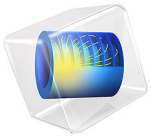


Model created in COMSOL Multiphysics 6.4

Oxide Jacking of Reinforced Concrete

Introduction

Oxide jacking is the process by which reinforced concrete cracks, due to the corrosion of the reinforcement bars. The corrosion process causes growth of an oxide layer on the rebar, which in turn causes internal stresses in the concrete. If the corrosion process is allowed to continue, the concrete will eventually crack, compromising the structure.

This tutorial investigates the oxide jacking of reinforced concrete. The corrosion process is driven by oxygen reduction, forming an oxide layer. Charge and oxygen transport are modeled in the concrete domain, where the electrolyte conductivity and oxygen diffusivity depend on the moisture content.

The rebar and concrete are modeled as linear elastic materials, where the volumetric strain or the rebar in each time-step is based on the thickness of the oxide layer. Cracking in the concrete caused by the volumetric expansion due to oxide formation is accounted for using a scalar damage model.

Model Definition

Figure 1 shows the model geometry, defining concrete as an electrolyte domain and a circular steel rebar. The geometry is defined in 2D.

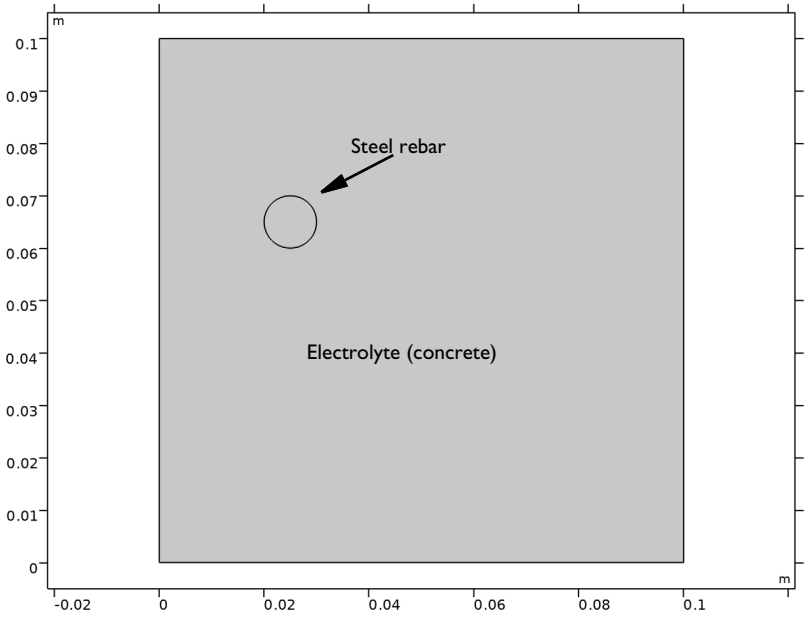


Figure 1: Model geometry.

Oxygen diffuses from one side of the concrete block, which is assumed to have a water pore saturation of 60%. The model is defined using the **Tertiary Current Distribution, Nernst–Planck** interface, solving for the electrolyte phase potential and the oxygen concentration, assuming a supporting electrolyte charge conservation model, defined in a similar way as in the Cathodic Protection of Steel in Reinforced Concrete tutorial.

The oxygen concentrations at the left most boundary is set to a reference concentration value of 8.6 $\mathrm{mol/m^3}$.

The following three different electrode reactions on the steel rebar boundary are considered: oxygen reduction, hydrogen evolution and the net iron oxidation.

Oxygen reduction reaction:

$$4\mathrm{H^+} + 4e^- + \mathrm{O_2} \rightarrow 2\mathrm{H_2O} \tag{1}$$

Hydrogen evolution reaction:

$$2H_2O + 2e^- \rightarrow H_2 + 2OH^- \tag{2}$$

The net iron oxidation reaction is considered to follow the following reaction scheme.

