Galvanic Corrosion with Electrode Deformation

Introduction

This example models the galvanic corrosion and deformation of a magnesium alloy (AE44) in contact with mild steel in brine solution. While similar to the Galvanic Corrosion of a Magnesium Alloy in Contact with Steel example, the present model also investigates the deformation of the corroding electrode over time.

The example is based on a paper by Deshpande (Ref. 1).

Model Definition

The model geometry is shown in Figure 1. Use one single electrolyte domain. The left part of the bottom boundary is the surface of the mild steel material, the right part is the corroding magnesium alloy. Because the alloy corrodes in the model, the right boundary is displaced downward in the geometry. Introduce a small height step of 0.1 mm in the negative y direction at the origin in the geometry to ensure that the topology of the geometry is preserved during the simulation. Let the vertical boundary of the step belong to the steel surface.

Electrolyte (salt water)

Cathode
(mild steel)

Anode
(magnesium alloy)

$x = 0$
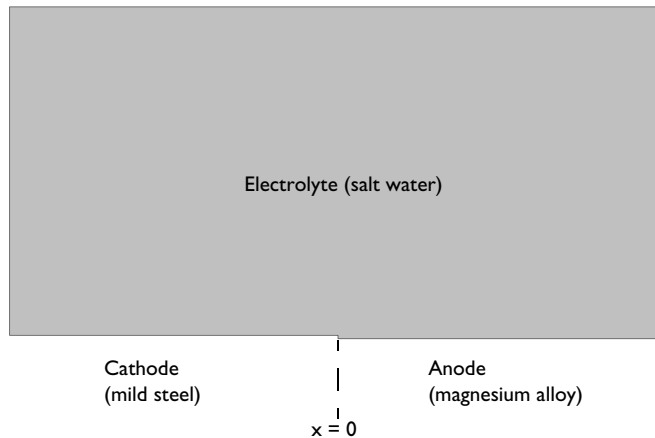
Figure 1: Model geometry.

The electrolyte is well mixed so that a secondary current distribution can be assumed, solving for the electrolyte potential, ϕ_1 (V), in the domain. Set the electrolyte conductivity to 5 S/m.

The magnesium alloy is an anode of the galvanic couple, oxidizing magnesium according to

$$Mg(s) \rightarrow Mg^{2+}(aq) + 2e^-$$
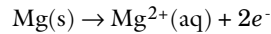
The alloy consists mainly of magnesium, the oxidation reactions of the other alloying elements are neglected in this model.

The mild steel acts as a cathode for this galvanic couple.

The electrode kinetics at both the mild steel and magnesium alloy surfaces is described using the experimental polarization data available in corrosion material library.

The dissolution of magnesium metal causes the electrode boundary to move, with a velocity in the normal direction, v (SI unit: m/s), according to

$$v = \frac{i_{an}}{2F}\frac{M}{\rho}$$

where i_{an} (SI unit: A/m^2) is the anodic electrode reaction current density, M is the mean molar mass (25 g/mol) and ρ the density (1820 kg/m^3) of the magnesium alloy.

Solve the model in a time-dependent study, simulating the corrosion for three days of immersion in salt water.

Results and Discussion

Figure 2 shows the electrode current densities at the beginning and the end of the simulation. As expected, the highest electrode current densities are found at the contact point between the two metals.
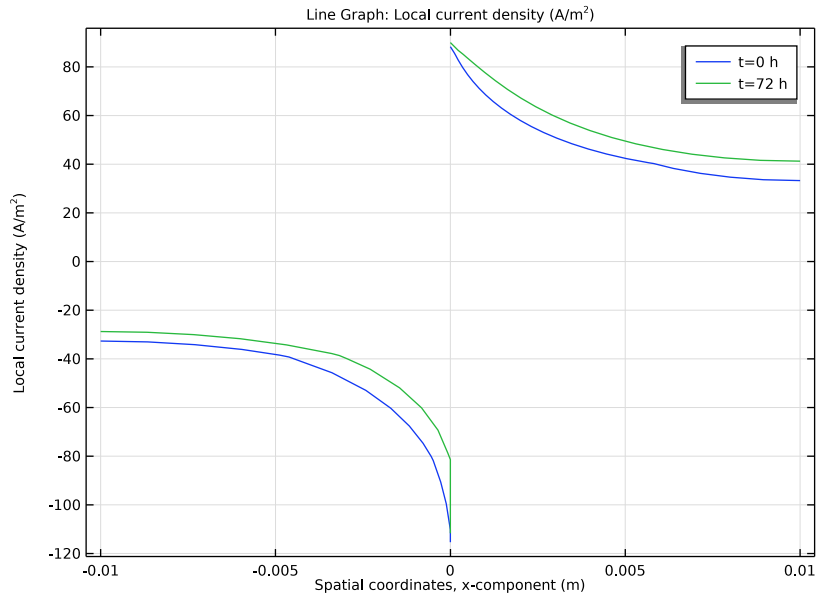

