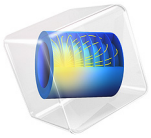


Model created in COMSOL Multiphysics 6.4

Biodegradation of a Magnesium Stent

Introduction

Biodegradable metallic biomaterials such as Magnesium (Mg) are gathering attention for biomedical applications due to their favorable properties. While degrading, magnesium parts undergo geometrical changes, and the dissolution of metal ions may give rise to harmful changes in pH in human tissue. The present model simulates dissolution of a Mg stent placed in a blood vessel.

In the first study of the model, the Level Set interface is used to model the geometrical changes of the stent when subject to a local constant dissolution rate over time.

The resulting stent shapes at various stages of dissolution are then used in a second study in order to calculate the concentration of Mg ions in the tissue and vessel surrounding the stent, and the corresponding pH levels.

Model Definition

Figure 1 shows the full geometry of a biomedical stent. The highlighted region shows the circumferential symmetry in the stent geometry.

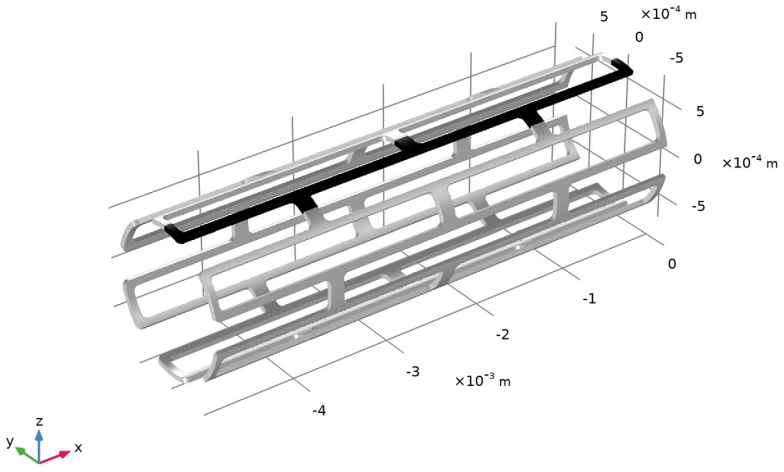


Figure 1: Full Mg stent geometry along with minimal symmetry region highlighted.

Due to this symmetry, only one-twelfth of the full stent geometry is considered in the model. The reduced geometry of the Mg stent placed in the tissue and blood vessel is shown in Figure 2.

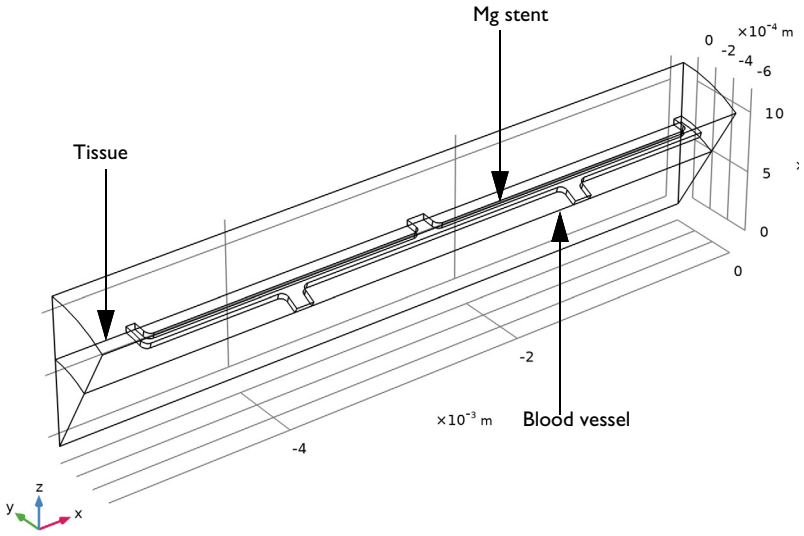


Figure 2: Reduced Mg stent geometry considered in the model due to symmetry.

DISSOLUTION INTERFACE TRACKING

The Level Set interface is used to keep track of the Mg stent dissolution due to uniform corrosion. The Level Set interface automatically sets up the equations for the movement of the interface between the Mg stent and the tissue. The level set variable varies from 1 in the tissue and blood vessel domains to 0 in the Mg stent domain. The interface is represented by the 0.5 contour of the level set variable ϕ. The transport of the level set variable is given by:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \quad (1)$$

The ε parameter determines the thickness of the interface and is defined as $\varepsilon = h_{\text{stent}}$, where h_{stent} is the mesh element size at the stent surface. The γ parameter determines the amount of reinitialization. A suitable value for γ is the maximum velocity magnitude occurring in the model.

The level-set variable is advected by a constant normal velocity, v_n, which is set to a value of 2 mm/y (Ref. 2).

The level set delta function is approximated by

$$\delta = 6|\phi(1-\phi)||\nabla\phi| \tag{2}$$

AQUEOUS ELECTROLYTE TRANSPORT INTERFACE

The interface is used to define material balances accounting for the mass transport of species, i, and various sources in the tissue and blood vessel domains:

$$\varepsilon_l \frac{\partial c}{\partial t} + \nabla \cdot \boldsymbol{J}_i + \mathbf{u} \cdot \nabla c = S \tag{3}$$

In the equation, ε_l is the plasma volume fraction, $\boldsymbol{J}_i$ is the diffusion and migration flux, and S any type of source (mol/(m^3·s)). The velocity field, $\mathbf{u}$, is set using an analytical expression to mimic Hagen–Poiseuille flow in the blood vessel, and it is set to 0 in the stent and tissue domains.

