



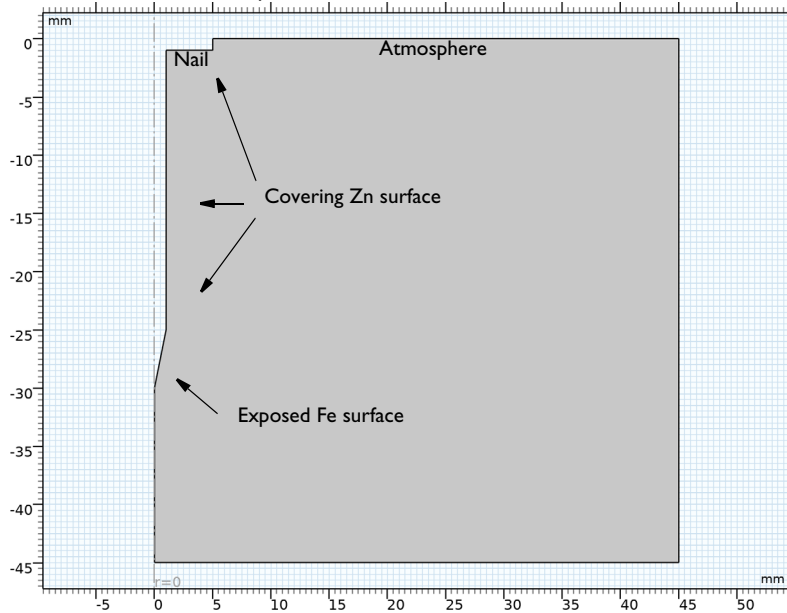
# Galvanized Nail

## Introduction

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This tutorial model serves as an introduction to the Corrosion Module and models the metal oxidation and oxygen reduction current densities on the surface of a galvanized nail, surrounded by a piece of wet wood, which acts as electrolyte.

The protecting zinc layer on the nail is not fully covering, so that at the tip of the nail the underlying iron surface is exposed. First the electrolyte conductivity and the electrode reaction kinetics are modeled to obtain a secondary current distribution (concentration variations in the cell are not accounted for), in a second part the oxygen transport is included to model a tertiary current distribution.



*Figure 1: Modeled geometry (2D axisymmetric). The nail surface has two parts: the main part is protected by zinc, on the tip the underlying iron is exposed. The top boundary is in contact with the atmosphere.*

## Model Definition

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Figure 1 shows the model geometry. Due to the symmetry of the problem the geometry is made 2D axisymmetric, and consists of one single domain, the electrolyte. The actual nail is not included in the model geometry as a domain since the metal electric potential

can be considered constant due to the high conductivity of the metal, in combination with the low expected current densities.

The surface of the nail consists of two parts, the zinc covered part, and the tip, where the zinc has been scratched off to expose the underlying iron. The top electrolyte boundary is in contact with the atmosphere, all other boundaries are insulating.

### ELECTROLYTE CHARGE TRANSPORT

The currents expected are small in relation to the total amount of charge carrying ions in the electrolyte. This implies that a constant conductivity can be assumed, use the Secondary Current Distribution interface to solve for the electrolyte potential,  $\phi_l$  (SI unit: V), according to:

$$\begin{aligned}\mathbf{i}_l &= -\sigma_l \nabla \phi_l \\ \nabla \cdot \mathbf{i}_l &= 0\end{aligned}$$

where  $\mathbf{i}_l$  (SI unit: A/m<sup>2</sup>) is the electrolyte current density vector and  $\sigma_l$  (SI unit: S/m) is the electrolyte conductivity. Use the default insulating conditions for all boundaries except the nail surface:

$$\mathbf{n} \cdot \mathbf{i}_l = 0$$

Where  $\mathbf{n}$  is the normal vector, pointing out of the domain.

