Model created in COMSOL Multiphysics 6.4

Corrosion Under an Evans Droplet

Introduction

An Evans droplet experiment is a century-old corrosion experiment for demonstrating oxygen transport-limited corrosion. A droplet of water is placed on a metal surface, and over time the surface features differences in the radial direction of the surface in terms of amount of corroded material and deposited corrosion products.

This tutorial model defines corrosion of an iron surface in contact with an aqueous sodium-chloride solution droplet in a surrounding atmosphere containing both carbon dioxide and oxygen. The model accounts for charge and mass transport of multiple species as well as iron dissolution, oxygen reduction, carbonic acid equilibria, iron hydrolysis, and precipitation of ferrous hydroxide and ferrous carbonate corrosion products.

The model computes the transient and spatial distributions of the various species within the droplet. A spatial gradient in pH is demonstrated and is attributed to the complex dynamic interplay between the dissolved iron, corrosion products, and dissolved atmospheric gases.

The model is based on several journal papers (Ref. 1–Ref. 4).

Model Definition

Figure 1 shows the model geometry, defining an elliptical electrolyte droplet (with a 90° wetting angle) covering an iron metal surface. The geometry is defined in 2D with axial symmetry. As an assumption, the geometry is fixed throughout the simulation.

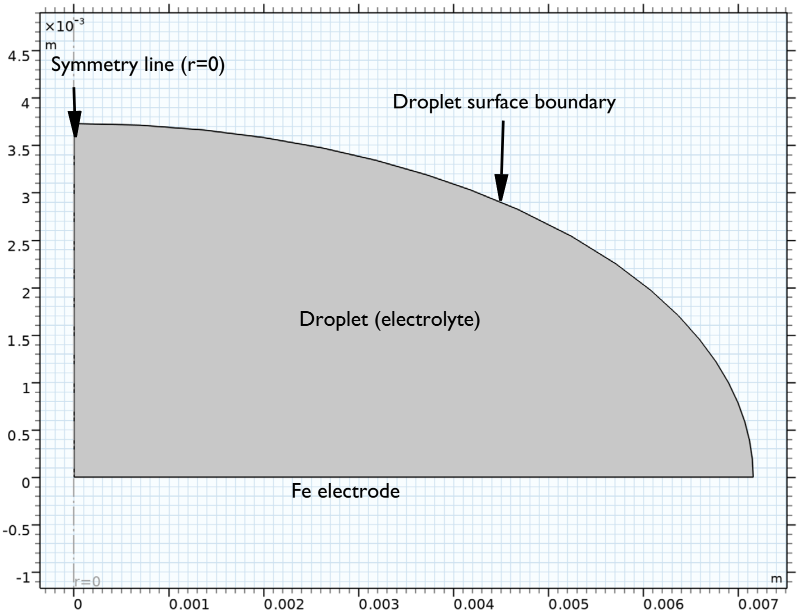

Figure 1: Model geometry.

The model is defined using the **Aqueous Electrolyte Transport** interface, solving for the electrolyte phase potential and the concentrations of the electrolyte species H^+, OH^-, Fe^{2+}, $FeOH^+$, $Fe(OH)_2$(aq), $FeCO_3$(aq), O_2(aq), CO_2(aq), H_2CO_3, HCO_3^-, CO_3^{2-}, Na^+, and Cl^-.

Oxygen reduction occurs on the metal surface, which, due to limited oxygen diffusion, is more dominant toward the periphery of the droplet:

$$4\mathrm{H}^+ + 4e^- + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O} \tag{1}$$

Iron is oxidized to counterbalance the oxygen reduction reaction:

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

Butler–Volmer electrode kinetics expressions are used for both the oxygen-reduction and iron-dissolution reactions. The combination of these two reactions gives rise to a mixed electrode potential of the metal surface.

Dissolved iron precipitates as ferrous hydroxide and ferrous carbonate corrosion products at the electrode surface due to the following reactions:

$$\mathrm{Fe}^{2+} + 2\mathrm{OH}^{-} \rightarrow \mathrm{Fe(OH)_2(s)} \qquad (3)$$

$$\mathrm{Fe}^{2+} + \mathrm{CO}_3^{2-} \rightarrow \mathrm{FeCO_3(s)} \qquad (4)$$

The reactions are defined as irreversible and precipitation takes place once the solubility product is exceeded. The corrosion products are said to cover the metallic surface and are assumed to only inhibit the metal dissolution, that is, the products passivate the iron. The corrosion-product coverage degree, θ, is computed with the expression

$$\theta = 1 - e^{-\frac{c_{\mathrm{tot,\,s}}}{c_{\mathrm{available,\,s}}}} \qquad (5)$$

With the use of the above expression, the coverage can reach a maximum value of 1 with precipitation. $c_{\mathrm{tot,s}}$ is the total molar amount per surface area of precipitated corrosion products and $c_{\mathrm{available,s}}$ is the molar availability per surface area and monolayer for corrosion-product precipitation. The inhibition of the metal dissolution is modeled by multiplying the local current density of the metal dissolution reaction with the uncovered surface fraction, $1 - \theta$. Note that with the expression above more than $c_{\mathrm{available,s}}$ needs to precipitate for full passivation.

