Model created in COMSOL Multiphysics 6.4

Accelerated Corrosion Test of a Scratched Galvanized Steel Sample

Introduction

An established method for benchmarking the atmospheric corrosion resistance of materials is the use of accelerated corrosion tests (ACT) performed in climate chambers. The main purpose of ACTs is to make reliable and fast predictions of the long-time behavior. The tests expose samples to cyclic conditions during a few weeks. Elevated temperature, repeated drying and wetting together with salt addition are conditions that typically speed up corrosion and characterize ACTs. The samples can be of all shapes and sizes, in setups targeting crevice or galvanic corrosion, or have artificial damage.

This example studies a galvanized steel sample with crossing scratches that fully penetrate the zinc coating and expose the underlying steel. The corrosion is simulated for a dummy ACT running for 7 days. The model solves for a thin liquid film that covers the sample surface. Local variations in pH, corrosion products, and coating damage are shown.

Model Definition

GEOMETRY

The 2D sample and model geometries with scratches are shown in Figure 1.

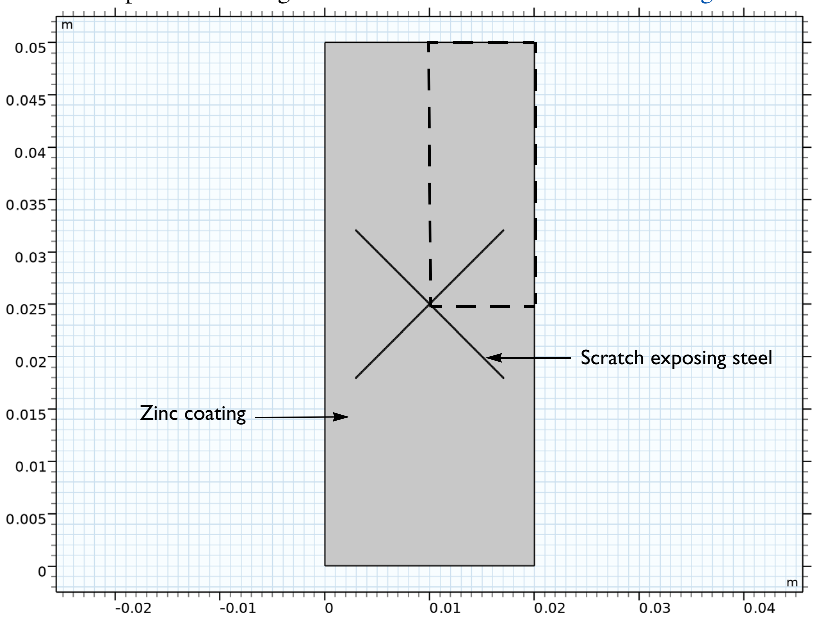


Figure 1: The galvanized steel sample geometry with 0.1 mm wide scratches exposing the steel. The model geometry is marked with dashed lines.

As indicated in the figure, due to symmetry, only one quarter of the sample is needed to investigate the full sample surface. The 2D geometry neglects the thickness of the liquid film. Since the atmospheric corrosion is limited to thin films, in the range of up to tens of micrometers, negligible gradients across the film thickness are expected and makes the thickness dimension redundant.

More information on atmospheric corrosion can be found in the Atmospheric Corrosion example.

ACCELERATED CORROSION TEST MODEL

The ACT is displayed in Figure 2. The temperature interval is between 278.15 K and 323.15 K, and the relative humidity ranges between 70% and 95%. The low RH periods are oscillating around the deliquescence of the NaCl salt (~RH 75%). 1 wt% NaCl solution is sprayed onto the sample at the beginning of day 1, 3, and 6.