### METAL OXIDATION REACTIONS

The nail is not included as a domain in the model, therefore use the Electrode Surface boundary node to model the nail surface, and set the potential of the metal phase  $\phi_s$  (SI unit: V) to 0 on this boundary.

The Electrode Surface sets the boundary condition for the electrolyte potential to

$$\mathbf{n} \cdot \mathbf{i}_l = \sum_m i_{\text{loc}, m}$$

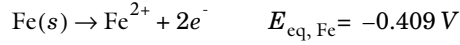
where  $i_{\text{loc}, m}$  (SI unit: A/m<sup>2</sup>) are the local individual electrode reaction current densities.

Add Electrode Reaction nodes to the Electrode Surface to define the individual electrode reactions.

On the zinc surface, oxidation occurs according to



whereas on the exposed iron surface, iron is oxidized according to



where  $E_{\text{eq},m}$  (SI unit: V) is the equilibrium potential of the electrode reaction.

Use an anodic Tafel expression to model these reactions, this sets the local current density to

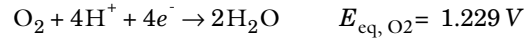
$$i_{\text{loc}, m} = i_{0, m} 10^{\frac{\eta_m}{A_m}}$$

for each reaction, where  $i_{0,m}$  is the exchange current density,  $A_m$  (SI unit: V) is the Tafel slope and the overpotential  $\eta$  (SI unit: V) is calculated from

$$\eta = \phi_s - \phi_l - E_{\text{eq},m} \quad (1)$$

#### OXYGEN REDUCTION AND OXYGEN TRANSPORT

Oxygen is reduced on both the zinc and iron electrode surfaces according to



Use a cathodic Tafel expression to model this reaction, which sets the local current density to

$$i_{\text{loc, O}_2} = -i_{0, \text{O}_2} 10^{\frac{\eta_{\text{O}_2}}{A_{\text{O}_2}}}$$

Since zinc and iron have different catalytic properties for oxygen reduction, use different parameter values for  $A_{\text{O}_2}$  and  $i_{0, \text{O}_2}$  on the different surfaces.

It is often good modeling practice to solve for a secondary current distribution first, before adding mass transfer. Once one has obtained a satisfactory solution for the secondary problem, one can proceed to increase the complexity of the model.

For this model, solve for the Secondary Current Distribution interface first then add a Transport of Diluted Species interface to model oxygen transport by Fickian diffusion:

$$\begin{aligned} \mathbf{N} &= -D\nabla c \\ \nabla \cdot \mathbf{N} &= 0 \end{aligned}$$

where  $c$  (SI unit:  $\text{mol}/\text{m}^3$ ) is the oxygen concentration,  $\mathbf{N}$  (SI unit:  $\text{mol}/(\text{m}^2 \cdot \text{s})$ ) the flux vector, and  $D$  (SI unit:  $\text{m}^2/\text{s}$ ) the diffusion coefficient.

Use the default No Flux conditions for the right and bottom boundary:

$$\mathbf{n} \cdot \mathbf{N} = 0$$

The top boundary is in contact with the surrounding air, set the concentration to a fixed value on this boundary.

$$c = c_{\text{ref}}$$

On the nail surface, couple the oxygen flux over the boundary to the oxygen reduction current density by using an Electrode-Electrolyte Interface Coupling boundary condition. This sets the flux to be proportional to the electrode current density according to Faraday's law:

$$\mathbf{n} \cdot \mathbf{N} = \frac{v i_{\text{loc, O2}}}{nF}$$

where  $F$  is Faraday's constant (96,485 C/mol),  $v$  the stoichiometric coefficient for oxygen in the reduction reaction and  $n$  the number of electrons in the reaction.

The sign convention for  $v$  is that it should be negative for reactants and positive for products in a reduction reaction (A reaction with the electrons participating as reactants).  $n$  is always positive. Set  $v$  to -1 and  $n$  to 4 for this model.

