

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.

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

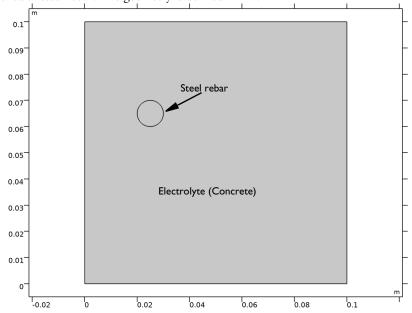


Figure 1: Model geometry.

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 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:

$$4H^{+} + 4e^{-} + O_{2} \rightarrow 2H_{2}O$$
 (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:

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

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

$$2 \text{FeO(OH)} \rightarrow \text{Fe}_2 \text{O}_3 + \text{H}_2 \text{O} \tag{5}$$

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

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

The iron oxide layer thickness, $s_{b, {\rm tot}}$ (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 **Tertary Current Distribution**, **Nernst-Planck** interface according to

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

The **Initial Strain 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.

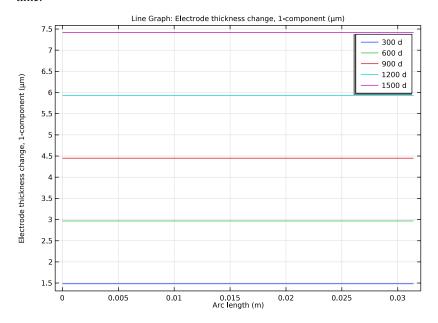
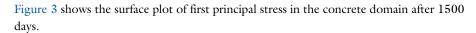


Figure 2: Iron oxide layer thickness at different times.



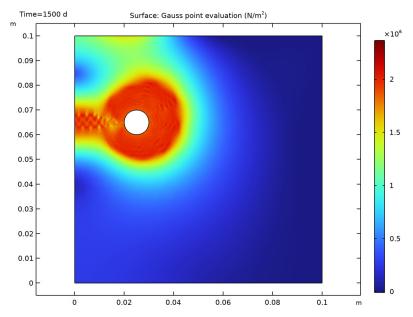
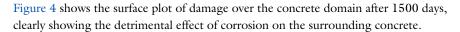


Figure 3: First principal stress distribution in the concrete domain after 1500 days.



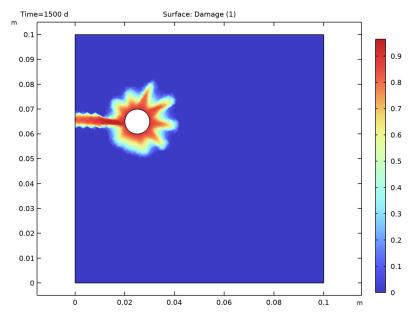


Figure 4: Damage distribution over concrete domain after 1500 days.

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 towards the outer surface of concrete.

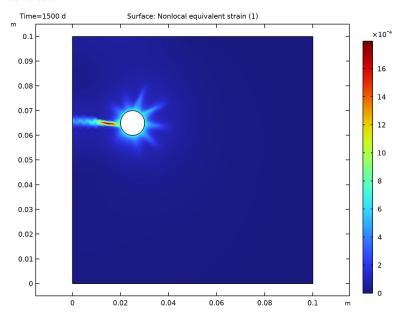


Figure 5: Nonlocal equivalent strain distribution indicating crack propagation over concrete domain after 1500 days.

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

- I In the Model Wizard window, click 9 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** table, enter the following settings:

С

- 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.

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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 I

Draw the model geometry.

Square I (sq1)

- I 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 check box.
- 6 Click | Build Selected.