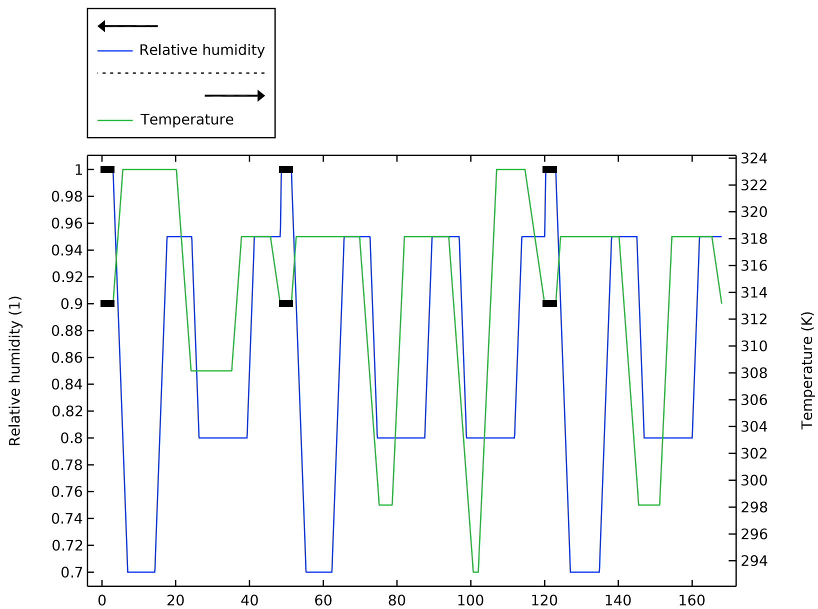


Figure 2: ACT. Solid black line indicates periods of spraying 1 wt% NaCl solution onto the sample.

During spray periods, the liquid film thickness is assumed to be constant at 100 µm and the film volume is fully replenished ten times. When not sprayed, the thickness depends on both the salt load density and the relative humidity. Low RH dries up the film while higher RH leads to condensation of gaseous water which thickens the film. Below the deliquescence RH, the film is assumed to be discontinuous.

The dependence of RH on film thickness and (other properties) is described in the Atmospheric Corrosion example. A general approximation from that example and throughout this model is that parameters that possibly could depend on the total aqueous species concentration in the film (or ionic strength) are dependent on the NaCl concentration only. The weak temperature dependence that is characteristic for the NaCl salt solubility and deliquescence is also practiced.

Mass transport of several relevant species, reactions (electrochemical, homogeneous, and heterogeneous) and interactions with atmosphere (gas dissolution and drying/condensation) are all phenomena considered during the ACT. For simplicity a horizontal sample orientation is considered.

AQUEOUS ELECTROLYTE TRANSPORT INTERFACE

The interface is used to define material balances accounting for the mass transport of species, i, and various sources in a liquid film covering the galvanized steel sample:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot J_i = S \tag{1}$$

In the equation, J_i is the diffusion and migration flux, and S any type of source (mol/(m^3·s)).

With the use of **Highly Conductive Porous Electrode** and **Species Source** nodes, reactions at the metal surface and at the atmosphere-liquid boundary are accounted for on the 2D geometry. The approach assumes that the liquid film is thin with no gradients along the film. The **Include out-of-plane thickness in time-derivative in material balances** setting is by default activated (on the physics top node) and is left untouched. In this manner if the film grows and shrinks due to evaporation and condensation, respectively, concentrations will change.

Electrochemical Reactions

The electrochemical reactions on zinc and steel are defined using polarization data available in the **Corrosion** folder in the **Material Library**. Metal dissolution is set at zinc and oxygen reduction on steel. Thus these two reactions are accounted for:

$$\mathrm{Zn(s)} \rightarrow \mathrm{Zn^{2+}} + 2\mathrm{e^-}$$
$$\frac{1}{2}\mathrm{O_2} + \mathrm{H_2O} + 2\mathrm{e^-} \rightarrow 2\mathrm{OH^-}$$