EQUILIBRIUM REACTIONS

The following equilibrium reactions are accounted for in the electrolyte:

$$\begin{aligned}
&H_2O \Leftrightarrow H^+ + OH^- && K_1 = 6.418 \cdot 10^{-3} \\
&CO_2(aq) + H_2O \Leftrightarrow H_2CO_3 && K_2 = 2.580 \cdot 10^{-3} \\
&H_2CO_3 \Leftrightarrow H^+ + HCO_3^- && K_3 = 1.251 \cdot 10^{-4} \\
&HCO_3^- \Leftrightarrow H^+ + CO_3^{2-} && K_4 = 1.382 \cdot 10^{-10} \\
&Fe^{2+} + H_2O \Leftrightarrow FeOH^+ + H^+ && K_5 = 3.162 \cdot 10^{-10} \\
&FeOH^+ + H_2O \Leftrightarrow Fe(OH)_2(aq) + H^+ && K_6 = 7.943 \cdot 10^{-12} \\
&FeCO_3(aq) \Leftrightarrow Fe^{2+} + CO_3^{2-} && K_7 = 2.692 \cdot 10^{-7}
\end{aligned} \tag{6}$$

K_1 through K_7 are the equilibrium constants. Values have been chosen for temperatures near room temperature (293.15 K).

The water dissociation equilibrium reaction is built-in for the Aqueous Electrolyte Transport interface. All three carbonic acid reactions can be captured by adding the Carbonic Acid feature to the Electrolyte domain node. The Ampholyte feature is used to model the two iron hydrolysis reactions. Finally, the Complex Species feature allows for easy representation of the iron carbonate species. These equilibrium reaction features simultaneously calculate the concentration of all aqueous species based on equilibrium expressions, which are based on the reaction stoichiometry and the equilibrium constant K_k according to

$$K_k = \prod_i (c_i)^{v_{ik}} \tag{7}$$

where c_i (SI unit: mol/m^3) is the concentration of species i and v_{ik} is the stoichiometric coefficient of species i in reaction k.

As a result of the above equilibrium reactions, the gaseous CO_2 dissolved at the droplet surface forms carbonic acid, which generally lowers the pH.

The model is solved using a time-dependent solver, simulating the transient and spatial evolution of the species considered for 300 seconds. Inward fluxes of O_2 and CO_2 are set relatively high at the upper droplet boundary facing the surrounding atmosphere such that the gas concentrations are approximately constant and equal to the saturation concentrations (O_2(aq, sat) and CO_2(aq, sat)) at the droplet surface.

Results and Discussion

Figure 2 shows the iron ion concentration distribution within the Evans droplet at 10 s (left) and 300 s (right). It can be seen that the concentration is lower within a ring expanding inward from the droplet periphery compared to the central parts of the droplet. At the 300 s, this ring with lower iron ion concentration has become approximately 1 mm wide.

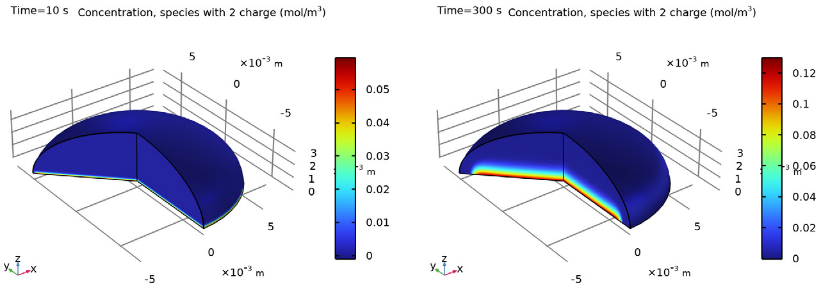

Figure 2: Iron ion concentration distribution within the droplet at t = 10 s (left) and t = 300 s (right).