Iron oxidizes and dissolves:

$$2Fe(s) \rightarrow 2Fe^{2+} + 4e^- \tag{3}$$

Dissolved iron ions then react with water and oxygen:

$$2Fe^{2+} + \frac{1}{2}O_2 + 3H_2O \rightarrow 2FeO(OH) + 4H^+ \tag{4}$$

The final corrosion product iron oxide is the formed according to:

$$2FeO(OH) \rightarrow Fe_2O_3 + H_2O \tag{5}$$

Thus, the net iron oxidation reaction considered in the model is:

$$2Fe(s) + \frac{1}{2}O_2 + 2H_2O \rightarrow Fe_2O_3 + 4H^+ + 4e^- \tag{6}$$

The iron oxide layer thickness, $s_{b,\mathrm{tot}}$ (m) along the rebar-concrete interface is computed using the **Dissolving–Depositing Species** functionality of the **Electrode Surface** node.

The **Solid Mechanics** interface is used for structural analysis using two **Linear Elastic Material** nodes to model the steel rebar and concrete domains. A scalar damage model is used to describe cracking of the concrete domain, using a **Damage** subnode.

The average areal strain of the rebar is computed based on the oxide thickness layer obtained from the **Tertiary Current Distribution, Nernst–Planck** interface according to

$$\varepsilon_A = \frac{\int s_{b,\,\mathrm{tot}} d\Omega}{\pi r_{\mathrm{rebar}}^2} \tag{7}$$

The **Initial Stress and Strain** node of the Linear Elastic Material node defining the rebar domain is used to define the strain ε_0 in the x and y directions according to

$$\varepsilon_{0,\,x} = \varepsilon_{0,\,y} = \frac{\varepsilon_A}{2} \tag{8}$$

The model is solved in a time-dependent solver, simulating the oxide jacking during 1500 days.

Results and Discussion

Figure 2 shows the line plot of iron oxide corrosion product layer thickness along the rebar surface for different times. It can be seen that the iron oxide layer continuously grows with time.

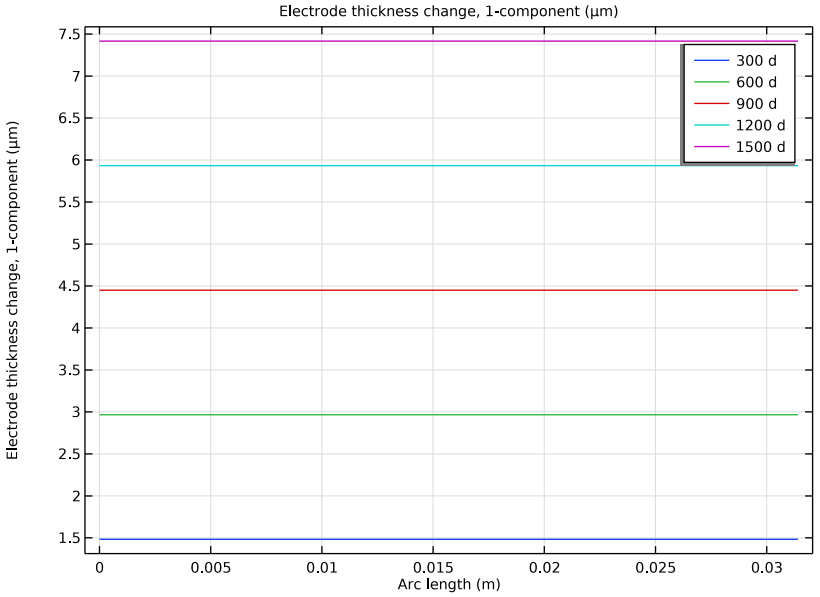


Figure 2: Iron oxide layer thickness at different times.

Figure 3 shows the surface plot of first principal stress in the concrete domain after 1500 days.