When including oxygen transport in the model, also change the electrode kinetics for the oxygen reduction reaction to the following expression:

$$i_{\text{loc, O2}} = -\left(\frac{c}{c_{\text{ref}}}\right) i_{0, \text{O2}} 10^{\frac{\eta_{\text{O2}}}{A_{\text{O2}}}}$$

## Results and Discussion

Figure 2 shows the electrode reaction current densities for the secondary current distribution model. Zinc oxidation dominates on the zinc surface, with a maximum at the point between the iron and zinc surfaces. Oxygen reduction dominates on the iron surface.

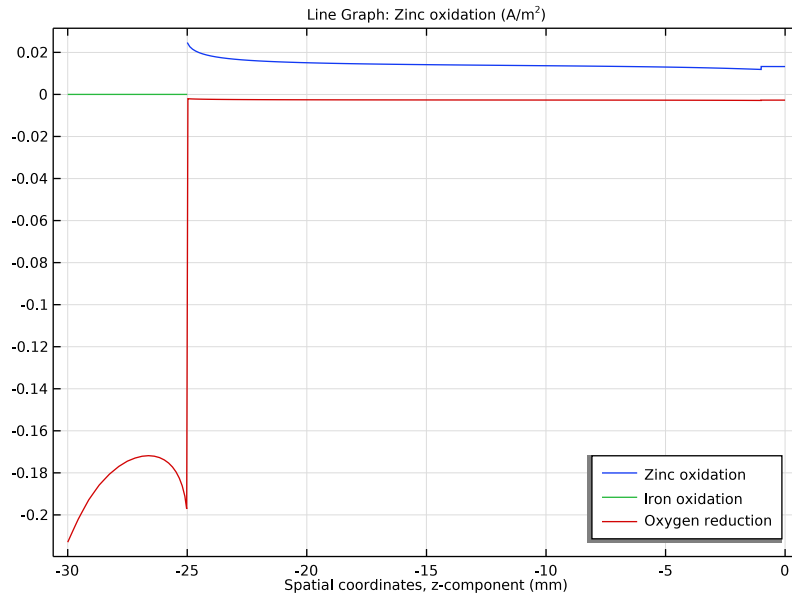


Figure 2: Individual electrode reaction current densities.

Figure 3 shows the concentration of oxygen for the second study step when oxygen transport has been included in the model, for the tertiary current distribution. The concentration of oxygen decreases toward the tip of the nail.

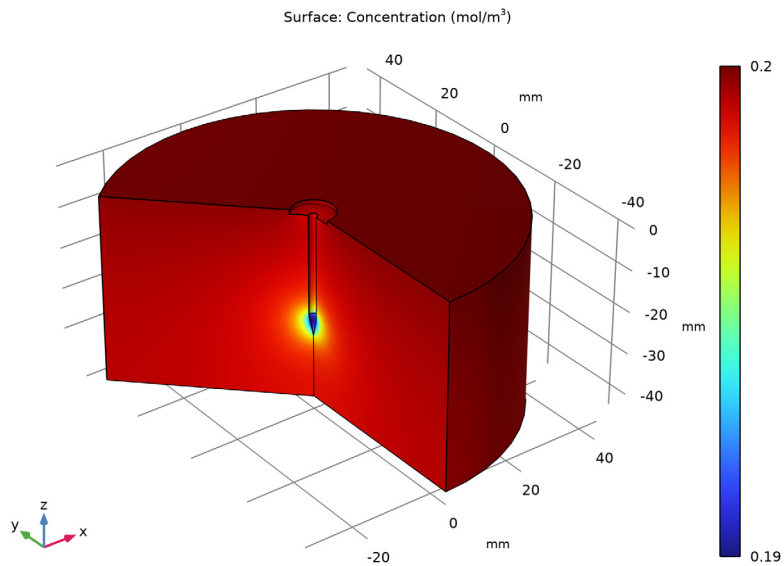


Figure 3: Oxygen concentration in the electrolyte.