In Figure 3, the current density distributions and the corrosion-product coverage degree along the iron surface underneath the droplet at 300 s are displayed. The observed lower iron-ion concentration can be explained by the lower anodic metal-dissolution reaction which in turn is affected by the higher corrosion-product coverage degree at the same location. The short-time behavior in Figure 2 (left) is likewise explained by the coverage, which is less and means that the iron dissolution initially is present over almost the whole droplet covered surface.

The cathodic oxygen reduction is larger near the rim of the droplet due to limited oxygen transport, in combination with the limited electrolyte conductivity. The total current density shows that the anodic activity dominates the central parts of the droplet and the cathodic the periphery of the droplet.

Note that the droplet rim has a different behavior due to the acidifying CO_2 from the atmosphere. This acidity counteracts any corrosion-product precipitation.

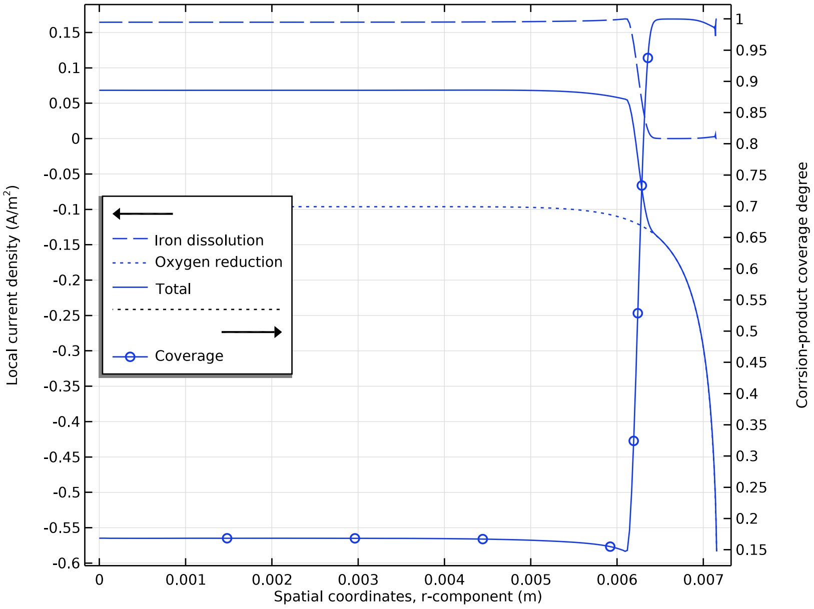

Figure 3: Iron dissolution, oxygen reduction, and total current density distributions along the iron surface at t = 300 s.

Figure 4 shows the CO_2(aq) concentration distribution within the droplet at 10 s (left) and 300 s (right). It can be seen that the concentration is reduced close to the iron surface, since it is consumed in a homogeneous reaction.

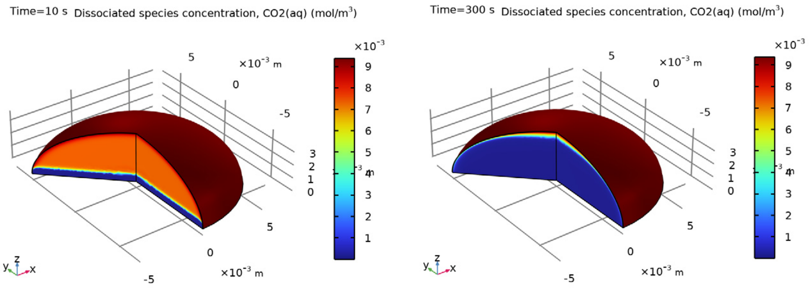

Figure 4: CO_2 concentration distribution within the droplet at t = 10 s (left) and t = 300 s (right).

Figure 5 shows the pH distribution within the droplet at 10 s (left) and 300 s (right). The pH changes over time are substantial. It can also be seen that the pH is increased in the vicinity of the metal surface, when compared to the pH closer to the droplet periphery. At the droplet rim, the pH is the lowest due to the CO_2 in the atmosphere. The pH changes are generally attributed to the dissolution of iron atoms which need to be counter-balanced by hydroxide ions from water autoprotolysis. The iron hydrolysis is insufficient to acidify the electrolyte near the iron surface.

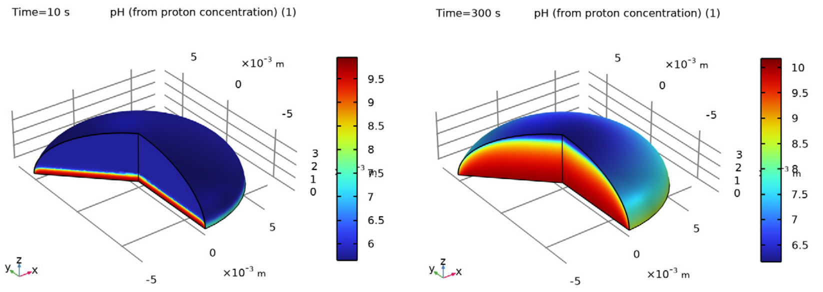

Figure 5: pH distribution within the droplet at t = 10 s (left) and t = 300 s (right).