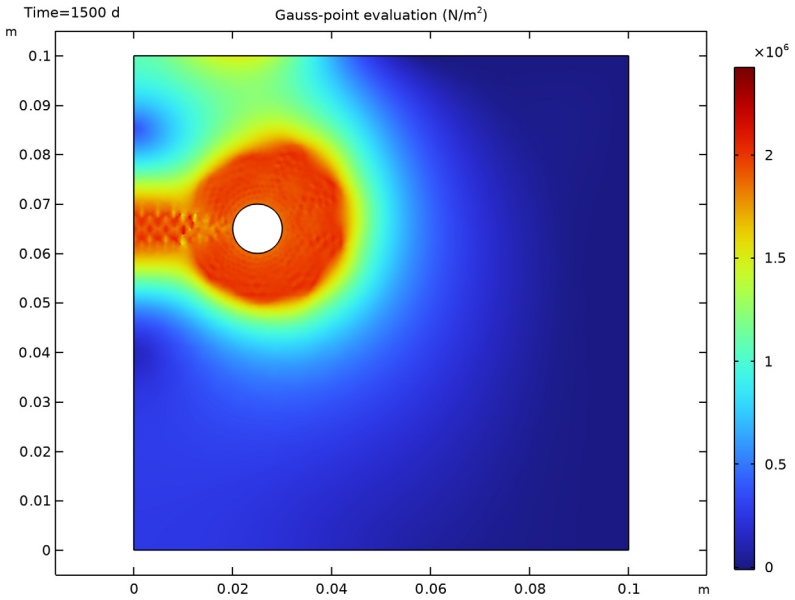


Figure 3: First principal stress distribution in the concrete domain after 1500 days.

Figure 4 shows the surface plot of damage over the concrete domain after 1500 days, clearly showing the detrimental effect of corrosion on the surrounding concrete.

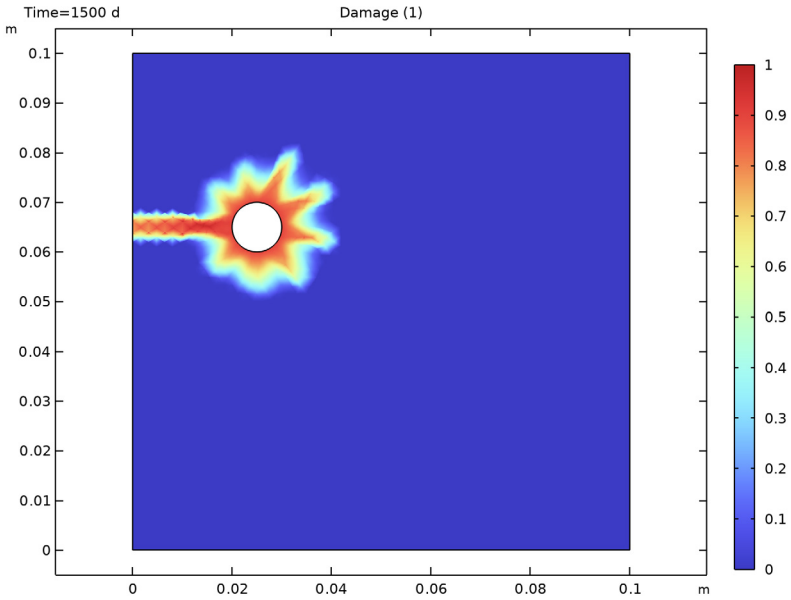


Figure 4: Damage distribution over concrete domain after 1500 days.

Figure 5 shows the surface plot of nonlocal equivalent strain over the concrete domain after 1500 days. It can be seen that a crack is formed at the rebar surface as the stiffness of

concrete degrades. The crack is seen to be propagating toward the outer surface of concrete.

