Inhomogeneous swelling (Ref. 2)	Uniaxial consolidation (Ref. 1)
G	40 kPa	40 kPa
K_{mix}	40 MPa	40 MPa
χ	0.1	0.2
V_{m}	$6.022 \cdot 10^{-5}$ $\mathrm{m}^3/\mathrm{mol}$	$6.022 \cdot 10^{-5}$ $\mathrm{m}^3/\mathrm{mol}$
D	10^3 m^2/s	$8 \cdot 10^{-10}$ m^2/s
μ_{ref}	$-2.6376 \cdot 10^5$ Pa	0 Pa
λ_0	2.0	3.215

Results and Discussion

The swelling ratio J relative to the dry polymer network is shown in Figure 1 for cylindrical gels bonded to a rigid substrate and swollen to reach equilibrium with a pure solvent. The results are displayed for gels with three different aspect ratios (D/H), and they agree well with the deformed shapes reported in Ref. 2, see Figure 7 therein. Note that, most obvious in the case $D/H = 10$, the free lateral edge deforms strongly by folding over and making contact with the rigid substrate. Furthermore, note that the swelling ratio (and thus the solvent concentration) is inhomogeneous within the gel and along its outer boundaries.

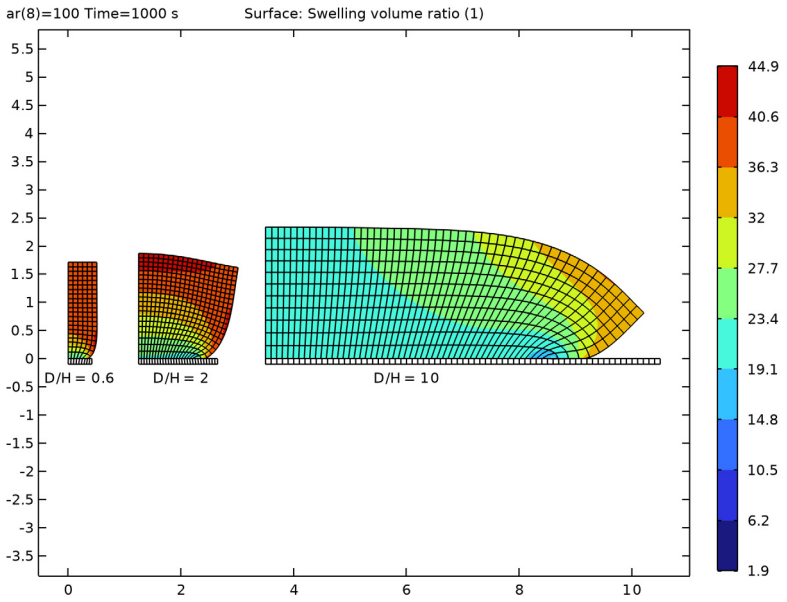


Figure 1: Swelling ratio in a cylindrical polymer hydrogel bonded to a rigid substrate.

Figure 2 shows the change in gel height as a function of the aspect ratio of the cylinder. For thin, pillar-like gels, the gel height approaches that predicted by homogeneous free swelling (green curve), as most of the domain is unaffected by the constraint. In contrast,

for wide, disk-like gels (high D/H), the gel is constrained in the in-plane directions and the state of swelling is close to uniaxial (red curve).

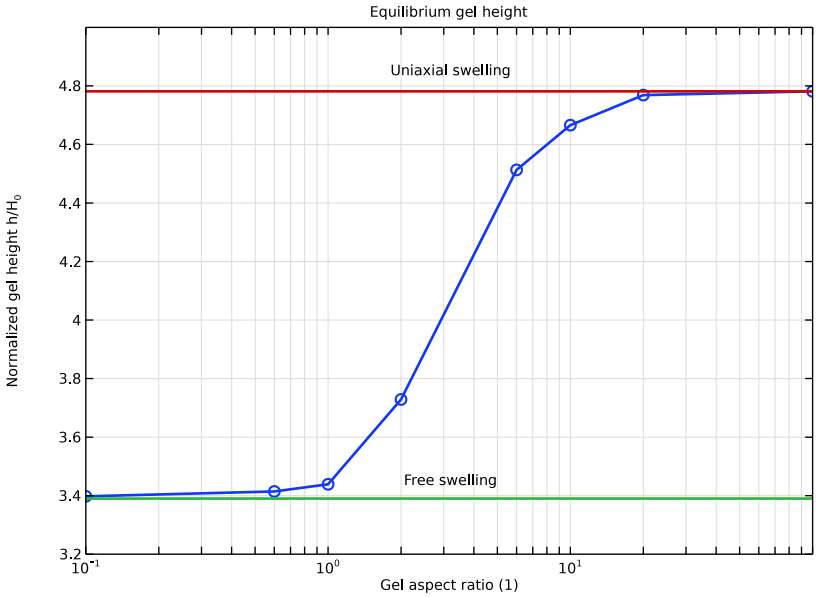


Figure 2: Equilibrium swelling ratio in the thickness direction as a function of gel aspect ratio.

Next, consider the time-dependent solution under uniaxial consolidation. In Figure 3, surface plots of the normal stress and the chemical potential are shown in the spatial frame at dimensionless time $Dt/H_0^2 = 200$. Note that the normal stress is constant through the thickness, as required by the momentum balance. At the bottom of the gel, most of the load is borne by fluid pressurization, whereas at the top of the gel, the load is borne primarily by the polymer network.

The stretch in the thickness direction is shown as a function of the normalized reference coordinate for a few selected time points in Figure 4. For easier comparison with Ref. 1 (see Figure 4 therein), the direction of the Z-axis has been reversed, now going from top to bottom. Both the short- and long-term limits as well as the temporal evolution are in excellent agreement with the results reported in Ref. 1.