Figure 6 shows the surface plot of precipitated corrosion products per area along the iron surface underneath the droplet and the streamline plot of the electrolyte current density over the droplet domain at 300 s. Most has precipitated in the ring region where the low iron-ion concentration is observed. A comparison with the coverage degree in Figure 3 indicates that ferrous carbonate almost exclusively makes up the coverage in that region. The access to carbonates in the form of carbonate ions near the droplet periphery is the main cause for this. The streamlines show the ionic current flow from the core toward the rim of the droplet.

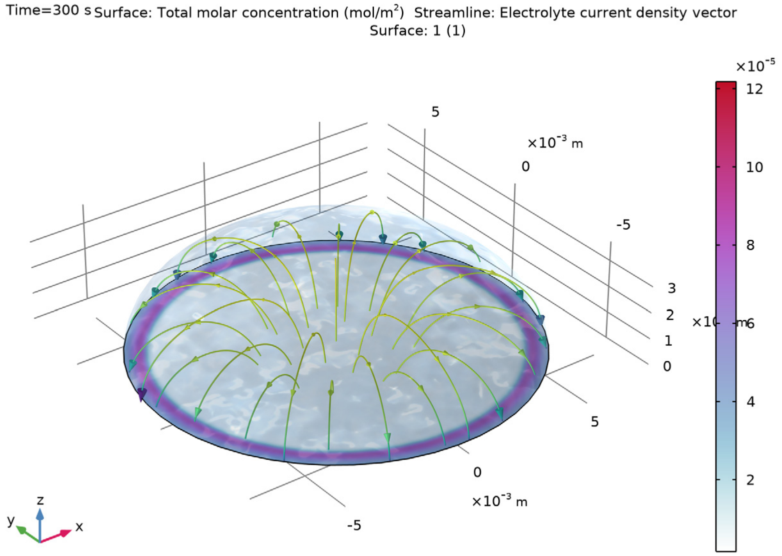

Figure 6: Precipitated ferrous carbonate and ferrous oxide at the iron surface and streamline plot of the electrolyte current density at t = 300 s.

References

1. B.G. Koushik, N. Van den Steen, M.H. Mamme, Y. Van Ingelgem, and H. Terryn, “Review on modelling of corrosion under droplet electrolyte for predicting atmospheric corrosion rate,” *J. Mater. Sci. Technol.*, vol. 62, pp. 254–267, 2021.

2. M. Nordsveen, S. Nesic, R. Nyborg, and A. Stangeland, “A Mechanistic Model for Carbon Dioxide Corrosion of Mild Steel in the Presence of Protective Iron Carbonate Films-Part 1: Theory and Verification,” *Corrosion*, vol. 59, no. 5, pp. 443–456, 2003.

3. P.L. Fosboel and K. Thomsen, “Review and recommended thermodynamic properties of $FeCO_3$,” *Corros. Sci. Technol.*, vol. 45, no. 2, pp. 115–135, 2010.

4. F.J. Millero, W. Yao, and J. Aicher, “The speciation of Fe(II) and Fe(III) in natural waters,” *Marine Chemistry*, vol. 50, pp. 21–39, 1995.

Application Library path: `Corrosion_Module/Atmospheric_Corrosion/evans_droplet`

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 Axisymmetric**.
2. In the **Select Physics** tree, select **Electrochemistry** > **Aqueous Electrolyte Transport (aqt)**.
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**.

GLOBAL DEFINITIONS

Load the model parameters form 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 `evans_droplet_parameters.txt`.

GEOMETRY 1

Ellipse 1 (e1)

The geometry consists of a sector of an ellipse.

1. In the **Geometry** toolbar, click **Ellipse**.
2. In the **Settings** window for **Ellipse**, locate the **Size and Shape** section.

3 In the **a-semiaxis** text field, type `a`.

4 In the **b-semiaxis** text field, type `b`.

5 In the **Sector angle** text field, type `90`.

6 Click **Build All Objects**.

DEFINITIONS

Load the model variables from a text file. These include precipitation and passivation definitions.

Variables 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** node.