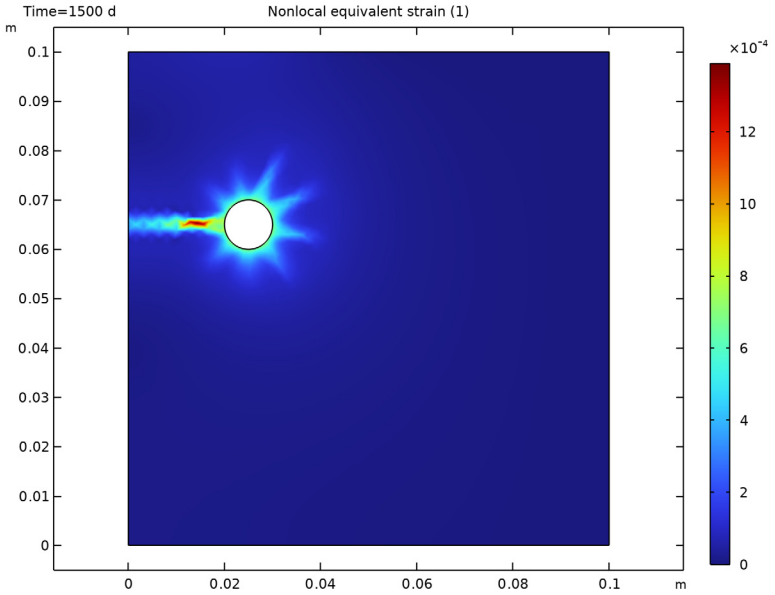


Figure 5: Nonlocal equivalent strain distribution indicating crack propagation over concrete domain after 1500 days.

Application Library path: `Corrosion_Module/General_Corrosion/oxide_jacking`

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**.

2 In the **Select Physics** tree, select **Electrochemistry** > **Tertiary Current Distribution, Nernst–Planck** > **Tertiary, Supporting Electrolyte (tcd)**.

3 Click **Add**.

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

5 In the **Concentrations (mol/m³)** table, enter the following settings:

c

6 In the **Select Physics** tree, select **Structural Mechanics** > **Solid Mechanics (solid)**.

7 Click **Add**.

8 Click **Study**.

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

10 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

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 `oxide_jacking_parameters.txt`.

GEOMETRY 1

Draw the model geometry.

Square 1 (sq1)

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

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

3 In the **Side length** text field, type `10[cm]`.

4 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	0.05

5 Select the **Layers to the left** checkbox.

6 Click **Build Selected**.

Circle 1 (c1)

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

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

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

4 Locate the **Position** section. In the **x** text field, type `2.5[cm]`.

5 In the **y** text field, type `6.5[cm]`.

6 Click **Build All Objects**.

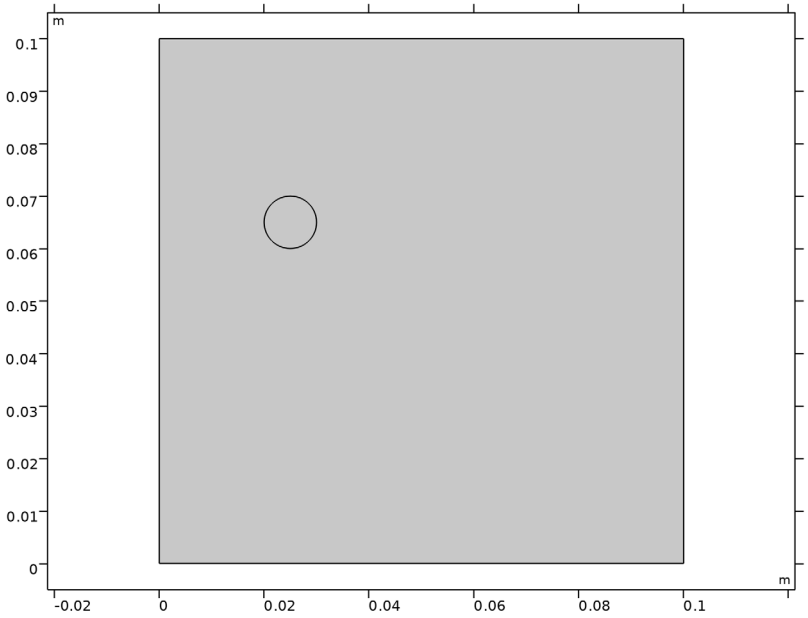
Mesh Control Domains 1 (mcd1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Mesh Control Domains**.