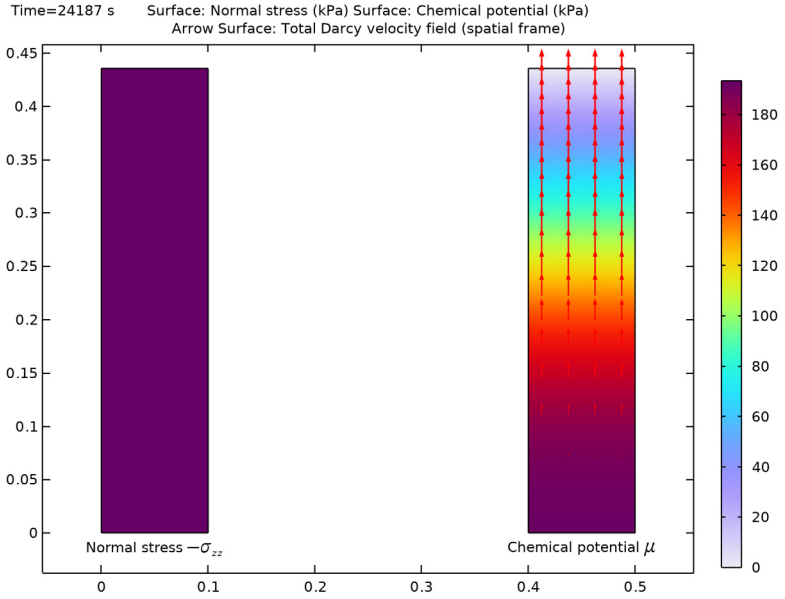


Figure 3: Normal stress (left) and chemical potential and solvent flux (right) in a gel under uniaxial consolidation at dimensionless time $Dt/H_0 = 200$. *Note that the normal stress is constant through the thickness. The chemical potential is maximal at the bottom surface and minimal at the top surface where the load is applied through a porous filter and the free flow boundary condition applies.*

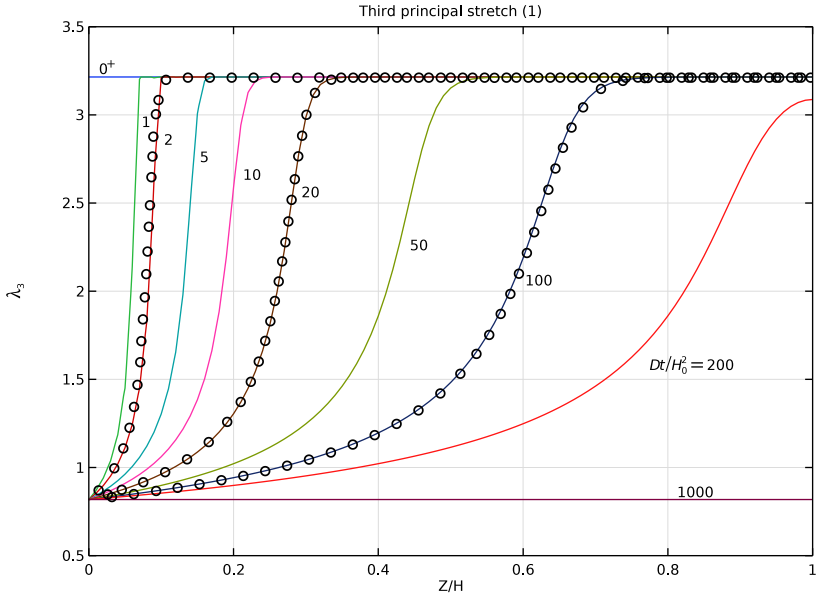


Figure 4: Stretch in the thickness direction during uniaxial consolidation as a function of the position along the gel thickness, shown for various dimensionless times. The data are in excellent agreement with the benchmark in Ref. 1 *(circles).*

Notes About the COMSOL Implementation

This multiphysics model is implemented by combining the Solid Mechanics and the Darcy's Law interfaces using the **Poroelasticity** multiphysics coupling for solving the coupled momentum and volume balance equations. Since both the polymer network and the solvent are assumed materially incompressible, the **Biphasic** poroelasticity model is used. In addition, the Global ODEs and DAEs interface is used to solve the nonlinear algebraic equations for free and uniaxial homogeneous swelling. The geometry and the displacement field are discretized using *quadratic Lagrange* shape functions, whereas linear shape functions are used for the chemical potential; these choices ensure a consistent interpolation order when computing the stresses.

The free energy density is implemented as a user-defined **Hyperelastic** material. The load contribution from the chemical potential is added automatically in the **Poroelasticity** coupling node. Note that the stress variables `solid.sij` correspond to the so-called effective stress; that is, they do not include the contribution from the pore pressure. The total Cauchy stress corresponding to Equation 12 is available from the multiphysics

coupling node in the variables `poro1.sij`, `poro1` being the **Name** of the **Poroelasticity** node.

In problems where the contact patch is changing during a simulation, the boundary condition for the solvent flux depends on the contact status. In case of a gel coming into contact with an impermeable surface, a **No Flow** boundary condition applies for the portion of the gel boundary in contact with the surface, whereas free flow applies elsewhere. Such complex boundary conditions can be implemented with an if-statement embedded in a **Pressure** node.

References

1. W. Hong, X. Zhao, J. Zhou, and Z. Suo, "A theory of coupled diffusion and large deformation in polymeric gels," *J. Mech. Phys. Solids*, vol. 56, pp. 1779–1793, 2008.

2. W. Hong, Z. Liu, and Z. Suo, "Inhomogeneous swelling of a gel in equilibrium with a solvent and mechanical load," *Int. J. Solids Struct.*, vol. 46, pp. 2382–3289, 2009.

Application Library path: `Porous_Media_Flow_Module/Poromechanics/hydrogel_swelling`

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 Axisymmetric**.