Figure 4 shows a comparison of the iron oxidation current densities between the secondary and tertiary current distribution models. The current density decreases slightly when including oxygen transport in the model.

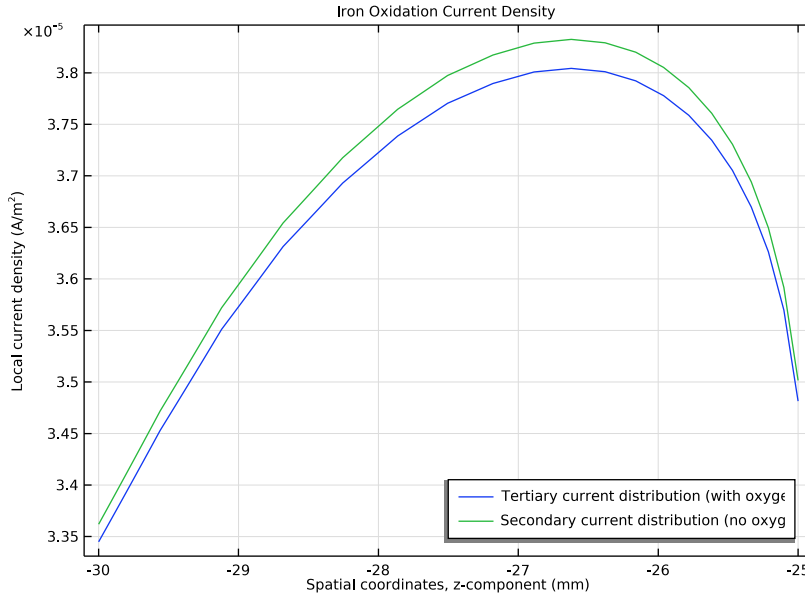


Figure 4: Iron oxidation current densities. Effect of including oxygen transport in the model.

### Notes About the COMSOL Implementation

The initial value for the electrolyte potential is set to  $-E_{\text{eq,Zn}}$  to reduce the computational time. It is generally good practice to set initial values for the potentials, if they can be derived.

In this case it was assumed that the zinc reaction would be governing due to the larger area of the zinc surface, and the faster reaction kinetics of the zinc reaction in relation to the oxygen reduction reaction. Assuming zero overpotential for the zinc reaction, and using Equation 1, the initial value for the electrolyte potential can be calculated according to:

$$\phi_{l,0} = \phi_s - E_{\text{eq,Zn}} = -E_{\text{eq,Zn}}$$



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**Application Library path:** Corrosion\_Module/Galvanic\_Corrosion/  
galvanized\_nail


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### *Modeling Instructions*




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From the **File** menu, choose **New**.

#### **NEW**

In the **New** window, click  **Model Wizard**.

#### **MODEL WIZARD**


- 1 In the **Model Wizard** window, Make use of symmetry to model the nail using a 2D axisymmetric geometry.
- 2 click  **2D Axisymmetric**.  
Create the model in two steps: First, model a Secondary Current Distribution and solve for it in a Stationary study. Then, add more physics in a later step to include oxygen transport, and solve that model in a second study step.
- 3 In the **Select Physics** tree, select **Electrochemistry>Primary and Secondary Current Distribution>Secondary Current Distribution (cd)**.
- 4 Click **Add**.
- 5 Click  **Study**.
- 6 In the **Select Study** tree, select **General Studies>Stationary**.
- 7 Click  **Done**.

#### **GEOMETRY I**

Load the model parameters from a text file.

#### **GLOBAL DEFINITIONS**

##### *Parameters I*

- 1 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 `galvanized_nail_parameters.txt`.

## GEOMETRY I


Draw the geometry as the difference between a square (the electrolyte) and a polygon (the nail). Set the length unit so that the default unit is millimeters when specifying the polygon.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.
- 2 In the **Settings** window for **Geometry**, locate the **Units** section.
- 3 From the **Length unit** list, choose **mm**.