2 On the object **fin**, select Domains 1, 3, and 4 only.

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

The model geometry should look like this.



DEFINITIONS

Next add an integration operator, variables and interpolation functions for electrolyte conductivity and diffusivity.

Rebar boundary integration

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

2 In the **Settings** window for **Integration**, type `Rebar boundary integration` in the **Label** text field.

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

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog, type `5-8` in the **Selection** text field.

6 Click **OK**.

Variables 1

Next, load some variables from a text file.

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

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

3 Click **Load from File**.

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

Interpolation 1 (int1)

Add an interpolation function for the electrolyte conductivity.

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

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

3 In the **Function name** text field, type `sigma`.

4 Click **Load from File**.

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

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

Function	Unit
sigma	S/m

Interpolation 2 (int2)

Add an interpolation function also for the oxygen diffusivity.

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

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

3 In the **Function name** text field, type `D_O2`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `oxide_jacking_D_O2.txt`.

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

Function	Unit
D_O2	`m^2/s`

MATERIALS

Next, add some materials from Material Library for the structural analysis.

ADD MATERIAL

1 In the **Materials** toolbar, click **Add Material** to open the **Add Material** window.

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

3 In the tree, select **Built-in** > **Steel AISI 4340**.

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

MATERIALS

Steel AISI 4340 (mat1)

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

2 In the list box, select **1**.

3 Click **Remove from Selection**.

4 Select Domain 2 only.

ADD MATERIAL

1 Go to the **Add Material** window.

2 In the tree, select **Built-in** > **Concrete**.

3 Click the **Add to Component** button in the window toolbar.

MATERIALS

Concrete (mat2)

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

2 Click **Paste Selection**.

3 In the **Paste Selection** dialog, type `1` in the **Selection** text field.

4 Click **OK**.

5 Select Domain 1 only.

6 In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

ADD MATERIAL

1 In the **Materials** toolbar, click **Add Material** to open the **Add Material** window.

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

3 In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

TERTIARY CURRENT DISTRIBUTION, NERNST–PLANCK (TCD)

Start setting up the physics for the electrochemistry.

Select Domain 1 only.

Electrolyte 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck (tcd)** click **Electrolyte 1**.

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

3 In the D_c text field, type `D_O2(PS)`.

4 Locate the **Solvent** section. From the σ_l list, choose **User defined**. In the associated text field, type `sigma(PS)`.

Concentration 1

Set the concentration at the leftmost boundaries of the domain.

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

2 Select Boundary 1 only.

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

4 Select the **Species c** checkbox.

5 In the $c_{0,c}$ text field, type `C_O2_ref`.

Electrode Surface 1

Set the boundary conditions at the rebar surface.

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

2 Select Boundaries 5–8 only.

3 In the **Settings** window for **Electrode Surface**, click to expand the **Dissolving–Depositing Species** section.

4 Click + **Add**.

5 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
oxide	rho_oxide	M_oxide

6 Click + **Add**.

7 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
Fe	rho_Fe	M_Fe

Oxygen reduction

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck (tcd)** > **Electrode Surface 1** click **Electrode Reaction 1**.

2 In the **Settings** window for **Electrode Reaction**, type `Oxygen reduction` in the **Label** text field.

3 Locate the **Stoichiometric Coefficients** section. In the n text field, type `4`.

4 In the ν_c text field, type `-1`.

5 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeq_O2`.

6 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Cathodic Tafel equation**.

7 In the i_0 text field, type `c/C_O2_ref*i0_O2`.

8 In the A_c text field, type `A_O2`.

Electrode Surface 1

In the **Model Builder** window, click **Electrode Surface 1**.

Iron oxidation

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode Reaction**.