2 In the **Select Physics** tree, select **Structural Mechanics** > **Poroelasticity** > **Poroelasticity, Solid**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GLOBAL DEFINITIONS

Geometrical Parameters

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

2 In the **Settings** window for **Parameters**, type `Geometrical Parameters` in the **Label** text field.

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

Name	Expression	Value	Description
height	1[mm]	0.001 m	Gel height
ar	0.2	0.2	Gel aspect ratio
radius	ar*height/2	1E-4 m	Gel radius
elsize	if(ar<=2,0.05*height, 0.10*height)	5E-5 m	Element size

Material Parameters

1 In the **Home** toolbar, click **Parameters** and choose **Add** > **Parameters**.

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

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

Name	Expression	Value	Description
G	4e4[Pa]	40000 Pa	Initial shear modulus
Kmix	4e7[Pa]	4E7 Pa	Bulk modulus of mixing
chi	0.1	0.1	Enthalpy of mixing
temp	293.15[K]	293.15 K	Reference temperature
Vm	1e-28[m^3]* N_A_const	6.0221E-5 m^3/mol	Solvent molar volume
D	1e3[m^2/s]	1000 m^2/s	Solvent diffusivity
M0	Vm*D/(N_A_const* k_B_const*temp)	2.4707E-5 $m^3 \cdot s/kg$	Solvent mobility
rhof	1[g/cm^3]	1000 kg/m^3	Solvent density
muf	1e-3[mPa*s]	1E-6 Pa·s	Solvent viscosity
kappa0	M0*muf	2.4707E-11 m^2	Permeability

Model Parameters

1 In the **Home** toolbar, click **Parameters** and choose **Add** > **Parameters**.

2 In the **Settings** window for **Parameters**, type `Model Parameters` in the **Label** text field.

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

Name	Expression	Value	Description
stretch0	2	2	Free swelling stretch
J0	stretch0^3	8	Free swelling volume ratio
mu_ref	G/J0*(stretch0^2-1)+Kmix*(log(1-1/J0)+1/J0+chi/(J0^2))	-2.6376E5 Pa	Reference chemical potential
mu_sw	0[Pa]	0 Pa	Chemical potential of pure solvent
poro0	1-1/J0	0.875	Initial porosity
t_end	1000[s]	1000 s	Duration
stress	0[Pa]	0 Pa	Applied stress

Interpolation 1 (int1)

1 In the **Home** toolbar, click **Functions** and choose **Global** > **Interpolation**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 In the table, enter the following settings:

t	f(t)
0	mu_ref
t_end	mu_sw

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

Function	Unit
int1	Pa

5 In the **Argument** table, enter the following settings:

Argument	Unit
t	s

GEOMETRY 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Geometry 1** node, then click **Geometry 1**.

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

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

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 `radius`.

4 In the **Height** text field, type `height`.

Rectangle 2 (r2)

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 `1.4*radius`.

4 In the **Height** text field, type `0.1*height`.

5 Locate the **Position** section. In the **z** text field, type `-0.1*height`.

Partition Edges 1 (pare1)

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

2 On the object **r2**, select Boundary 3 only.

3 In the **Settings** window for **Partition Edges**, locate the **Positions** section.

4 In the table, enter the following settings:

Relative arc length parameters
1/1.4

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

Form Union (fin)

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

2 In the **Settings** window for **Form Union/Assembly**, locate the **Form Union/Assembly** section.

3 From the **Action** list, choose **Form an assembly**.

4 Clear the **Create pairs** checkbox.

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

COMPONENT 1 (COMP1)

Set the geometry shape function to **Quadratic Lagrange** polynomials. We will use the same shape functions for the geometry as for the displacement field.

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

2 In the **Settings** window for **Component**, locate the **Curved Mesh Elements** section.

3 From the **Geometry shape function** list, choose **Quadratic Lagrange**.

DEFINITIONS

Create a **Contact Pair** between the free edge of the rigid substrate (source) and the lateral edge of the gel (destination), which can come into contact when the gel swells.

Contact Pair 1 (p1)

1 In the **Definitions** toolbar, click **Pairs** and choose **Contact Pair**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Pair**, locate the **Destination Boundaries** section.

4 Click to select the **Activate Selection** toggle button.

5 Select Boundary 9 only.

Variables 1

Define **Variables** for the free energy density, solvent mobility, and the permeability tensor. These are provided in a separate text file.

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

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

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

4 Select Domain 2 only.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `hydrogel_swelling_variables.txt`.

SOLID MECHANICS (SOLID)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Solid Mechanics (solid)**.

2 In the **Settings** window for **Solid Mechanics**, click to expand the **Discretization** section.

3 From the **Displacement field** list, choose **Quadratic Lagrange**.

Rigid Material 1

1 In the **Physics** toolbar, click **Domains** and choose **Rigid Material**.

2 Select Domain 1 only.

Fixed Constraint 1

In the **Physics** toolbar, click **Attributes** and choose **Fixed Constraint**.

Hyperelastic Material 1

1 In the **Physics** toolbar, click **Domains** and choose **Hyperelastic Material**.

2 Select Domain 2 only.

3 In the **Settings** window for **Hyperelastic Material**, locate the **Hyperelastic Material** section.

4 From the **Material model** list, choose **User defined**.

5 In the W_s text field, type `Psi_s+Psi_mix`.

6 Click to expand the **Advanced** section. In the E_{eq} text field, type `3*G`. When simulating contact, the equivalent Young's modulus is used to estimate the contact pressure. For soft materials like gels, the default value is too high, leading to an ill-conditioned problem.