### *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  $1.5 \cdot L_{\text{nail}}$ .
- 4 Locate the **Position** section. In the **z** text field, type  $-1.5 \cdot L_{\text{nail}}$ .


### *Polygon 1 (pol1)*




- 1 In the **Geometry** toolbar, click  **Polygon**.
- 2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.
- 3 In the table, enter the following settings:

r (mm)	z (mm)
0	0
5	0
5	-1
1	-1
1	$5 - L_{\text{nail}}$
0	$-L_{\text{nail}}$

- 4 Click  **Build Selected**.

### *Difference 1 (dif1)*


- 1 In the **Geometry** toolbar, click  **Booleans and Partitions** and choose **Difference**.
- 2 Select the object **sq1** only.
- 3 In the **Settings** window for **Difference**, locate the **Difference** section.

- 4 Find the **Objects to subtract** subsection. Click to select the  **Activate Selection** toggle button.
  - 5 Select the object **poll** only.
  - 6 Click  **Build All Objects**.
  - 7 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- The finished geometry should now look like [Figure 1](#).


## DEFINITIONS

Create explicit selections of the zinc and iron parts of the nail surface. Then create a selection for the whole nail surface by using a union. You will use the selections later on when specifying the physics, setting up the mesh, and plotting the results.



### *Zinc surface*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Zinc surface in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundaries 4–6 only.

### *Iron surface*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Iron surface in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundary 3 only.

### *Nail surface*

- 1 In the **Definitions** toolbar, click  **Union**.
- 2 In the **Settings** window for **Union**, type Nail surface in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Input Entities** section. Under **Selections to add**, click  **Add**.
- 5 In the **Add** dialog box, in the **Selections to add** list, choose **Zinc surface** and **Iron surface**.
- 6 Click **OK**.

## SECONDARY CURRENT DISTRIBUTION (CD)


Now specify the physics for the secondary current distribution problem. Start with the electrolyte conductivity.

### *Electrolyte 1*

- 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  $\sigma_1$  list, choose **User defined**. In the associated text field, type **sigma**.

### *Electrode Surface 1*

Model the two parts of the nail surface using Electrode Surfaces, onto which Electrode Reactions can be added. Keep the electric potential default value of zero (ground) on both parts of the surface. This is the potential of the metal in the nail.

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electrode Surface**.
- 2 In the **Settings** window for **Electrode Surface**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Zinc surface**.

### *Zinc reaction*


Set up the parameters for the two electrode reactions on the zinc surface.

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Secondary Current Distribution (cd)>Electrode Surface 1** click **Electrode Reaction 1**.
- 2 In the **Settings** window for **Electrode Reaction**, type **Zinc reaction** in the **Label** text field.
- 3 Locate the **Equilibrium Potential** section. In the  $E_{eq}$  text field, type **Eeq\_Zn**.
- 4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Anodic Tafel equation**.
- 5 In the  $i_0$  text field, type **i0\_Zn**.
- 6 In the  $A_a$  text field, type **A\_Zn**.

### *Electrode Surface 1*

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

### *Oxygen reaction*

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Electrode Reaction**.
- 2 In the **Settings** window for **Electrode Reaction**, type **Oxygen reaction** in the **Label** text field.
- 3 Locate the **Equilibrium Potential** section. In the  $E_{eq}$  text field, type **Eeq\_O2**.
- 4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Cathodic Tafel equation**.

5 In the  $i_0$  text field, type  $i0\_02\_on\_Zn$ .

6 In the  $A_c$  text field, type  $A\_02\_on\_Zn$ .

#### *Electrode Surface 1*

Use the duplicate functionality to make a copy of the zinc Electrode Surface and apply it to the iron part of the nail surface. Modify the kinetics parameters for this surface.