The metal dissolution data are adjusted for changes in salt concentration using a simplified linear dependence and the oxygen reduction reaction uses a simple linear dependence approximation of the dissolved oxygen concentration. Both reactions include an Arrhenius equation factor to incorporate the temperature fluctuations. The volumetric current formulations, $i_{v,Ox}$ and $i_{v,Red}$, are defined as:

$$i_{v,Ox} = \frac{1-\theta}{L} \cdot \frac{c_{NaCl}}{c_{NaCl,ref}} \cdot i_{loc,Zn} \cdot e^{\frac{E_a}{R_g}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)} \tag{2}$$

$$i_{v,Red} = \frac{1-\theta}{L} \cdot \frac{c_{O_2,sat}}{c_{O_2,sat,ref}} \cdot i_{loc,\ Fe} \cdot e^{\frac{E_a}{R_g}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)} \tag{3}$$

where $i_{loc,Zn}$ and $i_{loc,Fe}$ are the polarization data (current density versus potential) for the two reactions, θ the corrosion product surface coverage degree, E_a the activation energy, L the film thickness, and subscript "ref" indicate parameter values at experimental data conditions. The film discontinuity below RH deliquescence is accounted for in the reaction expressions, by turning the volumetric currents off using a **Ramp** function factor.

The electrochemical reactions are defined using the **User Defined** electrode kinetics option in the **Porous Electrode Reaction** available at the **Highly Conductive Porous Electrode** nodes. By setting the **Active Species Surface Area** to the inverse of the liquid film thickness, the settings are equal to that of a thin liquid film with no gradients along the film thickness (i.e. homogenized properties across the thickness).

Homogeneous Reactions in Liquid Film

Carbonates originating from the atmosphere are accounted for. Three dissociation steps are defined using the **Carbonic Acid** node, in which the following equilibrium reactions are accounted for:

$$CO_2(aq) + H_2O \Leftrightarrow H_2CO_3$$

$$H_2CO_3 \Leftrightarrow H^+ + HCO_3^-$$

$$HCO_3^- \Leftrightarrow H^+ + CO_3^{2-}$$

The node defines the mass balance accounting for all carbonate species: $CO_2(aq)$, H_2CO_3, HCO_3^-, and CO_3^{2-}.

Zinc ions from the dissolution of the zinc coating hydrolyze in four steps (Ref. 2):

$$Zn^{2+} + H_2O \Leftrightarrow Zn(OH)^+ + H^+$$

$$Zn(OH)^+ + H_2O \Leftrightarrow Zn(OH)_2(aq) + H^+$$

$$Zn(OH)_2(aq) + H_2O \Leftrightarrow Zn(OH)_3^- + H^+$$

$$Zn(OH)_3^- + H_2O \Leftrightarrow Zn(OH)_4^{2-} + H^+$$

The hydrolysis is defined with an **Ampholyte** node. Similar to the **Weak Acid** node, it sets up the mass balance accounting for the total of all reacting species, in this case: Zn^{2+}, $Zn(OH)^+$, $Zn(OH)_2(aq)$, $Zn(OH)_3^-$, and $Zn(OH)_4^{2-}$.

NaCl Salt Species

The film conductivity together with the salt dependent parameters requires the presence of sodium and chloride ions. Both ions are added to the model using the **Fully Dissociated Species** node.

Corrosion Products and Passivation

Corrosion products are formed and are considered to passivate the metallic surface. This example accounts for the formation of ZnO according to the following reaction:

$$Zn^{2+} + 2OH^- \Leftrightarrow ZnO(s) + H_2O$$

The reaction is defined as fully reversible (ZnO both precipitates and dissolves). It is defined as a reaction rate, R_{ZnO} (mol/(m^3·s)), in a **Reaction** node that is added at the **Highly Conductive Porous Electrode** nodes. The rate formulation is based on the corrosion product solubility, as follows:

$$R_{ZnO} = -\frac{k_{ZnO}}{L}(c_{Zn^{2+}}c_{OH^-}^2 - K_{S,ZnO}), \text{ if prec.; } (c_{Zn^{2+}}c_{OH^-}^2 - K_{SP,ZnO}) > 0 \qquad (4)$$

$$R_{ZnO} = -\theta\frac{k_{ZnO}}{L}(c_{Zn^{2+}}c_{OH^-}^2 - K_{S,ZnO}), \text{ if diss.; } (c_{Zn^{2+}}c_{OH^-}^2 - K_{SP,ZnO}) < 0 \qquad (5)$$

In the above, k_{ZnO} is the rate constant for the corrosion product conversion (mol/(m^2·s)) and $K_{S,ZnO}$ the equilibrium constant of the reaction.