Contact 1

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

2 In the **Settings** window for **Contact**, locate the **Contact Pressure Penalty Factor** section.

3 From the **Penalty factor control** list, choose **Manual tuning**.

4 In the f_p text field, type `10`.

Fixed Constraint 1

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

2 Select Boundary 7 only.

DARCY'S LAW (DL)

Now, set up the **Darcy's Law** interface in the hydrogel domain to solve the volume balance equation. Set the discretization to **Linear** to enable a standard P2–P1 interpolation of displacement and pressure.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Darcy's Law (dl)**.

2 Select Domain 2 only.

3 In the **Settings** window for **Darcy's Law**, click to expand the **Discretization** section.

4 From the **Pressure** list, choose **Linear**.

5 Click to expand the **Dependent Variables** section. In the **Pressure (Pa)** text field, type `mu`.

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Darcy's Law (dl)** > **Porous Medium 1** click **Fluid 1**.

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

3 From the **Fluid type** list, choose **Incompressible**.

4 From the ρ_{ref} list, choose **User defined**. In the associated text field, type `rhof`.

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

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 `poro0`.

4 From the κ list, choose **User defined**. From the list, choose **Symmetric**.

5 Specify the κ matrix as

KRR	KRZ
KRZ	KZZ

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Darcy's Law (dl)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the *mu* text field, type `mu_ref`.

Continuity 1

Disable the default **Continuity** condition for the contact pair. In this case, the proper contact condition needs to be set up manually.

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

2 In the **Settings** window for **Continuity**, locate the **Advanced** section.

3 Select the **Disconnect pair** checkbox.

Contact (Swelling)

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

2 In the **Settings** window for **Pressure**, type `Contact (Swelling)` in the **Label** text field.

3 Select Boundary 9 only.

4 Locate the **Pressure** section. In the p_0 text field, type `if(incontact_p1,mu,int1(t))`.

Free Flow (Swelling)

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

2 In the **Settings** window for **Pressure**, type `Free Flow (Swelling)` in the **Label** text field.

3 Locate the **Pressure** section. In the p_0 text field, type `int1(t)`.

4 Select Boundary 8 only.

MULTIPHYSICS

Poroelasticity 1 (poro1)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Multiphysics** click **Poroelasticity 1 (poro1)**.

2 In the **Settings** window for **Poroelasticity**, locate the **Poroelastic Coupling Properties** section.

3 From the **Poroelasticity model** list, choose **Biphasic**.

4 From the p_{ref} list, choose **Reference pressure level (dl)**.

MESH 1

Mapped 1

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

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

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

4 Select Domain 2 only.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 7 and 8 only.

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

4 In the **Number of elements** text field, type `floor(radius/elsize)+1`.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 6 and 9 only.

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

4 In the **Number of elements** text field, type `floor(height/elsize)+1`.

Mapped 2

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

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

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

4 Select Domain 1 only.

Distribution 1

1 Right-click **Mapped 2** and choose **Distribution**.

2 Select Boundary 2 only.

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

4 In the **Number of elements** text field, type `floor(1.4*radius/elsize)+1`.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 2** and choose **Distribution**.

2 Select Boundaries 1 and 5 only.

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

4 In the **Number of elements** text field, type `1`.

5 Click **Build All**.

INHOMOGENEOUS SWELLING

Set up a parametric time-dependent study to compute the inhomogeneous swelling of the constrained hydrogel under a change in the external chemical potential for different gel aspect ratios. Note that the diffusion coefficient has been set to a large value so that solvent equilibrium is achieved within the study duration.

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

2 In the **Settings** window for **Study**, type `Inhomogeneous Swelling` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

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
ar (Gel aspect ratio)	`0.1 0.6 1.0 2.0 6.0 10.0 20.0 100.0`	

Step 1: Time Dependent

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

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

3 In the **Output times** text field, type `range(0,0.1,1)*t_end`.

Solver Configurations

Modify the default solver suggestion to improve convergence.

Solution 1 (sol1)

1 In the **Model Builder** window, right-click **Solver Configurations** and choose **Show Default Solver**.

2 Expand the **Solution 1 (sol1)** node.

3 In the **Model Builder** window, expand the **Inhomogeneous Swelling** > **Solver Configurations** > **Solution 1 (sol1)** > **Dependent Variables 1** node, then click **Pressure (comp1.mu)**.

4 In the **Settings** window for **Field**, locate the **Scaling** section.

5 From the **Method** list, choose **Manual**.

6 In the **Scale** text field, type `1e5`.

7 In the **Model Builder** window, click **Displacement Field (comp1.u)**.

8 In the **Settings** window for **Field**, locate the **Scaling** section.

9 In the **Scale** text field, type `height`.

10 In the **Model Builder** window, click **Time-Dependent Solver 1**.

11 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

12 Clear the **Interpolate solution at end time** checkbox.

13 In the **Model Builder** window, expand the **Inhomogeneous Swelling** > **Solver Configurations** > **Solution 1 (sol1)** > **Time-Dependent Solver 1** node, then click **Direct**.

14 In the **Settings** window for **Direct**, locate the **General** section.

15 From the **Solver** list, choose **PARDISO**.

16 In the **Model Builder** window, click **Fully Coupled 1**.

17 In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.

18 From the **Nonlinear method** list, choose **Constant (Newton)**.

19 From the **Jacobian update** list, choose **Once per time step**.

20 In the **Maximum number of iterations** text field, type `10`.

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

RESULT TEMPLATES

Create a **Surface Plot** to visualize the swelling ratio of the gel in the deformed configuration for three different aspect ratios. Start from the **Predefined Plot** of the stress.

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 **Inhomogeneous Swelling/Parametric Solutions 1 (sol2)** > **Solid Mechanics** > **Stress (solid)**.

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

Swelling Ratio

1 In the **Settings** window for **2D Plot Group**, type `Swelling Ratio` in the **Label** text field.

2 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

3 In the **Title** text area, type `Surface: Swelling volume ratio (1)`.

4 Locate the **Plot Settings** section. From the **View** list, choose **New view**.

5 Clear the **Plot dataset edges** checkbox.

Surface 1

1 In the **Model Builder** window, expand the **Swelling Ratio** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `comp1.J`.