2 Right-click **Definitions** and choose **Local Variables**.

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

4 Click **Load from File**.

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

AQUEOUS ELECTROLYTE TRANSPORT (AQT)

Electrolyte 1

Add all aqueous species in the Electrolyte feature. This includes Carbonic acid, which encompasses CO2 and all associated species, as well as the iron species, supporting electrolyte, and dissolved oxygen.

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

Carbonic Acid 1

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

Electrolyte 1

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

Ampholyte - Fe

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

2 In the **Settings** window for **Ampholyte**, type `Ampholyte - Fe` in the **Label** text field.

3 Locate the **Ampholyte** section. In the **Species name** text field, type `Fe`.

4 In the table, enter the following settings:

Dissociation step (1)	pKa (1)
1	`-log10(KFeOH)`
2	`-log10(KFeOH2)`

5 In the z_0 text field, type `0`.

6 Locate the **Diffusion and Migration** section. In the D text field, type `DFe`.

Electrolyte 1

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

Uncharged Species - O2

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

2 In the **Settings** window for **Uncharged Species**, type `Uncharged Species - O2` in the **Label** text field.

3 Locate the **Uncharged Species** section. In the **Species name** text field, type `O2`.

4 Locate the **Diffusion** section. In the D text field, type `DO2`.

Electrolyte 1

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

Fully Dissociated Species - Na

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

2 In the **Settings** window for **Fully Dissociated Species**, type `Fully Dissociated Species - Na` in the **Label** text field.

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

4 In the z text field, type `zNa`.

5 Locate the **Diffusion and Migration** section. In the D text field, type `DNa`.

Electrolyte 1

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

Fully Dissociated Species - Cl

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

2 In the **Settings** window for **Fully Dissociated Species**, type `Fully Dissociated Species - Cl` in the **Label** text field.

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

4 In the z text field, type `zCl`.

5. Locate the **Diffusion and Migration** section. In the D text field, type `DCl`.

Electrolyte 1

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

Complex Species - FeCO3

1. In the **Physics** toolbar, click **Attributes** and choose **Complex Species**.
2. In the **Settings** window for **Complex Species**, type `Complex Species - FeCO3` in the **Label** text field.
3. Locate the **Diffusion** section. In the D text field, type `DFe`.
4. Locate the **Equilibrium Constant** section. In the K_{eq} text field, type `KFeCO3`.
5. Locate the **Stoichiometric Coefficients** section. Select the **CO3** checkbox.
6. In the $\nu_{\mathrm{CO3}}{}^{2-}$ text field, type `-1`.
7. Select the **Fe (+2)** checkbox.
8. In the $\nu_{\mathrm{Fe}}{}^{2+}$ text field, type `-1`.

Initial Values 1

Set the initial concentration of dissolved species here. Note that the species H2CO3 is the total concentration of all carbon dioxide-related species.

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Aqueous Electrolyte Transport (aqt)** click **Initial Values 1**.
2. In the **Settings** window for **Initial Values**, locate the **Electrolyte Potential** section.
3. In the $\phi_{1,0}$ text field, type `phil0`.
4. Locate the **Concentration** section. In the $c_{\mathrm{H2CO3,0}}$ text field, type `cCO20`.
5. In the $c_{\mathrm{O2,0}}$ text field, type `cO20`.
6. In the $c_{\mathrm{Na,0}}$ text field, type `cNaCl0`.
7. In the $c_{\mathrm{Cl,0}}$ text field, type `cNaCl0`.

Flux 1

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

   Set high fluxes of carbon dioxide and oxygen in to the droplet to maintain a constant surface concentration of dissolved gases.

2. Select Boundary 3 only.
3. In the **Settings** window for **Flux**, locate the **Inward Species Fluxes** section.
4. In the $N_{\mathrm{CO2}(aq)}$ text field, type `-k_CO2*(aqt.c4_H2CO3-cCO20)`.
5. In the N_{O2} text field, type `-k_O2*(aqt.c_O2-cO2s)`.

Electrode Surface 1

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

 Use the Dissolving-Depositing Species section to include precipitation of ferrous hydroxide and ferrous carbonate at the surface.

2 Select Boundary 2 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 name	Molar volume (m^3/mol)	Initial concentration (mol/m^2)
`FeOH2`	`M_FeOH2/rho_FeOH2`	`0[mol/m^2]`

6 Click + **Add**.

7 In the table, enter the following settings:

Species name	Molar volume (m^3/mol)	Initial concentration (mol/m^2)
`FeCO3`	`M_FeCO3/rho_FeCO3`	`0[mol/m^2]`

 Now set up all four reactions happening at the electrode surface, two electrochemical reactions and two precipitation reactions.