The precipitated ZnO is set to cover the sample surface and assumed to inhibit (passivate) both electrochemical reactions. The ZnO coverage degree, θ, is assumed to change according to the following expression (Ref. 3):

$$\theta = 1 - e^{-\frac{m_{ZnO}}{m_{tot,surf}}} \qquad (6)$$

where m_{ZnO} is the precipitated molar amount of ZnO per surface area (mol/m^2) and $m_{tot,surf}$ is the molar metal surface availability per surface area and monolayer for ZnO precipitation. Note that with the use of the expression above more than $m_{tot,surf}$ needs to precipitate for the surface to become fully passivated.

The precipitated ZnO concentration in the film is defined using the **Dissolving–Depositing Species** at **Highly Conductive Porous Electrode** top nodes.

Dissolved Atmospheric Gases

Two atmospheric gases are accounted for.

Carbon dioxide dissolves into the film and affects the carbonate concentration and pH. The aqueous carbon dioxide saturation concentration, $c_{CO2,sat}$, depends on the partial pressure, p_{CO2}, together with temperature and the salt concentration (Ref. 1). A reaction source, $S_{carbonate}$ ($mol/(m^3{\cdot}s)$), is defined in a **Species Source** node for the carbonate species. The source minimizes the difference between the carbonate concentration in the film and the saturation concentration, as follows:

$$S_{carbonate} = \varepsilon \frac{k_{CO_2,sat}}{L}(c_{CO_2,sat}(p_{CO_2}, T, c_{NaCl}) - c_{CO_2(aq)}) \qquad (7)$$

In the expression, $k_{CO2,sat}$ is the rate constant for the carbon dioxide (1/s).

Oxygen dissolves into the film as well which affects the oxygen reduction reaction. The dissolved oxygen concentration is set equal to the saturation concentration that is dependent on the oxygen content in the atmosphere, temperature and salt concentration (compare with Atmospheric Corrosion example).

Spraying

During spraying, aqueous species concentrations are replaced with the compositions of the 1 wt% NaCl spray solution, $c_{i,spray}$. This is defined using **Species Source** nodes for the species. The generalized source expression used is as follows:

$$S_{NaCl} = k_{spray}(c_{i,\,spray} - c_i) \qquad (8)$$

The rate constant, k_{spray} (1/s), controls how well the solution is replenished.

Results and Discussion

Several variables are monitored during the run giving indications of the aggressiveness of the ACT (Figure 3, Figure 4, and Figure 5). In Figure 6 and Figure 7, the corrosion damage is shown in terms of loss of zinc coating mass and maximum decrease in coating thickness. At low RH the corrosion progresses very slowly. The precipitated amount of ZnO increases with time(Figure 6) and, as seen in both Figure 4 and Figure 7, acts to decrease the corrosion rate.

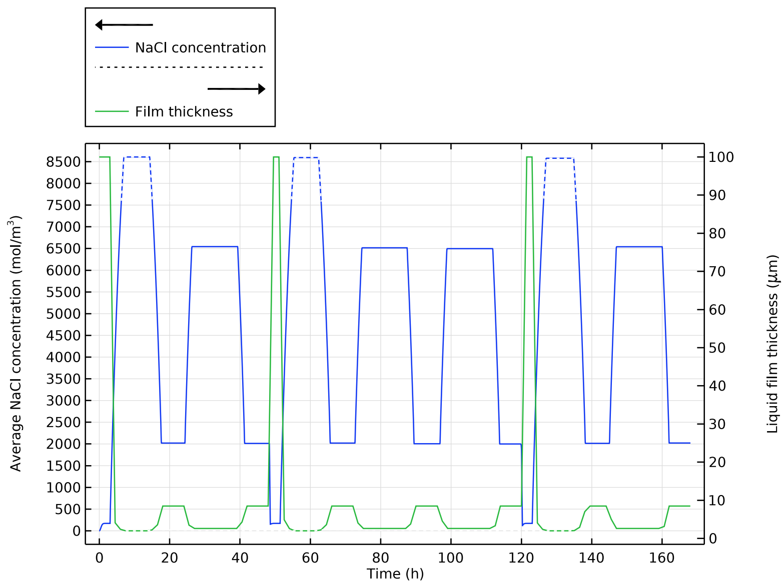


Figure 3: Salt concentration and liquid film thickness during ACT.