4 Locate the **Data** section. From the **Dataset** list, choose **Inhomogeneous Swelling/Parametric Solutions 1 (sol2)**.

5 From the **Parameter value (ar)** list, choose **0.6**.

6 Locate the **Coloring and Style** section. From the **Color table** list, choose **Rainbow**.

7 From the **Color table type** list, choose **Discrete**.

Mesh 1

1 In the **Model Builder** window, right-click **Swelling Ratio** and choose **Mesh**.

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

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

4 From the **Parameter value (ar)** list, choose **0.6**.

5 Locate the **Coloring and Style** section. From the **Element color** list, choose **None**.

6 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

Deformation 1

Right-click **Mesh 1** and choose **Deformation**.

Mesh 1, Surface 1

Right-click and choose **Duplicate**.

Surface 2

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

2 From the **Parameter value (ar)** list, choose **2**.

3 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

Transformation 1

1 Right-click **Surface 2** and choose **Transformation**.

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

3 In the **R** text field, type `1.25`.

Mesh 2

1 In the **Model Builder** window, under **Results** > **Swelling Ratio** click **Mesh 2**.

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

3 From the **Parameter value (ar)** list, choose **2**.

Transformation 1

1 Right-click **Mesh 2** and choose **Transformation**.

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

3 In the **R** text field, type `1.25`.

Mesh 2, Surface 2

1 In the **Model Builder** window, under **Results** > **Swelling Ratio**, Ctrl-click to select **Surface 2** and **Mesh 2**.

2 Right-click and choose **Duplicate**.

Surface 3

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

2 From the **Parameter value (ar)** list, choose **10**.

Transformation 1

1 In the **Model Builder** window, expand the **Surface 3** node, then click **Transformation 1**.

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

3 In the **R** text field, type `3.5`.

Mesh 3

1 In the **Model Builder** window, under **Results** > **Swelling Ratio** click **Mesh 3**.

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

3 From the **Parameter value (ar)** list, choose **10**.

Transformation 1

1 In the **Model Builder** window, expand the **Mesh 3** node, then click **Transformation 1**.

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

3 In the **R** text field, type `3.5`.

Swelling Ratio

In the **Model Builder** window, under **Results** click **Swelling Ratio**.

Table Annotation 1

1 In the **Swelling Ratio** toolbar, click **More Plots** and choose **Table Annotation**.

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

3 From the **Source** list, choose **Local table**.

4 In the table, enter the following settings:

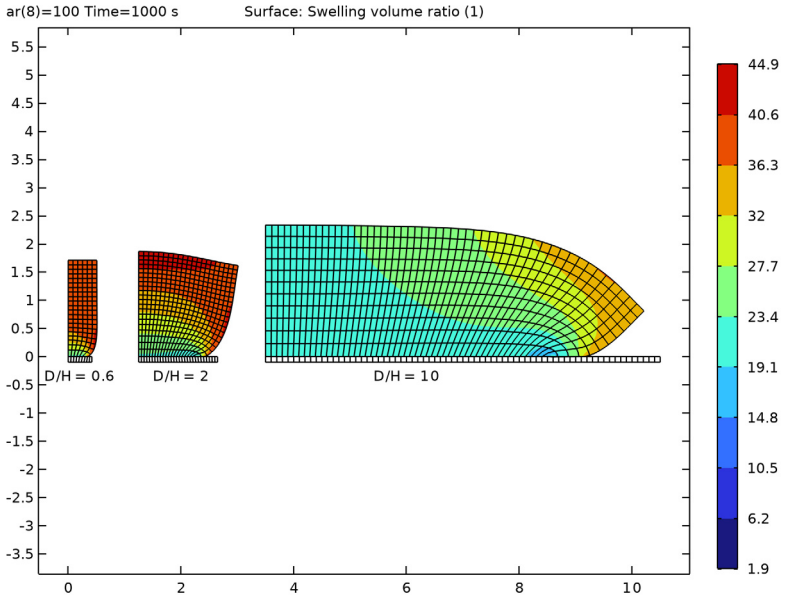
x-coordinate	y-coordinate	Annotation
0.2	-0.35	D/H = 0.6
2.0	-0.35	D/H = 2
6.0	-0.35	D/H = 10

5 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

6 From the **Anchor point** list, choose **Center**.

7 In the **Swelling Ratio** toolbar, click **Plot**.

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



Gel Height

Create a plot of the normalized gel height, similar to Fig. 6 in Ref. 2.

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

2 In the **Settings** window for **1D Plot Group**, type `Gel Height` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Inhomogeneous Swelling/ Parametric Solutions 1 (sol2)**.

4 From the **Time selection** list, choose **Last**.

5 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Equilibrium gel height`.

7 Locate the **Plot Settings** section.

8 Select the **x-axis label** checkbox. In the associated text field, type `Gel aspect ratio (1)`.

9 Select the **y-axis label** checkbox. In the associated text field, type `Normalized gel height h/H<sub>0</sub>`.

10 Locate the **Axis** section. Select the **Manual axis limits** checkbox.

11 In the **x minimum** text field, type `0.1`.

12 In the **x maximum** text field, type `100`.

13 In the **y minimum** text field, type `3.2`.

14 In the **y maximum** text field, type `5`.

15 Select the **x-axis log scale** checkbox.

16 Locate the **Grid** section. Select the **Manual spacing** checkbox.

17 In the **y spacing** text field, type `0.2`.

18 Locate the **Legend** section. Clear the **Show legends** checkbox.

Point Graph 1

1 Right-click **Gel Height** and choose **Point Graph**.

2 Select Point 7 only.

3 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `(height+w)/(height/stretch0)`.