2 In the **Settings** window for **Electrode Reaction**, type `Iron oxidation` in the **Label** text field.

3 Locate the **Stoichiometric Coefficients** section. In the n text field, type `4`.

4 In the ν_c text field, type `0.5`.

5 In the **Stoichiometric coefficients for dissolving–depositing species:** table, enter the following settings:

Species	Stoichiometric coefficient (1)
oxide	-1
Fe	2

6 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeq_Fe`.

7 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Anodic Tafel equation**.

8 In the i_0 text field, type `i0_Fe`.

9 In the A_a text field, type `A_Fe`.

Electrode Surface 1

In the **Model Builder** window, click **Electrode Surface 1**.

Hydrogen evolution

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode Reaction**.

2 In the **Settings** window for **Electrode Reaction**, type `Hydrogen evolution` in the **Label** text field.

3 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeq_H2`.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Cathodic Tafel equation**.

5 In the i_0 text field, type `i0_H2`.

6 In the A_c text field, type `A_H2`.

Initial Values 1

Set the initial value for oxygen concentration.

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck (tcd)** click **Initial Values 1**.

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

3 In the c text field, type `C_O2_ref`.

SOLID MECHANICS (SOLID)

Next, set up the physics for the structural analysis.

Linear Elastic Material 1

In the **Model Builder** window, expand the **Component 1 (comp1)** > **Solid Mechanics (solid)** > **Linear Elastic Material 1** node, then click **Linear Elastic Material 1**.

Initial Stress and Strain 1

1 In the **Physics** toolbar, click **Attributes** and choose **Initial Stress and Strain**.

2 In the **Settings** window for **Initial Stress and Strain**, locate the **Initial Stress and Strain** section.

3 Specify the ε_0 matrix as

e_init	0	0
0	e_init	0
0	0	0

Linear Elastic Material 2

Next, set a Damage condition for concrete domain.

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

2 Select Domain 1 only.

Damage 1

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

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

3 Find the **Damage evolution** subsection. From the σ_p list, choose **User defined**. In the associated text field, type `sigmap`.

4 From the G_f list, choose **User defined**. In the associated text field, type `Gf`.

5 Find the **Spatial regularization method** subsection. From the list, choose **Implicit gradient**.

6 In the l_{int} text field, type `lint`.

7 In the h_{dmg} text field, type `hdmg`.

Roller 1

Set a Roller condition at left- and bottom-most boundaries.

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

2 Select Boundaries 1 and 2 only.

MESH 1

Set the finer mesh near the rebar region.

Size 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Size**.

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

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

4 Select Domain 5 only.

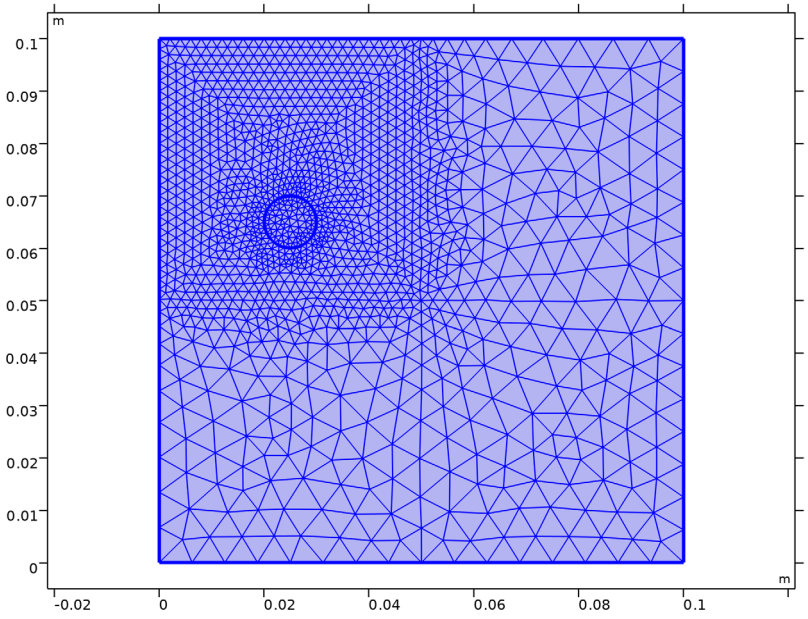
5 Locate the **Element Size** section. From the **Predefined** list, choose **Extra fine**.