Figure 2: Electrode current densities at t = 0 and t = 72 h.

Figure 3 shows the current density and potential distribution in the electrolyte, and the model geometry, at the beginning of the simulation.
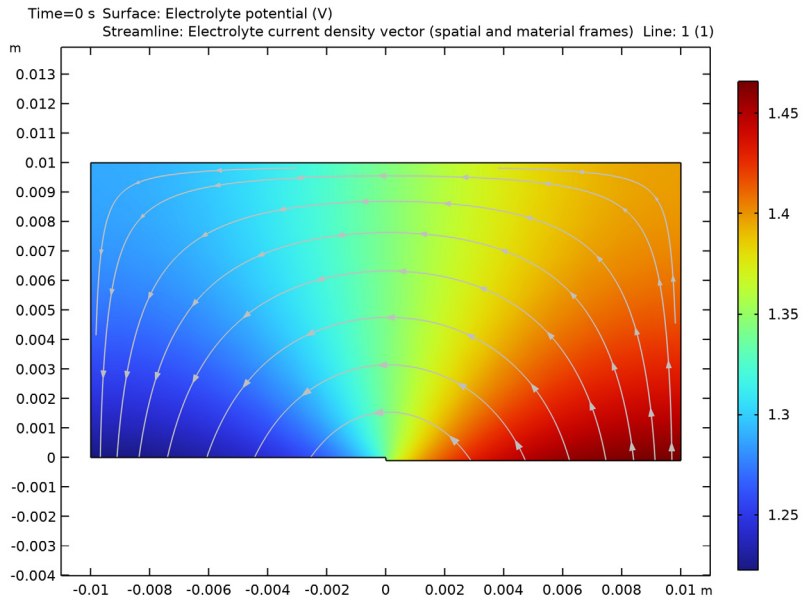

Figure 3: Model geometry, electrolyte potential, and current densities at t = 0.

Figure 4 shows the current density and potential distribution in the electrolyte and the changed geometry at the end of the simulation. Because the electrode current densities are highest at the contact point of the metals, the metal dissolution is also maximum at this point. When compared to Figure 3, the electrolyte potential is quite similar, which matches the results of Figure 2 with quite similar electrode current densities at the beginning and the end of the simulation.
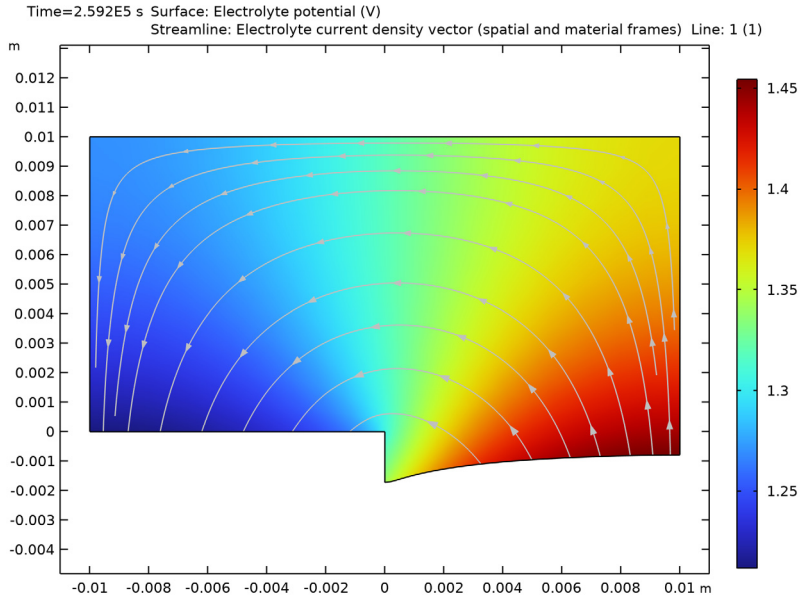
Figure 4: Model geometry, electrolyte potential, and current densities after 72 h.