Carbonic acid chemical equilibria are considered according to Table 1.

TABLE 1: CARBONIC ACID CHEMICAL EQUILIBRIA

REACTIONS	EQUILIBRIUM CONSTANT, K
$CO_2 + H_2O \Leftrightarrow H_2CO_3$	715
$H_2CO_3 \Leftrightarrow H^+ + HCO_3^-$	0.32 mol/m^3
$HCO_3^- \Leftrightarrow H^+ + CO_3^{2-}$	$5.01 \cdot 10^{-8}$ mol/m^3

Phosphoric acid chemical equilibria are considered according to Table 2.

TABLE 2: PHOSPHORIC ACID CHEMICAL EQUILIBRIA

REACTIONS	EQUILIBRIUM CONSTANT, K
$H_3PO_4 \Leftrightarrow H^+ + H_2PO_4^-$	7.5 mol/m^3
$H_2PO_4^- \Leftrightarrow H^+ + HPO_4^-$	$6.2 \cdot 10^{-5}$ mol/m^3

Two **Weak Acid** nodes are used to set the chemical equilibria of carbonic acid and phosphoric acid, respectively. The first two equilibrium reactions in carbonic acid chemical equilibria (Table 1) are clubbed together in the first dissociation step used in the **Weak Acid** node for carbonic acid. Values of the equilibrium constants are taken from Ref. 2 and Ref. 3. All species involved in chemical equilibria of carbonic acid and phosphoric acid are set as immobile species. The initial concentration of HCO_3^- and HPO_4^- ions are set to 25 mol/m^3 and 1 mol/m^3, respectively.

Since the net current on the Mg stent surface is zero, the induced electric field is assumed to be negligible. Hence, the electrolyte potential is not solved in this model. This also leads to the assumption of constant total concentrations of the CO_2 and H_3PO_4 buffer solutions in the tissue and blood vessel domains. Since the current densities are low and the transport is considered to be diffusion-convection dominated, only transport of Mg ions is solved for. The change in pH in the tissue and blood vessel is attributed to the change in Mg ion concentration, in combination with the equilibrium speciation of the two weak acids.

The transport of Mg ions is solved using the **Fully Dissociated Species** node. The source term, S_{Mg}, representing the dissolution of ions on the stent surface, is set in terms of the dissolution velocity, v_n, and the level set delta function according to

$$S_{\mathrm{Mg}} = v_n \frac{\rho_{\mathrm{Mg}}}{M_{\mathrm{Mg}}} \times \delta \tag{4}$$

where M_{Mg} is the molar mass (24.3 g/mol) and ρ_{Mg} is the density (1735 kg/m^3) of Mg. The **Inflow** and **Outflow** boundary nodes are set at the two non-symmetry exterior boundaries of the blood vessel domain. The initial concentration of Mg ions is set to 1.5 mol/m^3.

To account for all remaining ions in the blood, another **Fully Dissociated Species** node is added to the model, also being set as immobile species. The concentration of these auxiliary ions are set in order to reach an inlet pH level of 7.4.

The corresponding pH and speciation of the weak acids vs the magnesium concentration in the buffer system are shown in Figure 3 and Figure 4, respectively.

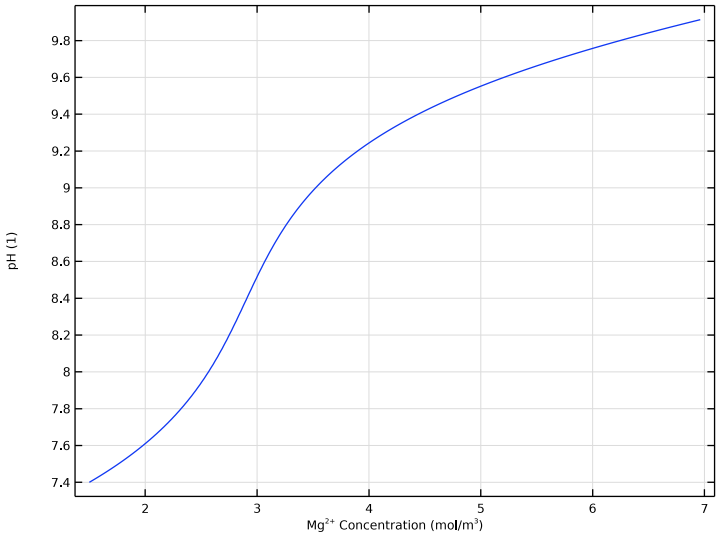


Figure 3: pH versus magnesium ion concentration for the carbonate and phosphoric acid buffer system for an initial/inlet Mg concentration of 1.5 mM.