Electrode Reaction - Fe Dissolution

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

2 In the **Settings** window for **Electrode Reaction**, type `Electrode Reaction - Fe Dissolution` in the **Label** text field.

3 Locate the **Stoichiometric Coefficients** section. In the $\nu_{\mathrm{Fe}}{}^{2+}$ text field, type `-1`.

4 Locate the **Equilibrium Potential** section. In the $E_{\mathrm{eq,ref}}(T)$ text field, type `Eeq_ref_Fe`.

5 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_Fe*(1-theta)`.

6 In the α_{a} text field, type `alphaa_Fe`.

Electrode Surface 1

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

Electrode Reaction 2

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

GLOBAL DEFINITIONS

Default Model Inputs

1. In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.
2. In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.
3. In the tree, select **General** > **Temperature (K) - minput.T**.
4. Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type `T`.

AQUEOUS ELECTROLYTE TRANSPORT (AQT)

Electrode Reaction - Oxygen Reduction

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Aqueous Electrolyte Transport (aqt)** > **Electrode Surface 1** click **Electrode Reaction 2**.
2. In the **Settings** window for **Electrode Reaction**, type `Electrode Reaction - Oxygen Reduction` in the **Label** text field.
3. Locate the **Stoichiometric Coefficients** section. In the ν_{O2} text field, type `-1`.
4. In the ν_{OH^-} text field, type `4`.
5. Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `Eeq_ref_O2`.
6. Click to expand the **Reference Concentrations** section. In the $c_{ref,O2}$ text field, type `cO2_sol`.
7. Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0_ref_O2`.
8. In the α_a text field, type `alphaa_O2`.

Electrode Surface 1

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

Reaction - FeOH2

1. In the **Physics** toolbar, click **Attributes** and choose **Reaction**.
2. In the **Settings** window for **Reaction**, type `Reaction - FeOH2` in the **Label** text field.
3. Locate the **Reaction Rate** section. In the R text field, type `rFeOH2`.
4. Locate the **Stoichiometric Coefficients** section. In the $\nu_{Fe^{2+}}$ text field, type `-1`.
5. In the ν_{OH^-} text field, type `-2`.

6. Find the **Stoichiometric coefficients for dissolving–depositing species** subsection. In the table, enter the following settings:

Species name	**Stoichiometric coefficient (1)**
FeOH2	1

Electrode Surface 1

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

Reaction - FeCO3

1. In the **Physics** toolbar, click **Attributes** and choose **Reaction**.
2. In the **Settings** window for **Reaction**, type `Reaction - FeCO3` in the **Label** text field.
3. Locate the **Reaction Rate** section. In the R text field, type `rFeCO3`.
4. Locate the **Stoichiometric Coefficients** section. In the $\nu_{\mathrm{CO3}}{}^{2-}$ text field, type `-1`.
5. In the $\nu_{\mathrm{Fe}}{}^{2+}$ text field, type `-1`.
6. Find the **Stoichiometric coefficients for dissolving–depositing species** subsection. In the table, enter the following settings:

Species name	**Stoichiometric coefficient (1)**
FeCO3	1

Build a mesh using a finer resolution at the electrode surface, gas-liquid boundary, and corner.

MESH 1

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
2. In the **Settings** window for **Mesh**, locate the **Sequence Type** section.
3. From the list, choose **User-controlled mesh**.

Size

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** click **Size**.
2. In the **Settings** window for **Size**, locate the **Element Size** section.
3. From the **Predefined** list, choose **Normal**.
4. Click to expand the **Element Size Parameters** section.

Distribution 1

1. In the **Model Builder** window, right-click **Free Triangular 1** and choose **Distribution**.
2. Select Boundaries 2 and 3 only.

3. In the **Settings** window for **Distribution**, locate the **Distribution** section.
4. From the **Distribution type** list, choose **Predefined**.
5. In the **Number of elements** text field, type `200`.
6. In the **Element ratio** text field, type `10`.

STUDY 1

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(0,10,300)`.
4. In the **Study** toolbar, click **Compute**.

RESULTS

Several plots are added by default. The following steps add additional useful plots, some of which appear in the Results and Discussion Section:

Total Corrosion Product Precipitation

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

   Start with a 2D image of the total Corrosion Product Precipitation.
2. In the **Settings** window for **2D Plot Group**, type `Total Corrosion Product Precipitation` in the **Label** text field.

Line 1

1. Right-click **Total Corrosion Product Precipitation** and choose **Line**.
2. Click the **Zoom Extents** button in the **Graphics** toolbar.
3. In the **Settings** window for **Line**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Aqueous Electrolyte Transport** > **Dissolving–depositing species** > **aqt.es1.ctot - Total molar concentration - mol/m²**.
4. In the **Total Corrosion Product Precipitation** toolbar, click **Plot**.