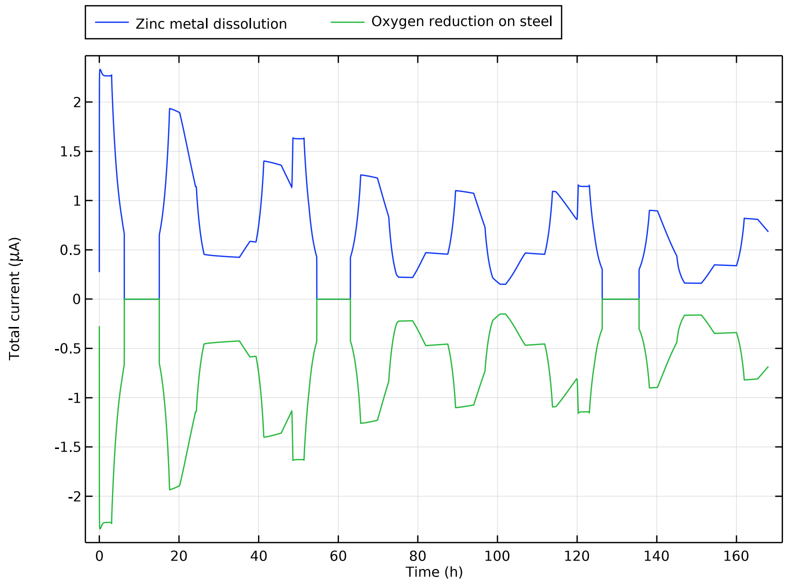


Figure 4: Total current of electrochemical reactions during ACT.

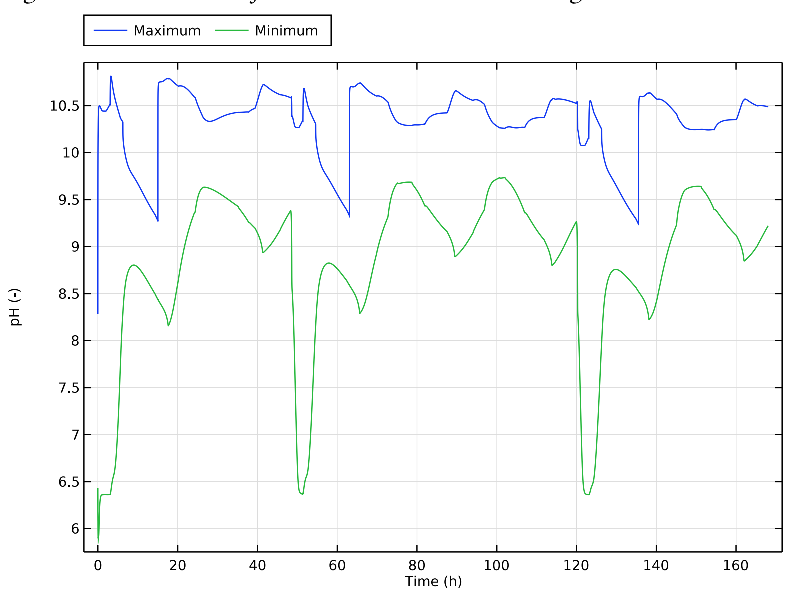


Figure 5: Maximum and minimum pH at sample during ACT.