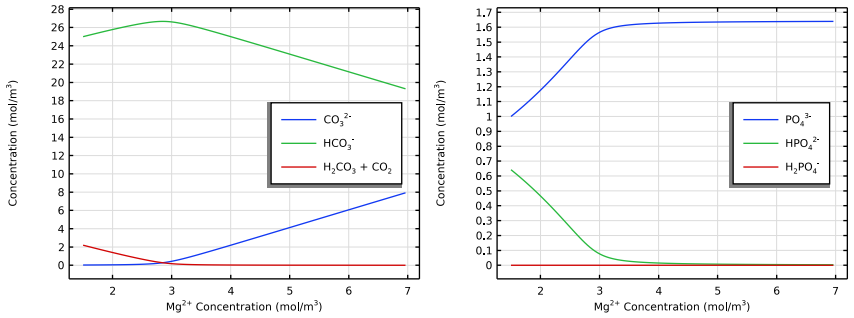


Figure 4: Speciation of carbonic (left) and phosphoric (right) acid.

STUDIES

The first study of the model, where the Level Set interface is solved, uses a time-dependent solver for 5 days. The second study of the model, where the Aqueous Electrolyte Transport interface is solved uses a quasi-stationary approach, where stationary analysis is performed for different stent shapes obtained from the first study of the model.

Figure 5 shows an isosurface plot of volume fraction of fluid 1 with a value of 0.5 representing the stent surface for the reduced geometry at 1 d (left) and 4 d (right). The change in Mg stent shape can be seen with time representing its dissolution in the tissue and blood vessel.

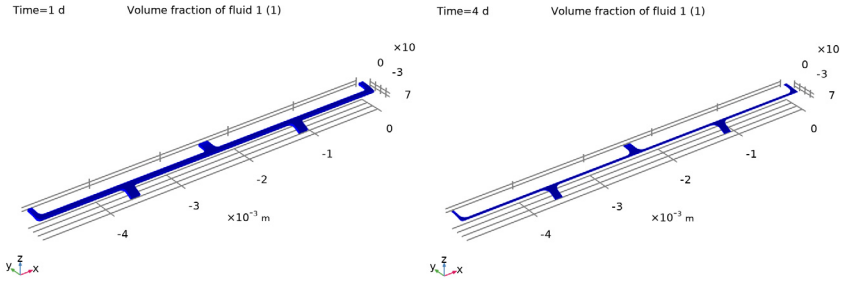


Figure 5: The isosurface plot of volume fraction of fluid 1 of value 0.5 for the reduced geometry of Mg stent at t = 1 d (left) and t = 4 d (right).

Figure 6 shows the isosurface plot of volume fraction of fluid 1 with a value of 0.5 representing the stent surface for the full Mg stent geometry at 1 d (left) and 4 d (right). The dissolution of the Mg stent leading to topological changes can be seen at 4 d.

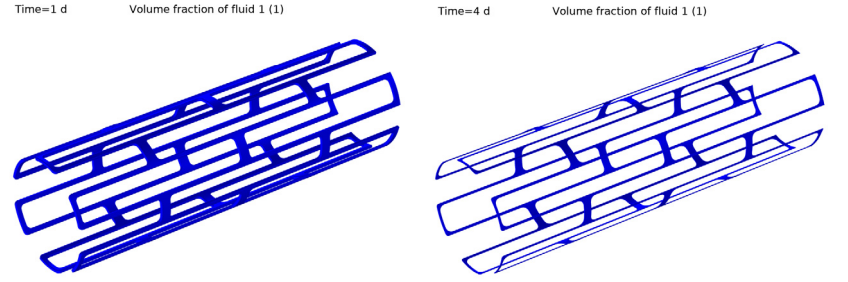


Figure 6: The isosurface plot of volume fraction of fluid 1 of value 0.5 for the full geometry of Mg stent at t = 1 d (left) and t = 4 d (right).

Figure 7 shows the change in the stent relative mass loss against time. It can seen that the dissolution rate is uniform until the Mg stent dissolves completely at around 5 d.

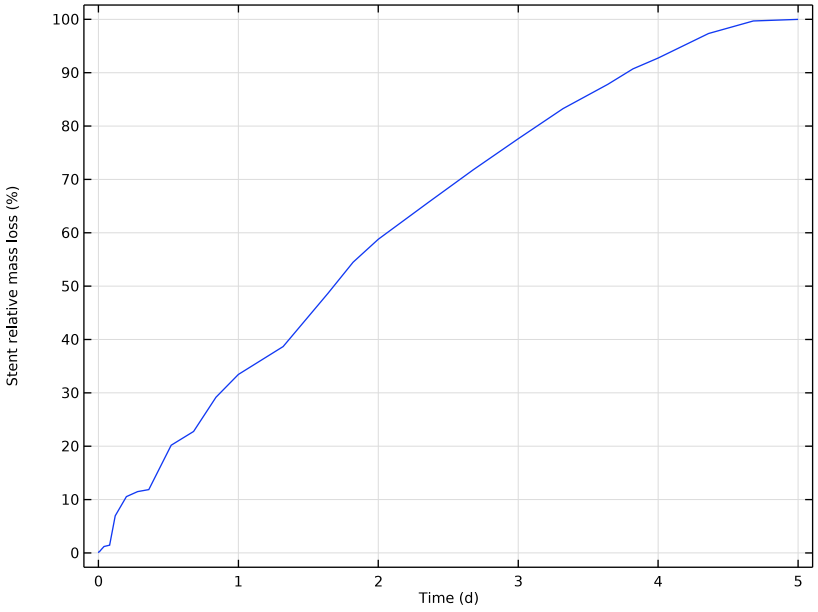


Figure 7: Change in Mg stent mass loss against time.