#### *Electrode Surface 2*

1 Right-click **Electrode Surface 1** and choose **Duplicate**.

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

3 From the **Selection** list, choose **Iron surface**.

#### *Iron Reaction*

1 In the **Model Builder** window, expand the **Electrode Surface 2** node, then click **Zinc reaction**.

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

3 Locate the **Equilibrium Potential** section. In the  $E_{eq}$  text field, type  $E_{eq\_Fe}$ .

4 Locate the **Electrode Kinetics** section. In the  $i_0$  text field, type  $i0\_Fe$ .

5 In the  $A_a$  text field, type  $A\_Fe$ .

#### *Oxygen reaction*

1 In the **Model Builder** window, click **Oxygen reaction**.

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

3 In the  $i_0$  text field, type  $i0\_02\_on\_Fe$ .

4 In the  $A_c$  text field, type  $A\_02\_on\_Fe$ .

#### *Initial Values 1*

Provide an initial guess for the electrolyte potential to reduce computational time.

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

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

3 In the *phil* text field, type  $-E_{eq\_Zn}$ .

#### **MESH 1**

Create a mesh with higher resolution at the electrode boundaries. Using a finer mesh close to the electrode surface resolves the contact between the two metal surfaces.

### Size

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

#### Size 1

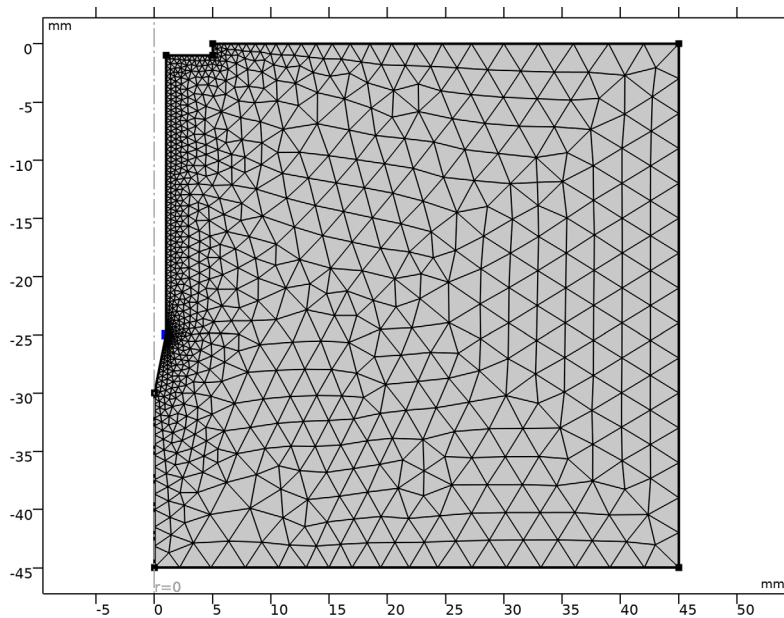
- 1 In the **Model Builder** window, right-click **Free Triangular 1** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 From the **Selection** list, choose **Nail surface**.
- 5 Locate the **Element Size** section. From the **Predefined** list, choose **Extremely fine**.

#### Size 2

- 1 Right-click **Free Triangular 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 **Point**.
- 4 Select Point 3 only.
- 5 Locate the **Element Size** section. Click the **Custom** button.
- 6 Locate the **Element Size Parameters** section.
- 7 Select the **Maximum element size** check box. In the associated text field, type 0.1.


8 Click  **Build All**.

Your finished mesh should now look like this:



## STUDY 1


Now solve the secondary current distribution model.

In the **Home** toolbar, click  **Compute**.

## RESULTS

Plot the electrode reaction currents in the following way:

### Local Current Density

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Local Current Density in the **Label** text field.

### Line Graph 1

- 1 Right-click **Local Current Density** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Zinc surface**.