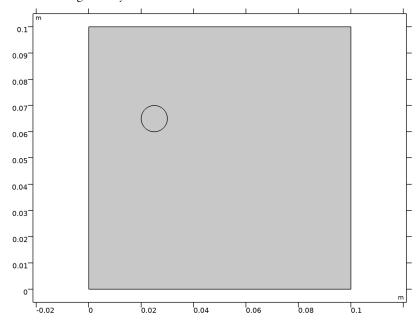
Circle I (c1)

- I 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 I (mcd1)

- I 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

- I In the Definitions toolbar, click Monlocal 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 box, type 5-8 in the Selection text field.
- 6 Click OK.

Variables 1

Next, load some variables from a text file.

- I In the **Definitions** toolbar, click **a= 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 I (int I)

Add an interpolation function for the electrolyte conductivity.

- I 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.

- I 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_02.
- 4 Click Load from File.
- **5** Browse to the model's Application Libraries folder and double-click the file oxide_jacking_D_02.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

- I In the Home 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 Add to Component in the window toolbar.

MATERIALS

Steel AISI 4340 (mat1)

- I In the Settings window for Material, locate the Geometric Entity Selection section.
- 2 In the list, select 1.
- 3 Click Remove from Selection.
- 4 Select Domain 2 only.

ADD MATERIAL

- I Go to the Add Material window.
- 2 In the tree, select Built-in>Concrete.
- 3 Click Add to Component in the window toolbar.

MATERIALS

Concrete (mat2)

- I In the Settings window for Material, locate the Geometric Entity Selection section.
- 2 Click Paste Selection.
- **3** In the **Paste Selection** dialog box, type 1 in the **Selection** text field.

- 4 Click OK.
- **5** Select Domain 1 only.
- 6 In the Home toolbar, click **Add Material** to close the Add Material window.

ADD MATERIAL

- I In the Home toolbar, click Radd Material to open the Add Material window.
- 2 Go to the Add Material window.
- 3 In the Home toolbar, click 4 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 I

- I In the Model Builder window, under Component I (compl)>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_02(PS).
- **4** Locate the **Solvent** section. From the σ_l list, choose **User defined**. In the associated text field, type sigma(PS).

Concentration I

Set the concentration at the leftmost boundaries of the domain.

- I 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** check box.
- **5** In the $c_{0,c}$ text field, type C_02_ref.

Electrode Surface 1

Set the boundary conditions at the rebar surface.

- I 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

- I In the Model Builder window, under Component I (compl)>Tertiary Current Distribution, Nernst-Planck (tcd)>Electrode Surface I click Electrode Reaction I.
- 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 v_c text field, type -1.
- 5 Locate the Equilibrium Potential section. From the $E_{\rm eq}$ list, choose User defined. In the associated text field, type Eeq_02.
- 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_02_ref*i0_02.
- **8** In the A_c text field, type A_02.

Electrode Surface 1

In the Model Builder window, click Electrode Surface 1.

Iron oxidation

- I 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 v_c text field, type 0.5.

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

Species	Stoichiometric coefficient (I)
oxide	-1
Fe	2

- **6** Locate the **Equilibrium Potential** section. From the $E_{\rm eq}$ 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 I

In the Model Builder window, click Electrode Surface 1.

Hydrogen evolution

- I 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 $E_{\rm eq}$ 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.

- I In the Model Builder window, under Component I (compl)>Tertiary Current Distribution, Nernst-Planck (tcd) click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** In the *c* text field, type C_02_ref.

SOLID MECHANICS (SOLID)

Next, set up the physics for the structural analysis.

Linear Elastic Material I

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

Initial Stress and Strain I

- I 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** In the ε_0 table, enter the following settings:

e_init	0	0
0	e_init	0
0	0	0

Linear Elastic Material 2

Next, set a Damage condition for concrete domain.

- I In the Physics toolbar, click **Domains** and choose **Linear Elastic Material**.
- 2 Select Domain 1 only.

Damage I

- I 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 $\sigma_{\rm p}$ 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 $h_{
 m dmg}$ text field, type hdmg.

Roller I

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

- I In the Physics toolbar, click Boundaries and choose Roller.
- 2 Select Boundaries 1 and 2 only.