Notes About the COMSOL Implementation

Use the Corrosion, Secondary entry from the Model Wizard for this model. It is a predefined multiphysics interface that contains a Secondary Current Distribution interface and a Deformed Geometry node. The Deformed Geometry node handles the deformed geometry (moving mesh/ALE) part of the problem.

For the mild steel surface, which is not deforming, use an Electrode Surface node to model the reduction reaction. For the magnesium alloy surface, use an Electrode Surface node with an added Dissolving-Depositing species, which sets up both the deformation of the geometry and the magnesium electrode reaction. Set the two electrode surfaces to the same electric potential in the metal phase.

Change the boundary condition setting of the default Non-Deforming Boundary node to Zero normal displacement. This imposes pointwise (instead of weak) constraints on the geometry displacement, and thereby fix the corners of the geometry.

Solve the model using a time-dependent study with automatic remeshing enabled.

Reference

1. K.B. Deshpande, "Validated numerical modelling of galvanic corrosion for couples: Magnesium alloy (AE44)-mild steel and AE44-aluminium alloy (AA6063) in brine solution", *Corrosion Science*, vol. 52, pp. 3514–3522, 2010.

Application Library path: `Corrosion_Module/Galvanic_Corrosion/`
`galvanic_corrosion_with_deformation`

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 Ω **2D**.

2 In the **Select Physics** tree, select **Electrochemistry>Corrosion, Deformed Geometry> Corrosion, Secondary**.

3 Click **Add**.

4 Click → **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Dependent with Initialization**.

6 Click ☑ **Done**.

GEOMETRY 1

Create the model geometry as a union of two rectangles.

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 0.01.

4 In the **Height** text field, type 0.01.

5 Locate the **Position** section. In the **x** text field, type -0.01.

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 0.01.

4 In the **Height** text field, type 0.01+1e-4.

5 Locate the **Position** section. In the **y** text field, type -1e-4.

Union 1 (uni1)

1 In the **Geometry** toolbar, click ▧ **Booleans and Partitions** and choose **Union**.

2 Click in the **Graphics** window and then press Ctrl+A to select both objects.

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

4 Clear the **Keep interior boundaries** check box.

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

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

GLOBAL DEFINITIONS

Load the model parameters from a text file.

Parameters 1

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

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

3 Click ▸ **Load from File**.

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

MATERIALS

Use the Corrosion Material Library to set up the material properties for the electrode kinetics at the magnesium and mild steel electrode surfaces.

ADD MATERIAL

1 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 **Corrosion>Iron Alloys (Steels)>Mild steel in 1.6 wt% NaCl**.