Precipitated FeCO3 Fraction, 3D

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

   The next plot shows the precipitated FeCO3 Fraction in 3D; it is also the thumbnail image.
2. Right-click **3D Plot Group 10** and choose **Rename**.

3. In the **Rename 3D Plot Group** dialog, type `Precipitated FeCO3 Fraction, 3D` in the **New label** text field.
4. Click **OK**.

Surface 1

Right-click **Precipitated FeCO3 Fraction, 3D** and choose **Surface**.

Revolution 2D 1

1. In the **Model Builder** window, expand the **Results** > **Datasets** node.
2. Right-click **Results** > **Datasets** and choose **Revolution 2D**.
3. In the **Settings** window for **Revolution 2D**, click to expand the **Revolution Layers** section.
4. Click to expand the **Advanced** section.

Revolution 2D 2

1. In the **Results** toolbar, click ▦ **More Datasets** and choose **Revolution 2D**.
2. In the **Settings** window for **Revolution 2D**, locate the **Revolution Layers** section.
3. In the **Start angle** text field, type `-90`.
4. In the **Revolution angle** text field, type `225`.

Precipitated FeCO3 Fraction, 3D

1. In the **Model Builder** window, under **Results** click **Precipitated FeCO3 Fraction, 3D**.
2. In the **Settings** window for **3D Plot Group**, locate the **Data** section.
3. From the **Dataset** list, choose **Revolution 2D 1**.

Surface 1

1. In the **Model Builder** window, click **Surface 1**.
2. In the **Settings** window for **Surface**, locate the **Expression** section.
3. In the **Expression** text field, type `comp1.aqt.es1.ctot`.
4. Locate the **Coloring and Style** section. From the **Color table** list, choose **Acanthaster**.

Streamline 1

1. In the **Model Builder** window, right-click **Precipitated FeCO3 Fraction, 3D** and choose **Streamline**.
2. In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
3. From the **Positioning** list, choose **Uniform density**.
4. In the **Density level** text field, type `7`.

5. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Tube**.
6. Select the **Radius scale factor** checkbox. In the associated text field, type `2.5e-5`.
7. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.
8. From the **Arrow length** list, choose **Logarithmic**.
9. From the **Color** list, choose **Green**.

Color Expression 1

1. Right-click **Streamline 1** and choose **Color Expression**.
2. In the **Settings** window for **Color Expression**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Aqueous Electrolyte Transport** > **aqt.IlMag - Electrolyte current density magnitude - A/m^2**.
3. Locate the **Coloring and Style** section. From the **Color table** list, choose **Viridis**.
4. From the **Color table transformation** list, choose **Reverse**.
5. Clear the **Color legend** checkbox.

Surface 2

1. In the **Model Builder** window, right-click **Precipitated FeCO3 Fraction, 3D** and choose **Surface**.
2. In the **Settings** window for **Surface**, locate the **Expression** section.
3. In the **Expression** text field, type `1`.

Selection 1

1. Right-click **Surface 2** and choose **Selection**.
2. Select Domain 1 only.

Transparency 1

1. In the **Model Builder** window, right-click **Surface 2** and choose **Transparency**.
2. In the **Settings** window for **Transparency**, locate the **Transparency** section.
3. Find the **Transparency** subsection. In the **Transparency** text field, type `0.85`.

Material Appearance 1

1. Right-click **Surface 2** and choose **Material Appearance**.
2. In the **Settings** window for **Material Appearance**, locate the **Appearance** section.
3. From the **Appearance** list, choose **Custom**.
4. From the **Material type** list, choose **Water**.
5. In the **Precipitated FeCO3 Fraction, 3D** toolbar, click **Plot**.

Precipitated FeCO3 Fraction, 3D

1. In the **Model Builder** window, under **Results** click **Precipitated FeCO3 Fraction, 3D**.
2. Click **Plot**.

pH, 3D

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

   Next, plot the pH in 3D.
2. Right-click **3D Plot Group 11** and choose **Rename**.
3. In the **Rename 3D Plot Group** dialog, type `pH, 3D` in the **New label** text field.
4. Click **OK**.

Surface 1

Right-click **pH, 3D** and choose **Surface**.

pH, 3D

1. In the **Settings** window for **3D Plot Group**, locate the **Data** section.
2. From the **Dataset** list, choose **Revolution 2D 2**.
3. In the **pH, 3D** toolbar, click **Plot**.
4. From the **Time (s)** list, choose **10**.
5. In the **pH, 3D** toolbar, click **Plot**.
6. From the **Time (s)** list, choose **300**.
7. In the **pH, 3D** toolbar, click **Plot**.