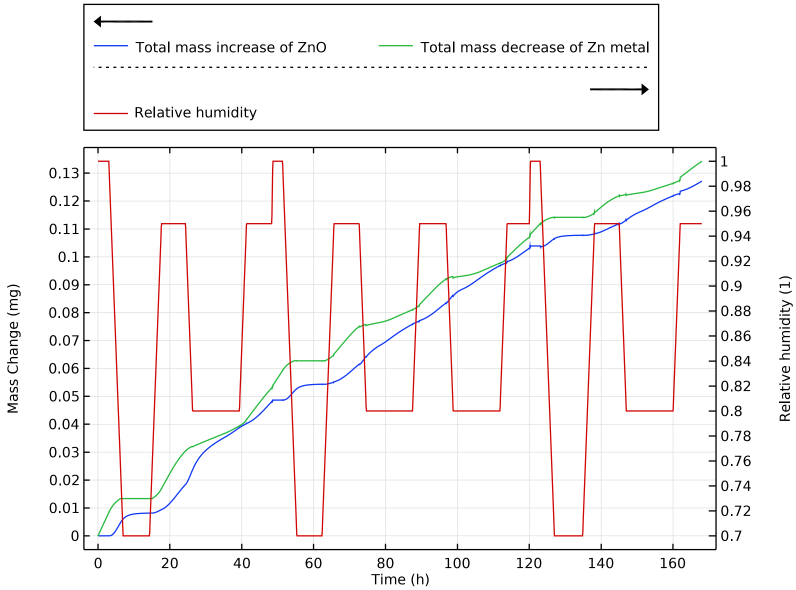


Figure 6: Mass changes over sample during ACT.

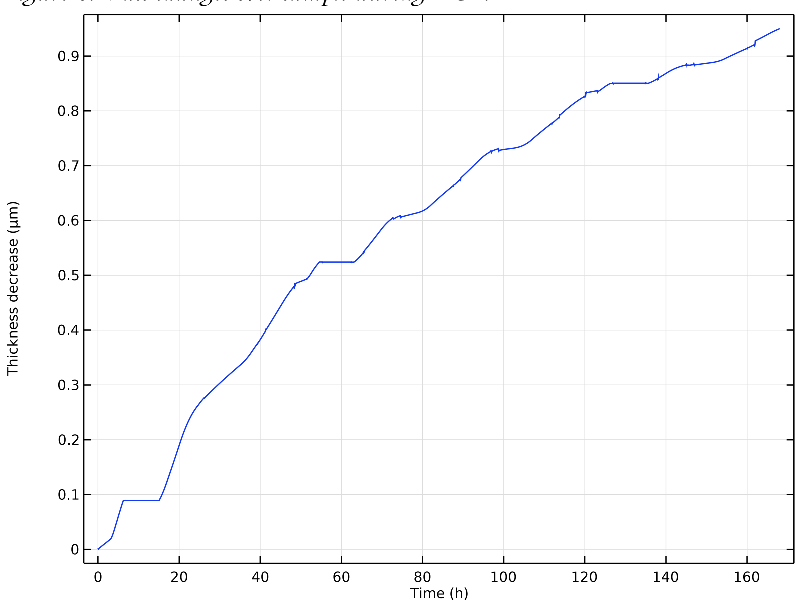


Figure 7: Maximum thickness decrease of coating during ACT.

The coating thickness after 7 days is shown in Figure 9. The coating is mainly consumed near the scratches and especially near the crossing of the scratches.

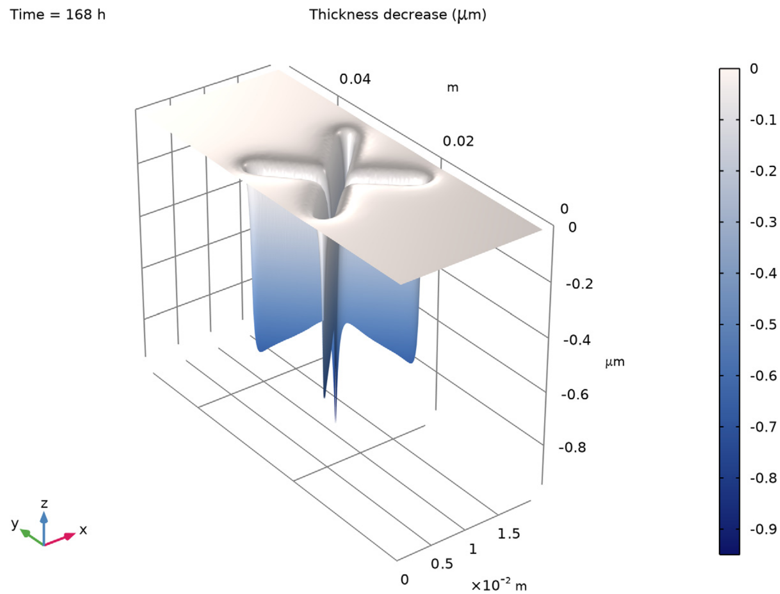


Figure 8: Local coating thickness decrease after 7 days.