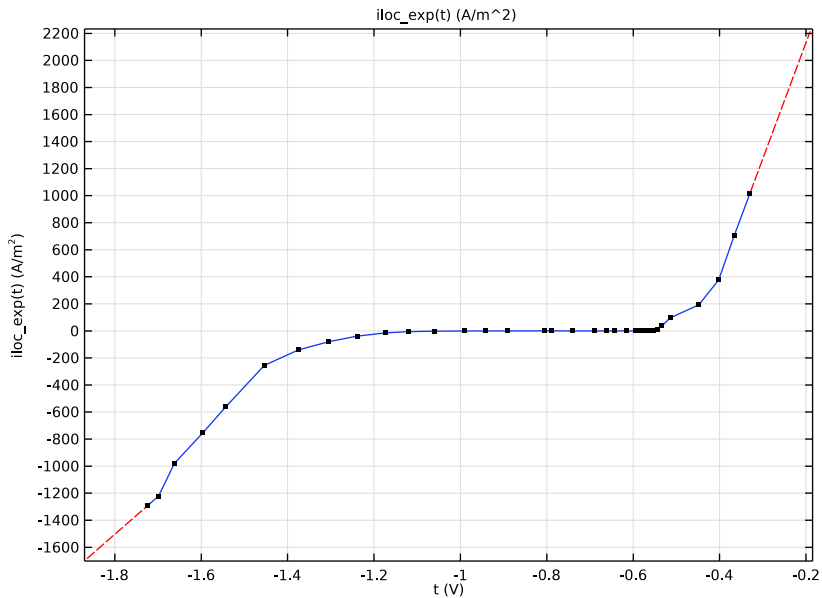**4** Click **Add to Component** in the window toolbar.

Mild steel in 1.6 wt% NaCl (mat1)

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

2 From the **Geometric entity level** list, choose **Boundary**.

3 Select Boundaries 2 and 4 only.

4 In the **Model Builder** window, expand the **Mild steel in 1.6 wt% NaCl (mat1)** node.

Interpolation 1 (iloc_exp)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials> Mild steel in 1.6 wt% NaCl (mat1)>Local current density (lcd)** node, then click **Interpolation 1 (iloc_exp)**.

2 In the **Settings** window for **Interpolation**, click 🔁 **Plot**.

The function plot should look like this:

ADD MATERIAL

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

2 In the tree, select **Corrosion>Magnesium Alloys>AE44 in 1.6 wt% NaCl**.

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

MATERIALS

AE44 in 1.6 wt% NaCl (mat2)

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

2 From the **Geometric entity level** list, choose **Boundary**.

3 Select Boundary 5 only.

4 In the **Model Builder** window, expand the **AE44 in 1.6 wt% NaCl (mat2)** node.

Interpolation 1 (iloc_exp)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials> AE44 in 1.6 wt% NaCl (mat2)>Local current density (lcd)** node, then click **Interpolation 1 (iloc_exp)**.

2 In the **Settings** window for **Interpolation**, click ⊡ **Plot**.

The function plot should look like this:
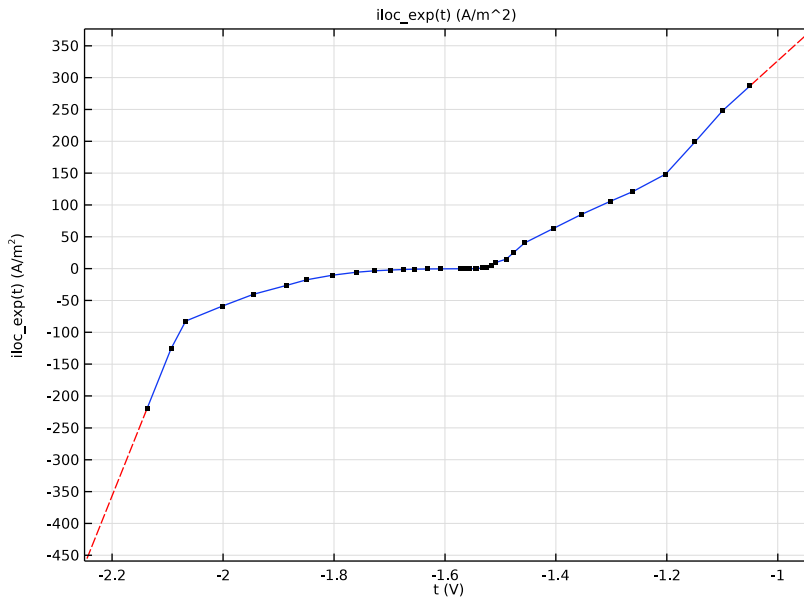
3 In the **Home** toolbar, click ▦ **Add Material** to close the **Add Material** window.