Free Triangular 1

1 In the **Mesh** toolbar, click **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.

The mesh should look like this:



STUDY 1

Set the Output times of the time-dependent solver.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: 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(0,25,1500)`.

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 From the **Maximum step constraint** list, choose **Constant**.

6 In the **Maximum step** text field, type 10.

7 In the **Model Builder** window, expand the **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Time-Dependent Solver 1** node, then click **Fully Coupled 1**.

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

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

10 From the **Jacobian update** list, choose **On every iteration**.

11 In the **Maximum number of iterations** text field, type 12.

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

RESULTS

Several plots are added by default. Now, first add a line plot for the corrosion product layer thickness along the rebar.

Corrosion Product Layer Thickness

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

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

3 Locate the **Data** section. From the **Time selection** list, choose **From list**.

4 In the **Times (d)** list, choose **300**, **600**, **900**, **1200**, and **1500**.

Line Graph 1

1 In the **Corrosion Product Layer Thickness** toolbar, click **Line Graph**.

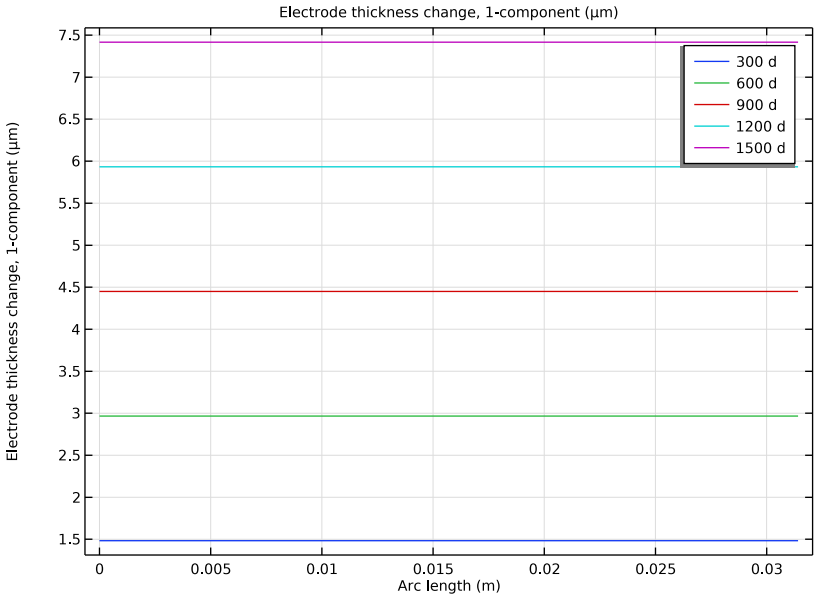
2 Select Boundaries 5–8 only.

3 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck** > **Dissolving–depositing species** > **Electrode thickness change - m** > **tcd.sb_oxide - Electrode thickness change, 1-component**.

4 Locate the **y-Axis Data** section. From the **Unit** list, choose **µm**.

5 Click to expand the **Legends** section. Select the **Show legends** checkbox.

6 In the **Corrosion Product Layer Thickness** toolbar, click **Plot**.



First Principal Stress Analysis

Next, plot the first principal stress.

1 In the **Model Builder** window, under **Results** click **Stress (solid)**.

2 In the **Settings** window for **2D Plot Group**, type `First Principal Stress Analysis` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **First Principal Stress Analysis** node, then click **Surface 1**.