5 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **ar**.

6 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

7 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

ADD PHYSICS

For comparison, compute the swelling stretches when the gel is allowed to swell homogeneously. The free and uniaxial swelling stretches can be computed by solving two nonlinear global DAEs.

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 **Mathematics** > **ODE and DAE Interfaces** > **Global ODEs and DAEs (ge)**.

4 Click the **Add to Component 1** button in the window toolbar.

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

GLOBAL ODES AND DAES (GE)

Global Equations 1 (ODE1)

1 In the **Settings** window for **Global Equations**, locate the **Global Equations** section.

2 In the table, enter the following settings:

Name	f(u,ut,utt,t) (1)	Initial value (u_0) (1)	Initial value (ut_0) (1/s)	Description
lam0_free	G/(lam0_free^3)*(lam0_free^2-1)+Kmix*(log(1-lam0_free^(-3))+lam0_free^(-3)+chi*lam0_free^(-6))-mu_sw	2	0	Free swelling ratio
lam0_ua	G/(stretch0^2*lam0_ua)*(lam0_ua^2-1)+Kmix*(log(1-1/(stretch0^2*lam0_ua))+1/(stretch0^2*lam0_ua)+chi/(stretch0^4*lam0_ua^2))-mu_sw	2	0	Uniaxial swelling ratio

3 Locate the **Units** section. Click **Define Source Term Unit**.

4 In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	Pa

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

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

HOMOGENEOUS SWELLING

1 In the **Settings** window for **Study**, type `Homogeneous Swelling` in the **Label** text field.

2 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

Step 1: Stationary

Disable all physics interfaces except for the **Global ODEs and DAEs** interface. Also, since only global DOFs are solved for, no mesh is required.

1 In the **Model Builder** window, under **Homogeneous Swelling** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Definitions** > **Contact Pair 1 (p1)**.

5 Click **Disable**.

6 In the tree, select **Component 1 (comp1)** > **Solid Mechanics (solid), Controls spatial frame** and **Component 1 (comp1)** > **Darcy's Law (dl)**.

7 Click **Disable in Model**.

8 In the tree, select **Component 1 (comp1)** > **Multiphysics** > **Poroelasticity 1 (poro1)**.

9 Click **Disable in Model**.

10 Click to expand the **Mesh Selection** section. In the table, enter the following settings:

Component	Mesh
Component 1	No mesh

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

RESULTS

Create an **Evaluation Group** to read out the homogeneous swelling stretches for use in the **Gel Height** plot.

Homogeneous Swelling Stretches

1 In the **Results** toolbar, click **Evaluation Group**.

2 In the **Settings** window for **Evaluation Group**, type `Homogeneous Swelling Stretches` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Homogeneous Swelling/ Solution 11 (sol11)**.

Global Evaluation 1

1 Right-click **Homogeneous Swelling Stretches** and choose **Global Evaluation**.

2 In the **Homogeneous Swelling Stretches** toolbar, click **Evaluate**.

Global 1

1 In the **Model Builder** window, right-click **Gel Height** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
3.3900	1	Free homogeneous swelling
4.7815	1	Uniaxial homogeneous swelling

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **ar**.

5 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

Gel Height

In the **Model Builder** window, click **Gel Height**.

Table Annotation 1

1 In the **Gel Height** toolbar, click **More Plots** and choose **Table Annotation**.

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

3 From the **Source** list, choose **Local table**.

4 In the table, enter the following settings:

x-coordinate	y-coordinate	Annotation
3.2	3.45	Free swelling
3.2	4.85	Uniaxial swelling

5 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

6 From the **Anchor point** list, choose **Center**.

7 In the **Gel Height** toolbar, click **Plot**.

GLOBAL DEFINITIONS

Now, set up the uniaxial consolidation load case. Start by adding parameter cases where some of the material parameters will be modified, see Table 1.

Material Parameters

1 In the **Home** toolbar, click **Parameter Case**.

2 In the **Settings** window for **Case**, type `Uniaxial Consolidation Case` in the **Label** text field.

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

Name	Expression	Description
chi	0.2	Enthalpy of mixing
D	8e-10[m^2/s]	Solvent diffusivity

Model Parameters

1 In the **Home** toolbar, click **Parameter Case**.

2 In the **Settings** window for **Case**, type `Uniaxial Consolidation Case` in the **Label** text field.

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

Name	Expression	Description
stretch0	`3.215`	Free swelling stretch
mu_ref	`0[Pa]`	Reference chemical potential
stress	`0.05*Kmix/(stretch0^2)`	Applied stress

Step 1 (step1)

Add a smooth **Step** function, which will be used to apply the creep load.

1 In the **Home** toolbar, click **Functions** and choose **Global** > **Step**.

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

3 In the **Location** text field, type `0[s]`.

4 Click to expand the **Smoothing** section. From the **Location definition** list, choose **Beginning of step**.

SOLID MECHANICS (SOLID)

Boundary Load 1

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

2 Select Boundary 8 only.

3 In the **Settings** window for **Boundary Load**, locate the **Force** section.

4 Specify the $\mathbf{f}_A$ vector as

`-stress*step1(t)`	`z`

Roller 1

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

2 Select Boundary 9 only.

DARCY'S LAW (DL)

Free Flow (Consolidation)

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

2 In the **Settings** window for **Pressure**, type `Free Flow (Consolidation)` in the **Label** text field.

3 Select Boundary 8 only.

4 Locate the **Pressure** section. In the p_0 text field, type `mu_ref`.

MESH 2

In the **Mesh** toolbar, click **Add Mesh** and choose **Add Mesh**.