SECONDARY CURRENT DISTRIBUTION (CD)

Now set up the physics for the current distribution. Start with selecting the reference electrode potential.

1 In the **Settings** window for **Secondary Current Distribution**, click to expand the **Physics vs. Materials Reference Electrode Potential** section.

2 From the list, choose **0.241 V (SCE vs. SHE)**.

Electrolyte 1
Set user defined electrolyte conductivity at the electrolyte domain.

1 In the **Model Builder** window, under **Component 1 (comp1)> Secondary Current Distribution (cd)** click **Electrolyte 1**.

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

3 From the σ_l list, choose **User defined**. In the associated text field, type sigma.

Electrode Surface 1
The following steps set up the cathodic reduction reaction.

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

2 Select Boundaries 2 and 4 only.

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

2 In the **Settings** window for **Electrode Reaction**, locate the **Electrode Kinetics** section.

3 From the $i_{loc,expr}$ list, choose **From material**.

Electrode Surface 2
The following steps set up the anodic corrosion reaction and the resulting boundary movement.

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

2 Select Boundary 5 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)
Mg	rho_Mg	M_Mg

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

2 In the **Settings** window for **Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the n text field, type 2.

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

Species	Stoichiometric coefficient (1)
Mg	1

5 Locate the **Electrode Kinetics** section. From the $i_{loc,expr}$ list, choose **From material**.

MULTIPHYSICS

Nondeforming Boundary 1 (ndbdg1)
The following applies a stronger constraint (than the default condition) for the planar nondepositing walls in order to enforce a zero boundary movement in the normal direction.

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Nondeforming Boundary 1 (ndbdg1)**.

2 In the **Settings** window for **Nondeforming Boundary**, locate the **Nondeforming Boundary** section.

3 From the **Boundary condition** list, choose **Zero normal displacement**.

Deforming Electrode Surface 1 (desdg1)
1 In the **Model Builder** window, click **Deforming Electrode Surface 1 (desdg1)**.

2 In the **Settings** window for **Deforming Electrode Surface**, locate the **Boundary Selection** section.

3 In the list, select **4**.

4 Click ▬ **Remove from Selection**.

5 Select Boundary 5 only.

STUDY 1
The simulation time is 72 h.

Step 2: Time Dependent
1 In the **Model Builder** window, under **Study 1** click **Step 2: 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, 12*3600, 3*24*3600).

4 Click to expand the **Study Extensions** section. Select the **Automatic remeshing** check box.

5 In the **Home** toolbar, click ![Compute icon] **Compute**.

RESULTS

The following reproduces the figures in the Results and Discussion section.

Electrolyte Potential (cd)

1 Click the ![Zoom Extents icon] **Zoom Extents** button in the **Graphics** toolbar.

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

3 Clear the **Plot dataset edges** check box.

Line 1

1 Right-click **Electrolyte Potential (cd)** and choose **Line**.

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

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

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

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

6 In the **Electrolyte Potential (cd)** toolbar, click ![Plot icon] **Plot**.

Electrolyte Potential (cd)

1 In the **Model Builder** window, click **Electrolyte Potential (cd)**.

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

3 From the **Time (s)** list, choose **0**.

4 In the **Electrolyte Potential (cd)** toolbar, click ![Plot icon] **Plot**.

1D Plot Group 5

In the **Home** toolbar, click ![Add Plot Group icon] **Add Plot Group** and choose **1D Plot Group**.

Line Graph 1

1 Right-click **1D Plot Group 5** and choose **Line Graph**.

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

3 From the **Dataset** list, choose **Study 1/Remeshed Solution 1 (sol3)**.

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

5 Select Boundaries 2, 4, and 5 only.

6 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Secondary Current Distribution>Electrode kinetics> cd.iloc_er1 - Local current density - A/m²**.

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

8 In the **Expression** text field, type x.

9 Click to expand the **Legends** section. Select the **Show legends** check box.

10 From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
t=0 h

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

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

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

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

5 Locate the **Legends** section. In the table, enter the following settings:

Legends
t=72 h

6 In the **1D Plot Group 5** toolbar, click **Plot**.