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

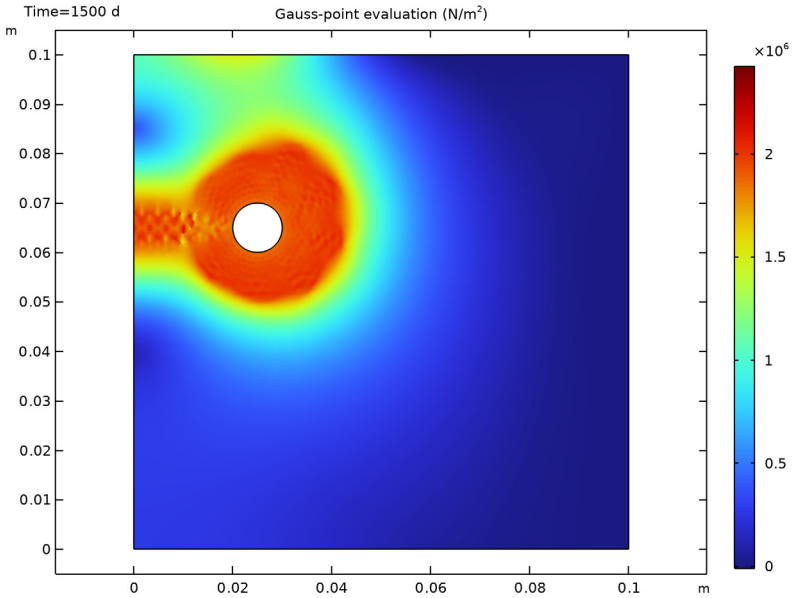
3 In the **Expression** text field, type `solid.gpeval(solid.sdp1)`.

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

Deformation

1 In the **Model Builder** window, expand the **Surface 1** node.

2 Right-click **Deformation** and choose **Disable**.



RESULT TEMPLATES

Next, plot the Damage.

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

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

3 In the tree, select **Study 1/Solution 1 (sol1)** > **Solid Mechanics** > **Damage (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

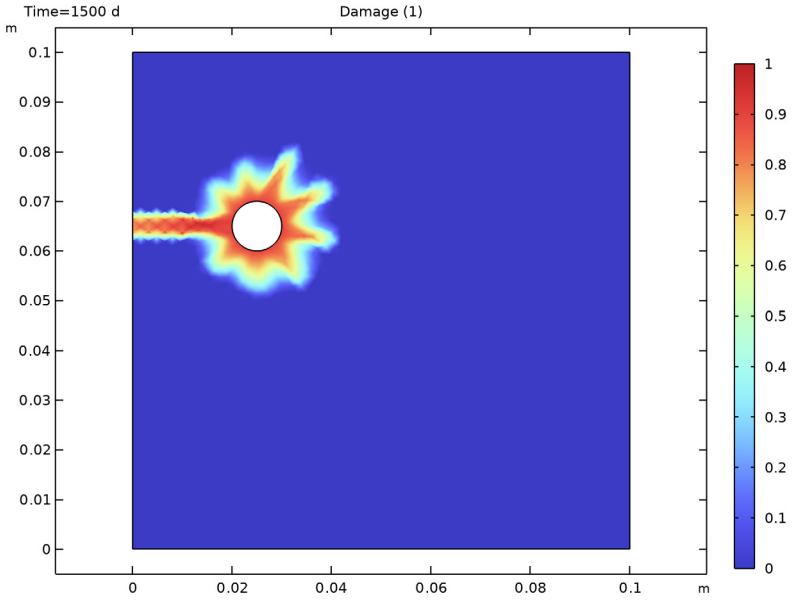
Surface 1

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

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

3 From the **Color table type** list, choose **Continuous**.

4 In the **Damage (solid)** toolbar, click **Plot**.



Crack

Next, plot the Crack.

1 In the **Results** toolbar, click **2D Plot Group**.

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

Surface 1

1 In the **Crack** toolbar, click **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Solid Mechanics** > **Damage** > **solid.eeqnl - Nonlocal equivalent strain - 1**.

3 In the **Crack** toolbar, click **Plot**.