Figure 8 shows the volume plot of Mg ion concentration and volume arrow plot of velocity in the blood vessel domain over a sector of the model geometry at 1 d (left) and 4 d (right). It can be seen that the Mg ion concentration is lower toward the inflow boundary and it gradually increases toward the outflow boundary. The higher value of Mg ion concentration is also seen over a small region at the stent/tissue interface.

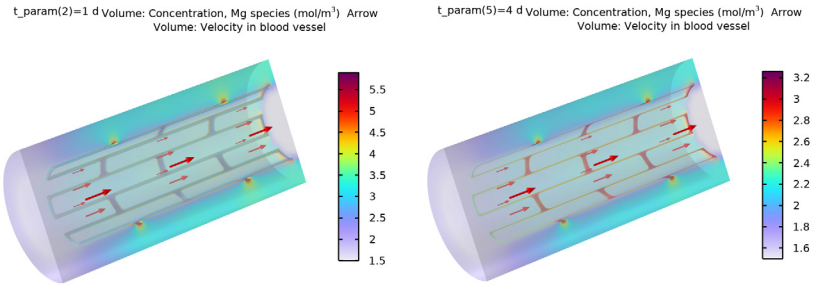


Figure 8: The volume plot of Mg ion concentration and arrow volume plot for velocity in blood vessel at t = 1 d (left) and t = 4 d (right).

Figure 9 shows the volume plot of pH and volume arrow plot of velocity in the blood vessel domain over a sector of the model geometry at 1 d (left) and 4 d (right). It can be seen that pH stays close to 7.4 (desired value) at the stent/blood vessel interface. The higher value of pH is seen over a small region at the stent/tissue interface. It should be noted that if pH gets too high, it could potentially damage the tissue. The higher value of pH at initial times and at the outer stent surface (stent/tissue interface) could be attributed to the longest transport distance to the blood vessel as well as the highest total Mg dissolution rate.

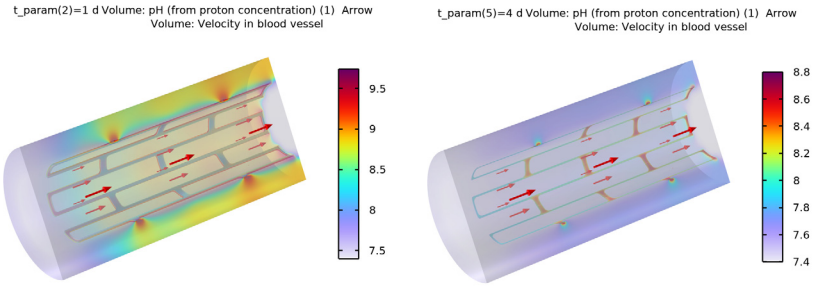


Figure 9: The volume plot of pH and arrow volume plot for velocity in blood vessel at t = 1 d (left) and t = 4 d (right).

References

1. M. Barzegari, D. Mei, S.V. Lamaka, and L. Geris, "Computational modeling of degradation process of biodegradable magnesium biomaterials," *Corros. Sci.*, vol. 190, no. 109674, pp. 1–11, 2021.

2. B. Zeller-Plumhoff, T. AlBaraghtheh, D. Hoche, and R. Willumeit-Romer, "Computational modelling of magnesium degradation in simulated body fluid under physiological conditions," *J. Magnes. Alloy*, vol. 10, issue 4, pp. 965–978, 2022.

3. D. Pines, J. Ditkovich, T. Mukra, Y. Miller, P.M. Kiefer, S. Daschakraborty, J.T. Hynes, and E. Pines, "How Acidic Is Carbonic Acid?," *J. Phys. Chem. B*, vol. 120, no. 9, pp. 2440–2451, 2016.

Application Library path: `Corrosion_Module/General_Corrosion/biodegradation_mg_stent`

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 **Mathematics** > **Moving Interface** > **Level Set (ls)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Time Dependent with Phase Initialization**.
6. Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Now load the model parameters.

1. In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
2. In the **Settings** window for **Parameters**, locate the **Parameters** section.
3. Click **Load from File**.
4. Browse to the model's Application Libraries folder and double-click the file `biodegradation_mg_stent_parameters.txt`.

GEOMETRY 1

Import 1 (imp1)

1. In the **Geometry** toolbar, click **Import**.
2. In the **Settings** window for **Import**, locate the **Source** section.
3. Click **Browse**.
4. Browse to the model's Application Libraries folder and double-click the file `biodegradation_mg_stent.mphbin`.
5. Click **Import**.

Work Plane 1 (wp1)

1 In the **Geometry** toolbar, click **Work Plane**.

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

3 From the **Plane** list, choose **yz-plane**.

4 In the **x-coordinate** text field, type `-5.5 [mm]`.

Work Plane 1 (wp1) > Plane Geometry

In the **Model Builder** window, click **Plane Geometry**.