Mapped 1

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

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

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

4 Select Domain 2 only.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 7 and 8 only.

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

4 In the **Number of elements** text field, type `1`.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 6 and 9 only.

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

4 In the **Number of elements** text field, type `100`.

Mapped 2

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

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

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

4 Select Domain 1 only.

Distribution 1

1 Right-click **Mapped 2** and choose **Distribution**.

2 Select Boundaries 1 and 5 only.

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

4 In the **Number of elements** text field, type `1`.

5 Click **Build All**.

ADD STUDY

Add a new time-dependent study to compute the consolidation load case. Modify the model configuration for the study to exclude the boundary conditions specific to the swelling load case.

1 In the **Study** 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** > **Time Dependent**.
4 Click the **Add Study** button in the window toolbar.
5 In the **Study** toolbar, click **Add Study** to close the **Add Study** window.

UNIAXIAL CONSOLIDATION

1 In the **Settings** window for **Study**, locate the **Study Settings** section.
2 Clear the **Generate default plots** checkbox.
3 In the **Label** text field, type `Uniaxial Consolidation`.

Parametric Sweep

Use a parameter switch to select the correct set of parameters for the uniaxial consolidation case.

1 In the **Study** toolbar, click **Parametric Sweep**.
2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.
3 From the **Sweep type** list, choose **Parameter switch**.
4 Click **Add** twice.
5 In the table, enter the following settings:

Switch	Cases	Case numbers
Material Parameters	User defined	1
Model Parameters	User defined	1

Step 1: Time Dependent

1 In the **Model Builder** window, click **Step 1: Time Dependent**.
2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
3 In the **Output times** text field, type `{0 1 2 5 10 20 50 100 200 1000}*(height/stretch0)^2/D`.

4 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** checkbox.

5 In the tree, select **Component 1 (comp1)** > **Definitions** > **Contact Pair 1 (p1)**.

6 Click **Disable**.

7 In the tree, select **Component 1 (comp1)** > **Darcy's Law (dl)** > **Contact (Swelling)** and **Component 1 (comp1)** > **Darcy's Law (dl)** > **Free Flow (Swelling)**.

8 Click **Disable**.

9 In the tree, select **Component 1 (comp1)** > **Global ODEs and DAEs (ge)**.

10 Click **Disable in Model**.

Solution 12 (sol12)

1 In the **Model Builder** window, right-click **Solver Configurations** and choose **Show Default Solver**.

2 Expand the **Solution 12 (sol12)** node.

3 In the **Model Builder** window, expand the **Uniaxial Consolidation** > **Solver Configurations** > **Solution 12 (sol12)** > **Dependent Variables 1** node, then click **Pressure (comp1.mu)**.

4 In the **Settings** window for **Field**, locate the **Scaling** section.

5 From the **Method** list, choose **Manual**.

6 In the **Scale** text field, type `1.0e5`.

7 In the **Model Builder** window, click **Displacement Field (comp1.u)**.

8 In the **Settings** window for **Field**, locate the **Scaling** section.

9 In the **Scale** text field, type `height`.

10 In the **Model Builder** window, click **Time-Dependent Solver 1**.

11 In the **Settings** window for **Time-Dependent Solver**, locate the **Time Stepping** section.

12 From the **Steps taken by solver** list, choose **Strict**.

13 Select the **Initial step** checkbox.

14 In the **Model Builder** window, expand the **Uniaxial Consolidation** > **Solver Configurations** > **Solution 12 (sol12)** > **Time-Dependent Solver 1** node, then click **Direct**.

15 In the **Settings** window for **Direct**, locate the **General** section.

16 From the **Solver** list, choose **PARDISO**.

17 In the **Model Builder** window, click **Fully Coupled 1**.

18 In the **Settings** window for **Fully Coupled**, locate the **Method and Termination** section.

19 From the **Jacobian update** list, choose **Once per time step**.

20 In the **Maximum number of iterations** text field, type 10.

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

RESULTS

Add a **Selection** to the **Dataset** for the Uniaxial Consolidation study to exclude the rigid substrate when creating surface plots.

Uniaxial Consolidation/Solution 12 (sol12)

In the **Model Builder** window, expand the **Results** > **Datasets** node, then click **Uniaxial Consolidation/Solution 12 (sol12)**.

Selection

1 In the **Results** toolbar, click **Attributes** and choose **Selection**.

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

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

4 Select Domain 2 only.

RESULT TEMPLATES

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 **Uniaxial Consolidation/Solution 12 (sol12)** > **Solid Mechanics** > **Stress (solid)**.

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

Stress and Chemical Potential

1 In the **Model Builder** window, expand the **Results** > **Stress (solid)** node, then click **Stress (solid)**.

2 In the **Settings** window for **2D Plot Group**, type `Stress and Chemical Potential` in the **Label** text field.

3 Locate the **Data** section. From the **Time (s)** list, choose **24187**.

4 Locate the **Plot Settings** section. From the **View** list, choose **New view**.

5 Click to expand the **Plot Array** section. Select the **Enable** checkbox.

6 From the **Displacement** list, choose **Absolute**.

7 In the **Cell displacement** text field, type `0.4`.

Mixture Stress

1 In the **Model Builder** window, under **Results** > **Stress and Chemical Potential** click **Surface 1**.

2 In the **Settings** window for **Surface**, type `Mixture Stress` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `-poro1.sGpzz`.

4 From the **Unit** list, choose **kPa**.

5 Select the **Description** checkbox. In the associated text field, type `Normal stress`.

Chemical Potential

1 Right-click **Mixture Stress** and choose **Duplicate**.

2 In the **Settings** window for **Surface**, type `Chemical Potential` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `mu`.

4 In the **Description** text field, type `Chemical potential`.

5 Locate the **Inherit Style** section. From the **Plot** list, choose **Mixture Stress**.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Stress and Chemical Potential** and choose **Arrow Surface**.

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

3 In the **R-component** text field, type `dl.u`.

4 In the **Z-component** text field, type `dl.w`.

5 Locate the **Arrow Positioning** section. Find the **R grid points** subsection. In the **Points** text field, type `4`.