MESH I

Set the finer mesh near the rebar region.

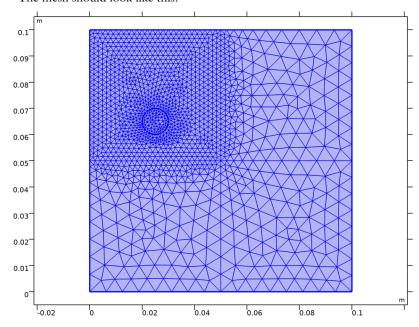
Size 1

- I In the Model Builder window, under Component I (compl) right-click Mesh I 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

- I 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 I

Set the Output times of the time-dependent solver.

Step 1: Time Dependent

- I In the Model Builder window, under Study I click Step I: 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 I (soll)

- I In the Study toolbar, click Show Default Solver.
- 2 In the Model Builder window, expand the Solution I (soll) node, then click Time-Dependent Solver I.
- 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 I>Solver Configurations> Solution I (soll)>Time-Dependent Solver I node, then click Fully Coupled I.
- 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.
- II 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.

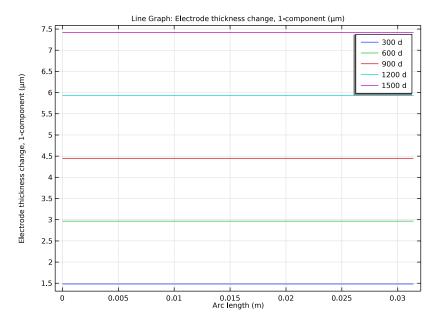
Corrosion Product Layer Thickness

- I In the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID 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 Grabh I

- I In the Corrosion Product Layer Thickness toolbar, click the 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 I (compl)>
 Tertiary Current Distribution, Nernst-Planck>Dissolving-depositing species>
 Electrode thickness change m>tcd.sb_oxide Electrode thickness change, I-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** check box.



First Principal Stress Analysis

Next, plot the first principal stress.

- I 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.

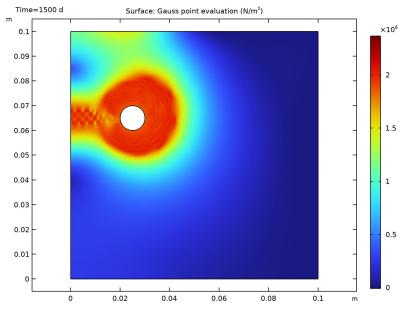
Surface I

- I 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. Click Change Color Table.
- 5 In the Color Table dialog box, select Rainbow>Rainbow in the tree.
- 6 Click OK.

Deformation

- I In the Model Builder window, expand the Surface I node.
- 2 Right-click Deformation and choose Disable.



Next, plot the Damage.

3 In the Home toolbar, click Add Predefined Plot.

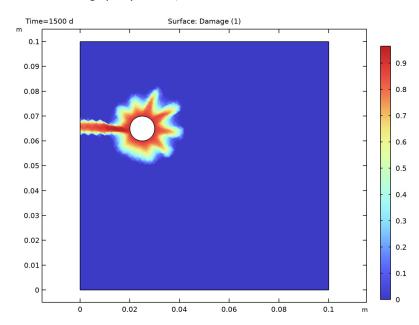
ADD PREDEFINED PLOT

- I Go to the Add Predefined Plot window.
- 2 In the tree, select Study I/Solution I (soll)>Solid Mechanics>Damage (solid).
- 3 Click Add Plot in the window toolbar.
- 4 In the Home toolbar, click Add Predefined Plot.

RESULTS

Surface I

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

- I In the Home toolbar, click Add Plot Group and choose 2D Plot Group.
- 2 In the Settings window for 2D Plot Group, type Crack in the Label text field.

Surface I

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

3 In the Crack toolbar, click Plot.