Work Plane 1 (wp1) > Circle 1 (c1)

1 In the **Work Plane** toolbar, click **Circle**.

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

3 In the **Radius** text field, type `R_tissue`.

4 In the **Sector angle** text field, type `30`.

5 Locate the **Rotation Angle** section. In the **Rotation** text field, type `90`.

Work Plane 1 (wp1) > Circle 2 (c2)

1 In the **Work Plane** toolbar, click **Circle**.

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

3 In the **Radius** text field, type `R_vessel`.

4 In the **Sector angle** text field, type `30`.

5 Locate the **Rotation Angle** section. In the **Rotation** text field, type `90`.

Extrude 1 (ext1)

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Extrude**.

2 In the **Settings** window for **Extrude**, locate the **Distances** section.

3 In the table, enter the following settings:

Distances (m)
`5.5[mm]`

4 Click the **Wireframe Rendering** button in the **Graphics** toolbar.

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

6 Click **Build All Objects**.

DEFINITIONS

Integration 1 (intop1)

Next, add an integration operator which will be used later during postprocessing.

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**.

Maximum 1 (maxop1)

Next, add a maximum operator which will be used later while setting up the model.

1. In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Maximum**.
2. In the **Settings** window for **Maximum**, locate the **Source Selection** section.
3. From the **Selection** list, choose **All domains**.

Global Variable Probe 1 (var1)

Next, add a global variable probe which will be used later during postprocessing.

1. In the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.
2. In the **Settings** window for **Global Variable Probe**, type `stent_mass_loss` in the **Variable name** text field.
3. Locate the **Expression** section. In the **Expression** text field, type `1-intop1(phils>0.5)/at(0,intop1(phils>0.5))`.
4. From the **Table and plot unit** list, choose **%**.
5. Select the **Description** checkbox. In the associated text field, type `Stent relative mass loss`.

Vessel

Next, create some selections to be used later while setting up the model.

1. In the **Definitions** toolbar, click **Explicit**.
2. In the **Settings** window for **Explicit**, type `Vessel` in the **Label** text field.
3. Select Domain 2 only.

Tissue

1. In the **Definitions** toolbar, click **Explicit**.
2. In the **Settings** window for **Explicit**, type `Tissue` in the **Label** text field.
3. Select Domain 1 only.

Stent

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, type `Stent` in the **Label** text field.

3 Select Domain 3 only.

Tissue and Stent

1 In the **Definitions** toolbar, click **Union**.

2 In the **Settings** window for **Union**, type `Tissue and Stent` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click **Add**.

4 In the **Add** dialog, in the **Selections to add** list, choose **Tissue** and **Stent**.

5 Click **OK**.

LEVEL SET (LS)

In the first part of the model, set the Level Set physics.

Level Set Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Level Set (ls)** click **Level Set Model 1**.

2 In the **Settings** window for **Level Set Model**, locate the **Level Set Model** section.

3 In the γ text field, type `max(maxop1(Vn),eps)`.

4 In the ε_{ls} text field, type `hstent`.

5 Locate the **Convection** section. Specify the $\mathbf{u}$ vector as

`Vn*ls.intnormx`	x
`Vn*ls.intnormy`	y
`Vn*ls.intnormz`	z

Initial Values, Fluid 2

1 In the **Model Builder** window, click **Initial Values, Fluid 2**.

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

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

MESH 1

Next, set a fine mesh near the stent domain.

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

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

3 From the list, choose **User-controlled mesh**.

Size 1

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

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

3 Clear the **Minimum element size** checkbox.

Free Triangular 1

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

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

3 Click  **Paste Selection**.

4 In the **Paste Selection** dialog, type 11 in the **Selection** text field.

5 Click **OK**.

Size 1

1 Right-click **Free Triangular 1** and choose **Size**.

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

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section.

5 Select the **Maximum element size** checkbox. In the associated text field, type `hstent`.

6 Select the **Minimum element size** checkbox. In the associated text field, type `1e-6`.

Swept 1

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

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

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

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

Distribution 1

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

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

3 In the **Number of elements** text field, type 10.

Free Triangular 1

In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** right-click **Free Triangular 1** and choose **Move Up**.

Swept 1

In the **Model Builder** window, right-click **Swept 1** and choose **Move Up**.

Boundary Layers 1

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

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

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

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

Boundary Layer Properties

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

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

3 Click  **Paste Selection**.

4 In the **Paste Selection** dialog, type `6, 12, 17, 23, 31, 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 `3`.

8 From the **Thickness specification** list, choose **First layer**.

9 In the **Thickness** text field, type `hstent/10`.

10 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.

STUDY 1

Step 1: Phase Initialization

1 In the **Model Builder** window, under **Study 1** click **Step 1: Phase Initialization**.

2 In the **Settings** window for **Phase Initialization**, click to expand the **Results While Solving** section.

3 From the **Probes** list, choose **None**.

Step 2: Time Dependent

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

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

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

4 In the **Output times** text field, type `range(0,1,5)`.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

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

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

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

RESULTS

The following steps reproduce the plots from the Results and Discussion section:

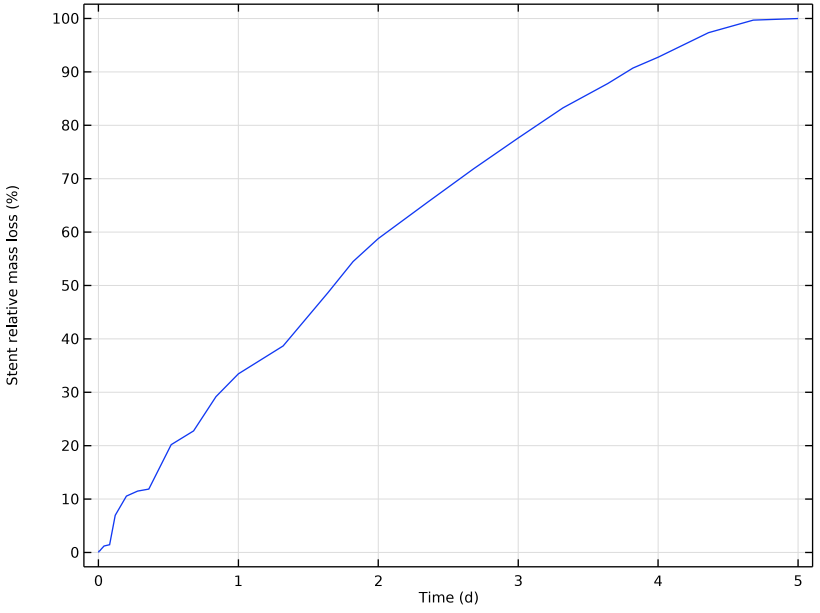
Stent Relative Mass Loss

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 1**.

2 In the **Settings** window for **1D Plot Group**, type `Stent Relative Mass Loss` in the **Label** text field.

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

4 In the **Stent Relative Mass Loss** toolbar, click **Plot**.



Volume Fraction of Fluid 1 (ls)

1 In the **Model Builder** window, click **Volume Fraction of Fluid 1 (ls)**.

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

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

4 Locate the **Color Legend** section. Clear the **Show legends** checkbox.

Slice 1

1 In the **Model Builder** window, expand the **Volume Fraction of Fluid 1 (ls)** node.

2 Right-click **Slice 1** and choose **Disable**.

Isosurface 1

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

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

3 From the **Color** list, choose **Blue**.

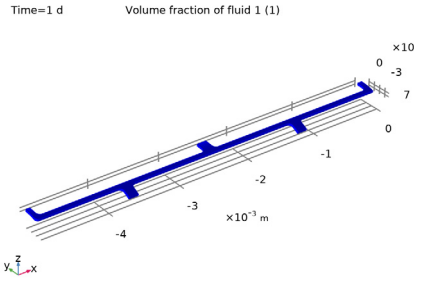
Stent Shape in Model Geometry

1 In the **Model Builder** window, under **Results** click **Volume Fraction of Fluid 1 (ls)**.

2 In the **Settings** window for **3D Plot Group**, type `Stent Shape in Model Geometry` in the **Label** text field.

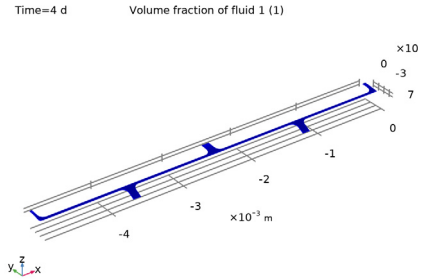
3 Locate the **Data** section. From the **Time (d)** list, choose **1**.

4 In the **Stent Shape in Model Geometry** toolbar, click **Plot**.



5 From the **Time (d)** list, choose **4**.

6 In the **Stent Shape in Model Geometry** toolbar, click **Plot**.



Mirror 3D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Mirror 3D**.

2 In the **Settings** window for **Mirror 3D**, locate the **Plane Data** section.

3 From the **Plane** list, choose **zx-planes**.

Sector 3D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Sector 3D**.

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

3 From the **Dataset** list, choose **Mirror 3D 1**.

4 Locate the **Axis Data** section. In row **Point 2**, set **x** to 1.

5 In row **Point 2**, set **z** to 0.

6 Locate the **Symmetry** section. In the **Number of sectors** text field, type 6.

3D Plot Group 3

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

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

3 From the **Dataset** list, choose **Sector 3D 1**.

Isosurface 1

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

2 In the **Settings** window for **Isosurface**, locate the **Levels** section.

3 From the **Entry method** list, choose **Levels**.

4 In the **Levels** text field, type 0.5.

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

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

Full Stent Shape

1 In the **Model Builder** window, under **Results** click **3D Plot Group 3**.

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

3 Locate the **Data** section. From the **Time (d)** list, choose **1**.

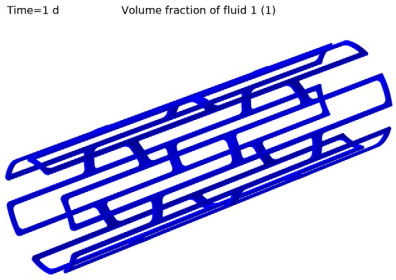
4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

5 Locate the **Color Legend** section. Clear the **Show legends** checkbox.

6 Click the **Show Grid** button in the **Graphics** toolbar.

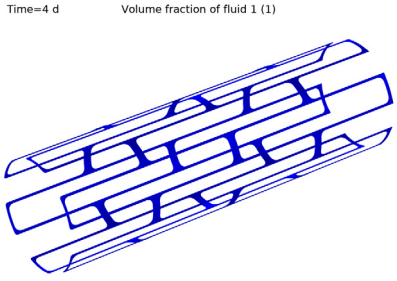
7 Click the **Show Axis Orientation** button in the **Graphics** toolbar.