- 4 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/m<sup>2</sup>**.
- 5 Locate the **y-Axis Data** section.
- 6 Select the **Description** check box. In the associated text field, type Zinc oxidation.
- 7 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 8 In the **Expression** text field, type z.
- 9 Click to expand the **Legends** section. Select the **Show legends** check box.
- 10 Find the **Include** subsection. Clear the **Solution** check box.
- 11 Select the **Description** check box.

#### *Line Graph 2*

- 1 Right-click **Line Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Iron surface**.
- 4 Locate the **y-Axis Data** section. In the **Description** text field, type Iron oxidation.
- 5 Click to expand the **Title** section. From the **Title type** list, choose **None**.

#### *Line Graph 3*

- 1 Right-click **Line Graph 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Nail surface**.
- 4 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\_er2 - Local current density - A/m<sup>2</sup>**.
- 5 Locate the **y-Axis Data** section. In the **Description** text field, type Oxygen reduction.

#### *Local Current Density*

- 1 In the **Model Builder** window, click **Local Current Density**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Legend** section.
- 3 From the **Position** list, choose **Lower right**.



The figure should now look like [Figure 2](#).



## COMPONENT 1 (COMP1)

Now expand the model by adding oxygen transport through the electrolyte, also modify the oxygen reduction kinetics expressions to be concentration dependent. Solve the model using two study steps.

### ADD PHYSICS

- 1 In the **Home** toolbar, click  **Add Physics** to open the **Add Physics** window.
- 2 Go to the **Add Physics** window.  
Add the Transport of Diluted Species physics to model oxygen transport by Fickian diffusion.
- 3 In the tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.
- 4 Click **Add to Component 1** in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Physics** to close the **Add Physics** window.

### TRANSPORT OF DILUTED SPECIES (TDS)

The electrolyte is quiescent so there is no need to model convection. Migration is not used either in this model. (Note that if migration and convection is enabled, Transport of Diluted Species models the full Nernst-Planck equations.)

- 1 In the **Settings** window for **Transport of Diluted Species**, locate the **Transport Mechanisms** section.
- 2 Clear the **Convection** check box.


#### *Transport Properties 1*

Set the diffusion coefficient in the electrolyte.

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Transport of Diluted Species (tds)** click **Transport Properties 1**.
- 2 In the **Settings** window for **Transport Properties**, locate the **Diffusion** section.
- 3 In the  $D_c$  text field, type  $D_{O_2}$ .

#### *Concentration 1*

Use a Concentration boundary condition on the top boundary to fix the concentration along this boundary, set the initial value for the concentration to the same value.

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Concentration**.
- 2 Select Boundary 7 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_O2_ref`.

#### *Initial Values 1*

- 1 In the **Model Builder** window, 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`.

#### *Electrode Surface Coupling 1*

Now couple the oxygen flux at the electrode boundary to the electrode reaction currents in the Secondary Current Distribution interface by using Electrode Surface coupling features. This will specify an oxygen flux according to Faraday's law.

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electrode Surface Coupling**.
- 2 In the **Settings** window for **Electrode Surface Coupling**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Zinc surface**.

#### *Reaction Coefficients 1*

- 1 In the **Model Builder** window, expand the **Electrode Surface Coupling 1** node, then click **Reaction Coefficients 1**.
- 2 In the **Settings** window for **Reaction Coefficients**, locate the **Model Inputs** section.
- 3 From the  $i_{loc}$  list, choose **Local current density, Oxygen reaction (cd/es1/er2)**.
- 4 Locate the **Stoichiometric Coefficients** section. In the  $n$  text field, type 4.
- 5 In the  $v_c$  text field, type -1.

The oxygen molecules are reactants when the oxygen reaction is written as a reduction reaction. Writing the reaction using four electrons the stoichiometric number for oxygen is -1.

#### *Electrode Surface Coupling 2*

- 1 In the **Model Builder** window, under **Component 1 (comp1)>** **Transport of Diluted Species (tds)** right-click **Electrode Surface Coupling 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Electrode Surface Coupling**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Iron surface**.