Local Current Density and Coverage

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

   Plot the local current density and surface coverage at the electrode surface in 1D as a function of the spatial dimension r.
2. In the **Settings** window for **1D Plot Group**, type `Local Current Density and Coverage` in the **Label** text field.
3. Click to expand the **Title** section. From the **Title type** list, choose **None**.
4. Locate the **Data** section. From the **Time selection** list, choose **Last**.
5. Locate the **Plot Settings** section. Select the **Two y-axes** checkbox.
6. Locate the **Legend** section. From the **Position** list, choose **Middle left**.
7. Locate the **Plot Settings** section.
8. Select the **y-axis label** checkbox. In the associated text field, type `Local current density (A/m<sup>2</sup>)`.

9 Select the **Secondary y-axis label** checkbox. In the associated text field, type `Corrosion-product coverage degree`.

10 Select the **x-axis label** checkbox. In the associated text field, type `Spatial coordinates, r-component (m)`.

Line Graph 1

1 Right-click **Local Current Density and Coverage** and choose **Line Graph**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `aqt.es1.er1.iloc`.

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

6 In the **Expression** text field, type `r`.

7 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

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

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

10 In the table, enter the following settings:

Legends
`Iron dissolution`

Line Graph 2

1 In the **Model Builder** window, right-click **Local Current Density and Coverage** and choose **Line Graph**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `aqt.es1.er2.iloc`.

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

6 In the **Expression** text field, type `r`.

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.

8 From the **Color** list, choose **Cycle (reset)**.

9 Locate the **Legends** section. Select the **Show legends** checkbox.

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

11 In the table, enter the following settings:

Legends
`Oxygen reduction`

Line Graph 3

1 Right-click **Local Current Density and Coverage** and choose **Line Graph**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `aqt.itot`.

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

6 In the **Expression** text field, type `r`.

7 Locate the **Coloring and Style** section. From the **Color** list, choose **Cycle (reset)**.

8 Locate the **Legends** section. Select the **Show legends** checkbox.

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

10 In the table, enter the following settings:

Legends
`Total`

Line Graph 4

1 Right-click **Local Current Density and Coverage** and choose **Line Graph**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `theta`.

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

6 In the **Expression** text field, type `r`.

7 Locate the **Coloring and Style** section. From the **Color** list, choose **Cycle (reset)**.

8 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

9 From the **Positioning** list, choose **Interpolated**.

10 Locate the **Legends** section. Select the **Show legends** checkbox.

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

12 In the table, enter the following settings:

Legends
`Coverage`

Local Current Density and Coverage

1 In the **Model Builder** window, click **Local Current Density and Coverage**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 In the table, select the **Plot on secondary y-axis** checkbox for **Line Graph 4**.

4 In the **Local Current Density and Coverage** toolbar, click **Plot**.

Concentration, Fe, 3D

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

Finish with two 3D plots of the local Fe and CO2 concentration.

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

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

4 In the **Label** text field, type `Concentration, Fe, 3D`.

Surface 1

1 Right-click **Concentration, Fe, 3D** and choose **Surface**.

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

3 In the **Expression** text field, type `aqt.c3_Fe`.

4 In the **Concentration, Fe, 3D** toolbar, click **Plot**.

Concentration, Fe, 3D

1 In the **Model Builder** window, click **Concentration, Fe, 3D**.

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

3 From the **Time (s)** list, choose **10**.

4 In the **Concentration, Fe, 3D** toolbar, click **Plot**.

5 From the **Time (s)** list, choose **300**.

6 In the **Concentration, Fe, 3D** toolbar, click **Plot**.

Concentration, CO2, 3D

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

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

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

4 In the **Label** text field, type `Concentration, CO2, 3D`.

Surface 1

1 Right-click **Concentration, CO2, 3D** 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)** > **Aqueous Electrolyte Transport** > **Carbonic Acid 1** > **aqt.c4_H2CO3 - Dissociated species concentration, CO2(aq) - mol/**m^3.

3 In the **Concentration, CO2, 3D** toolbar, click **Plot**.

Concentration, CO2, 3D

1 In the **Model Builder** window, click **Concentration, CO2, 3D**.

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

3 From the **Time (s)** list, choose **10**.

4 In the **Concentration, CO2, 3D** toolbar, click **Plot**.

5 From the **Time (s)** list, choose **300**.

6 In the **Concentration, CO2, 3D** toolbar, click **Plot**.