8 In the **Full Stent Shape** toolbar, click **Plot**.



9 Locate the **Data** section. From the **Time (d)** list, choose **4**.

10 In the **Full Stent Shape** toolbar, click **Plot**.



COMPONENT 1 (COMP1)

In the second part of the model, we do a quasi-stationary analysis of blood chemistry using the Aqueous Electrolyte Transport interface.

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 **Electrochemistry** > **Aqueous Electrolyte Transport (aqt)**.

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

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

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

GLOBAL DEFINITIONS

Acid Equilibria Parameters

Next, add parameters used for acid equilibria.

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

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

3 Locate the **Parameters** section. Click **Load from File**.

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

Next, set the temperature to T in the Default Model Inputs.

Default Model Inputs

1 In the **Model Builder** window, click **Default Model Inputs**.

2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.

3 In the tree, select **General** > **Temperature (K) - minput.T**.

4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type `T`.

DEFINITIONS

Now, add variables.

Variables 1

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

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

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

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

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

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

Variables 2

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

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

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

4 From the **Selection** list, choose **Tissue and Stent**.

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

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

AQUEOUS ELECTROLYTE TRANSPORT (AQT)

Now, start setting up the physics.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Aqueous Electrolyte Transport (aqt)**.

2 In the **Settings** window for **Aqueous Electrolyte Transport**, locate the **Transport Mechanisms** section.

3 Clear the **Solve for electrolyte phase potential** checkbox.

4 Select the **Convection** checkbox.

Electrolyte 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Aqueous Electrolyte Transport (aqt)** click **Electrolyte 1**.

2 In the **Settings** window for **Electrolyte**, locate the **Convection** section.

3 Specify the **u** vector as

u	x
0	y
0	z

Next, add acid equilibria for H2CO3 using the Weak Acid feature.

4 In the **Model Builder** window, click **Electrolyte 1**.

Weak Acid: H2CO3

1 In the **Physics** toolbar, click **Attributes** and choose **Weak Acid**.

2 In the **Settings** window for **Weak Acid**, type `Weak Acid: H2CO3` in the **Label** text field.

3 Locate the **Weak Acid** section. In the **Species name** text field, type `H2CO3`.

4 From the list, choose **Polyprotic**.

5 In the table, enter the following settings:

Dissociation step (I)	pKa (I)
1	pKa_H2CO3_1
2	pKa_H2CO3_2

6 Select the **Immobile species** checkbox.

7 In the *c* text field, type `cCO2tot`.

Electrolyte 1

Next, add acid equilibria for H3PO4 using the Weak Acid feature.

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

Weak Acid: H3PO4

1 In the **Physics** toolbar, click **Attributes** and choose **Weak Acid**.

2 In the **Settings** window for **Weak Acid**, type `Weak Acid: H3PO4` in the **Label** text field.

3 Locate the **Weak Acid** section. In the **Species name** text field, type `H3PO4`.

4 From the list, choose **Polyprotic**.

5 In the table, enter the following settings:

Dissociation step (I)	pKa (I)
1	pKa_H3PO4_1
2	pKa_H3PO4_2

6 Select the **Immobile species** checkbox.

7 In the *c* text field, type `cH3PO4tot`.

Electrolyte 1

Next, set mass transport and source term for magnesium species using the Fully Dissociated Species feature.

In the **Physics** toolbar, click **Attributes** and choose **Fully Dissociated Species**.

Fully Dissociated Species: Mg

1 In the **Settings** window for **Fully Dissociated Species**, type `Fully Dissociated Species: Mg` in the **Label** text field.

2 Locate the **Fully Dissociated Species** section. In the **Species name** text field, type `Mg`.

3 In the z text field, type `2`.

4 Locate the **Diffusion and Migration** section. In the D text field, type `DMg`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Aqueous Electrolyte Transport (aqt)** click **Initial Values 1**.

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

3 In the $c_{\mathrm{Mg},0}$ text field, type `cMg0`.

Species Source 1

1 In the **Physics** toolbar, click **Domains** and choose **Species Source**.

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

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

4 Locate the **Species Sources** section. In the $R_{\mathrm{Mg}^{2+}}$ text field, type `S_Mg*ls.delta`.

5 In the R_{OH^-} text field, type `2*S_Mg*ls.delta`.

Inflow 1

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

2 Select Boundary 4 only.

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

4 In the $c_{0,\mathrm{Mg}}$ text field, type `cMg0`.

5 Locate the **Boundary Condition Type** section. From the list, choose **Flux (Danckwerts)**.

Outflow 1

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

2 Select Boundary 44 only.

Electrolyte 1

Next, add all additional ions into an auxiliary species using the Fully Dissociated Species feature.

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

Fully Dissociated Species: Auxiliary Ions

1 In the **Physics** toolbar, click **Attributes** and choose **Fully Dissociated Species**.

2 In the **Settings** window for **Fully Dissociated Species**, type `Fully Dissociated Species: Auxiliary Ions` in the **Label** text field.

3 Locate the **Fully Dissociated Species** section. In the **Species name** text field, type `aux`.

4 In the *z* text field, type `1`.

5 Select the **Immobile species** checkbox.

6 In the *c* text field, type `cAux0`.

Separator 1

Next, set the plasma volume fraction using the Separator feature.

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

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

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

4 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `epsl`.