### *Reaction Coefficients 1*

- 1 In the **Model Builder** window, expand the **Electrode Surface Coupling 2** node, then click **Reaction Coefficients 1**.
- 2 In the **Settings** window for **Reaction Coefficients**, locate the **Model Inputs** section.
- 3 From the  $i_{loc}$  list, choose **Local current density, Oxygen reaction (cd/es2/er2)**.

### **ROOT**

Also couple the oxygen electrode reaction currents to the oxygen concentration by including the concentration variable in the exchange current density expressions.

### **SECONDARY CURRENT DISTRIBUTION (CD)**

#### *Oxygen reaction*

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Secondary Current Distribution (cd)>Electrode Surface 1** click **Oxygen reaction**.
- 2 In the **Settings** window for **Electrode Reaction**, locate the **Electrode Kinetics** section.
- 3 In the  $i_0$  text field, type  $i0\_02\_on\_Zn*c/c\_02\_ref$ .  
Now select "Oxygen reaction" under Electrode surface 2 to modify the exchange current density expression on the iron electrode surface as well.

#### *Oxygen reaction*

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Secondary Current Distribution (cd)>Electrode Surface 2** click **Oxygen reaction**.
- 2 In the **Settings** window for **Electrode Reaction**, locate the **Electrode Kinetics** section.
- 3 In the  $i_0$  text field, type  $i0\_02\_on\_Fe*c/c\_02\_ref$ .

### **STUDY 1**

It is general good practice to solve this type of problems by solving for the potentials first, and then the fully coupled problem. Disable Transport of Diluted Species from the first step, and add a second step to solve for the full problem.

#### *Step 1: Stationary*

- 1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.
- 2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
- 3 In the table, clear the **Solve for** check box for **Transport of Diluted Species (tds)**.

#### *Stationary 2*


- 1 In the **Study** toolbar, click  **Study Steps** and choose **Stationary>Stationary**.

- 2 Click  **Compute**.


## RESULTS

Plot the concentration profile on the revolved geometry, created from the 2D axisymmetric geometry, in the following way:

### *Oxygen Concentration*


- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Oxygen Concentration in the **Label** text field.

### *Surface 1*

- 1 Right-click **Oxygen Concentration** and choose **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)>Transport of Diluted Species>Species c>c - Concentration - mol/m<sup>3</sup>**.
- 3 In the **Oxygen Concentration** toolbar, click  **Plot**.  
The figure should now look like [Figure 3](#).

### *Iron Oxidation Current Density*

Finally, analyze the impact of introducing the oxygen concentration to the model by comparing the iron oxidation current densities from the two different study steps (Solution 1 and Solution 2). Since the first study step (Solution 2) does not solve for the oxygen concentration it is kept constant to its initial value.

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Iron Oxidation Current Density in the **Label** text field.

### *Line Graph 1*

- 1 Right-click **Iron Oxidation Current Density** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Iron surface**.
- 4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **cd.iloc\_er1 - Local current density - A/m<sup>2</sup>**.
- 5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 6 In the **Expression** text field, type **z**.
- 7 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

- 8 Locate the **Legends** section. Select the **Show legends** check box.
- 9 From the **Legends** list, choose **Manual**.
- 10 In the table, enter the following settings:

Legends
Tertiary current distribution (with oxygen transport limitation)

*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 **Dataset** list, choose **Study 1/Solution Store 1 (sol2)**.
- 4 Locate the **Legends** section. In the table, enter the following settings:

Legends
Secondary current distribution (no oxygen transport limitation)

*Iron Oxidation Current Density*

- 1 In the **Model Builder** window, click **Iron Oxidation Current Density**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Legend** section.
- 3 From the **Position** list, choose **Lower right**.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **Label**.  
 The figure should now look like [Figure 4](#).