6 Find the **Z grid points** subsection. In the **Points** text field, type `20`.

7 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Mixture Stress**.

8 Clear the **Arrow scale factor** checkbox.

9 Clear the **Color** checkbox.

10 Clear the **Color and data range** checkbox.

11 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

12 In the **Index** text field, type `1`.

Deformation 1

Right-click **Arrow Surface 1** and choose **Deformation**.

Table Annotation 1

1 In the **Stress and Chemical Potential** toolbar, click **More Plots** and choose **Table Annotation**.

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

3 From the **Source** list, choose **Local table**.

4 In the table, enter the following settings:

x-coordinate	y-coordinate	Annotation
0.05	-0.015	Normal stress $-\sigma_{zz}$
0.45	-0.015	Chemical potential μ

5 Select the **LaTeX markup** checkbox.

6 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

7 From the **Anchor point** list, choose **Center**.

Stress and Chemical Potential

1 In the **Model Builder** window, click **Stress and Chemical Potential**.

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

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type

```
Surface: Normal stress (kPa) Surface: Chemical potential (kPa)
Arrow Surface: Total Darcy velocity field (spatial frame)
```

on separate lines.

5 In the **Stress and Chemical Potential** toolbar, click **Plot**.

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

Thickness Stretch

Follow the instructions below to reproduce Fig. 4 in Ref. 1.

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

2 In the **Settings** window for **1D Plot Group**, type `Thickness Stretch` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Uniaxial Consolidation/ Solution 12 (sol12)**.

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Z/H`.

6 Select the **y-axis label** checkbox. In the associated text field, type `\lambda<sub>3</sub>`.

7 Locate the **Axis** section. Select the **Manual axis limits** checkbox.

8 In the **x minimum** text field, type `0`.

9 In the **y minimum** text field, type `0.5`.

10 In the **y maximum** text field, type `3.5`.

11 Locate the **Grid** section. Select the **Manual spacing** checkbox.

12 In the **x spacing** text field, type `0.2`.

13 In the **y spacing** text field, type `0.5`.

14 Locate the **Legend** section. Clear the **Show legends** checkbox.

Line Graph 1

1 Right-click **Thickness Stretch** and choose **Line Graph**.

2 Select Boundary 6 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `solid.stchp3*stretch0`.

5 Select the **Description** checkbox. In the associated text field, type `Third principal stretch`.

6 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

7 In the **Expression** text field, type `1-Z/height`.

8 Click to expand the **Coloring and Style** section. From the **Color cycle** list, choose **Long**.

Thickness Stretch

In the **Model Builder** window, click **Thickness Stretch**.

Table Annotation 1

1 In the **Thickness Stretch** toolbar, click **More Plots** and choose **Table Annotation**.

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

3 From the **Source** list, choose **Local table**.

4 In the table, enter the following settings:

x-coordinate	y-coordinate	Annotation
0	3.2	0^+
0.06	2.9	1
0.09	2.8	2

x-coordinate	y-coordinate	Annotation
0.14	2.7	5
0.2	2.6	10
0.28	2.5	20
0.43	2.2	50
0.59	2.0	100
0.76	1.5	$Dt/H_0^2 = 200$
0.8	0.8	1000

5 Select the **LaTeX markup** checkbox.

6 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

7 From the **Anchor point** list, choose **Lower left**.

8 In the **Thickness Stretch** toolbar, click **Plot**.

Reference Data, Hong and others (2008), t=2

Compare the results with data from Ref. 1 for a few time points.

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Reference Data, Hong and others (2008), t=2` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `hydrogel_swelling_uniaxial_t2.txt`.

Reference Data, Hong and others (2008), t=20

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Reference Data, Hong and others (2008), t=20` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `hydrogel_swelling_uniaxial_t20.txt`.

Reference Data, Hong and others (2008), t=100

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Reference Data, Hong and others (2008), t=100` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `hydrogel_swelling_uniaxial_t100.txt`.

Reference Data, Hong and others (2008), t=2

1 Right-click **Thickness Stretch** and choose **Table Graph**.

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

3 Find the **Line style** subsection. From the **Line** list, choose **None**.

4 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

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

6 In the **Label** text field, type `Reference Data, Hong and others (2008), t=2`.

Reference Data, Hong and others (2008), t=20

1 Right-click **Reference Data, Hong and others (2008), t=2** and choose **Duplicate**.

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

3 From the **Table** list, choose **Reference Data, Hong and others (2008), t=20**.

4 In the **Label** text field, type `Reference Data, Hong and others (2008), t=20`.

Reference Data, Hong and others (2008), t=100

1 Right-click **Reference Data, Hong and others (2008), t=20** and choose **Duplicate**.

2 In the **Settings** window for **Table Graph**, type `Reference Data, Hong and others (2008), t=100` in the **Label** text field.

3 Locate the **Data** section. From the **Table** list, choose **Reference Data, Hong and others (2008), t=100**.

4 In the **Thickness Stretch** toolbar, click  **Plot**.

INHOMOGENEOUS SWELLING

Finally, disable the boundary conditions added for the consolidation study in the settings for **Step 1: Time Dependent** under the **Inhomogeneous Swelling** study node if you want to recompute the swelling load case.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Inhomogeneous Swelling** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Global ODEs and DAEs (ge)**.

5 Click **Disable in Model**.

6 In the tree, select **Component 1 (comp1)** > **Solid Mechanics (solid), Controls spatial frame** > **Boundary Load 1** and **Component 1 (comp1)** > **Solid Mechanics (solid), Controls spatial frame** > **Roller 1**.

7 Click **Disable**.

8 In the tree, select **Component 1 (comp1)** > **Darcy's Law (dl)** > **Free Flow (Consolidation)**.

9 Click **Disable**.