ROOT

Finally, add a Study node to set a quasi-stationary analysis.

ADD STUDY

1 In the **Home** toolbar, click **Windows** and choose **Add Study**.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Some Physics Interfaces** > **Stationary**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkbox for **Level Set (ls)**.

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
t_param (Time parameter in Study 2)	`range(0,1,5)`	d

5 Locate the **Output While Solving** section. From the **Probes** list, choose **None**.

Step 1: Stationary

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

2 In the **Settings** window for **Stationary**, click to expand the **Values of Dependent Variables** section.

3 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

4 From the **Method** list, choose **Solution**.

5 From the **Study** list, choose **Study 1, Time Dependent**.

6 From the **Time (d)** list, choose **Interpolated**.

7 In the **Time** text field, type `t_param`.

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

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

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

The model is now ready for computations.

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

RESULTS

The following steps reproduce the plots from the Results and Discussion section:

Mirror 3D 2

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

2 Right-click **Results** > **Datasets** and choose **More 3D Datasets** > **Mirror 3D**.

3 In the **Settings** window for **Mirror 3D**, locate the **Data** section.

4 From the **Dataset** list, choose **Study 2/Parametric Solutions 1 (sol4)**.

5 Locate the **Plane Data** section. From the **Plane** list, choose **zx-planes**.

Sector 3D 2

1 In the **Results** toolbar, click **More Datasets** and choose **Sector 3D**.

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

3 From the **Dataset** list, choose **Mirror 3D 2**.

4 Locate the **Axis Data** section. In row **Point 2**, set **x** to 1.

5 In row **Point 2**, set **z** to 0.

6 Locate the **Symmetry** section. In the **Number of sectors** text field, type 6.

7 From the **Sectors to include** list, choose **Manual**.

8 In the **Start sector** text field, type `-3`.

9 In the **Number of sectors to include** text field, type `3`.

Concentration, Mg

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Sector 3D 2**.

4 From the **Parameter value (t_param (d))** list, choose **1**.

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

Volume 1

1 In the **Concentration, Mg** toolbar, click **Volume**.

2 In the **Settings** window for **Volume**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Aqueous Electrolyte Transport** > **Fully Dissociated Species: Mg** > **aqt.c_Mg - Concentration, Mg species - mol/m³**.

3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prism**.

Transparency 1

In the **Concentration, Mg** toolbar, click **Transparency**.

Volume 1

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

Filter 1

1 In the **Concentration, Mg** toolbar, click **Filter**.

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

3 In the **Logical expression for inclusion** text field, type `ls.Vf1>=0.5`.

Concentration, Mg

In the **Model Builder** window, under **Results** click **Concentration, Mg**.

Arrow Volume 1

1 In the **Concentration, Mg** toolbar, click **Arrow Volume**.

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

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

4 In the **y-component** text field, type `0`.

5 In the **z-component** text field, type `0`.

6 Select the **Description** checkbox. In the associated text field, type `Velocity in blood vessel`.

7 Locate the **Arrow Positioning** section. Find the **x grid points** subsection. In the **Points** text field, type `3`.

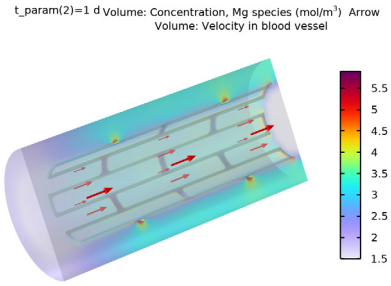
Concentration, Mg

1 Click the **Show Axis Orientation** button in the **Graphics** toolbar.

2 Click the **Show Grid** button in the **Graphics** toolbar.

3 In the **Model Builder** window, click **Concentration, Mg**.

4 In the **Concentration, Mg** toolbar, click **Plot**.

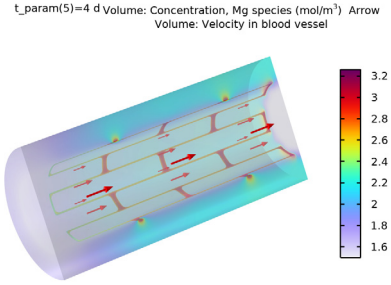


5 In the **Model Builder** window, click **Concentration, Mg**.

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

7 From the **Parameter value (t_param (d))** list, choose **4**.

8 In the **Concentration, Mg** toolbar, click **Plot**.



pH

1 Right-click **Concentration, Mg** and choose **Duplicate**.

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

Volume 1

1 In the **Model Builder** window, expand the **pH** node, then click **Volume 1**.

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

3 In the **Expression** text field, type `aqt.pH`.

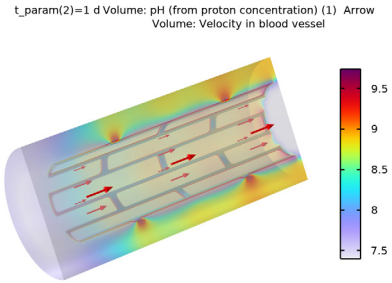
pH

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

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

3 From the **Parameter value (t_param (d))** list, choose **1**.

4 In the **pH** toolbar, click **Plot**.



5 In the **Model Builder** window, click **pH**.

6 From the **Parameter value (t_param (d))** list, choose **4**.

7 In the **pH** toolbar, click **Plot**.