The localized pH is displayed in Figure 9 for different times. The oxygen reduction reaction in the scratch keeps the pH basic there at all times, favoring passivation.

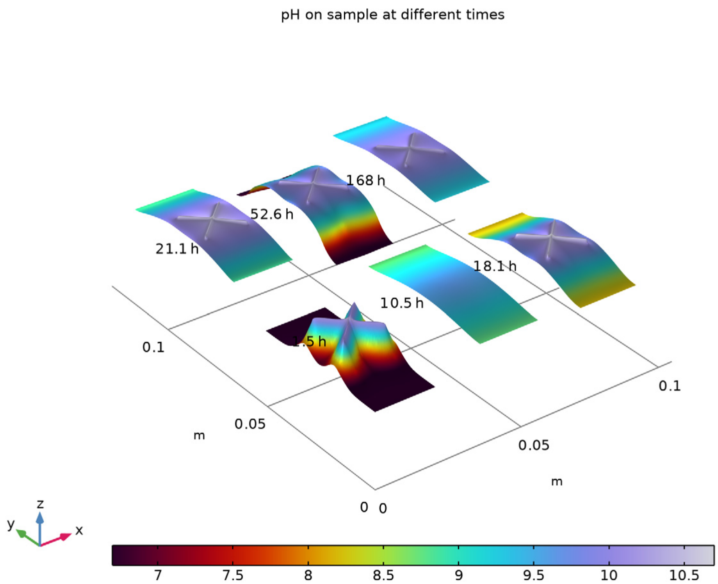


Figure 9: Local pH at the sample surface at different times during the ACT.

The corrosion product coverage after 7 days is substantial, as shown in Figure 10.

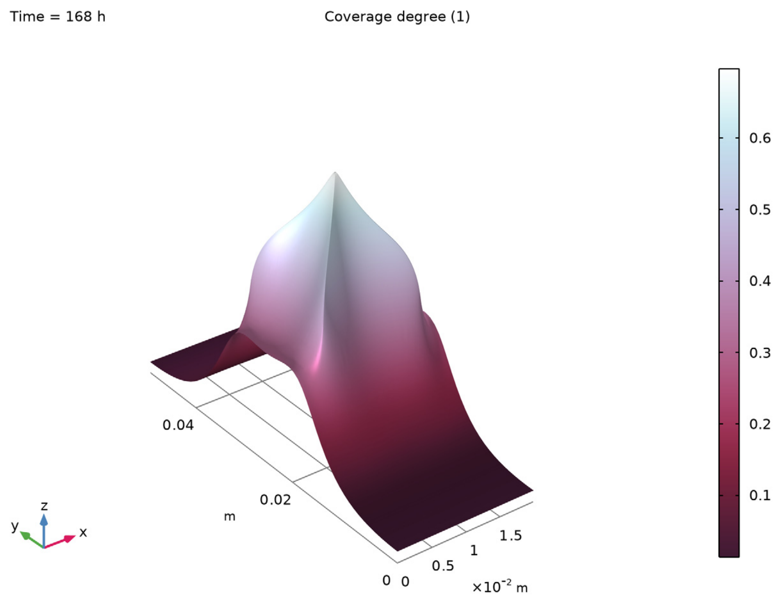


Figure 10: Local degree of coverage after 7 days.

References

1. 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. 443–455, 2023

2. V. Topa, A.S. Demeter, L. Hotoiu, D. Deconinck, and J. Deconinck, "A transient multi-ion transport model for galvanized steel corrosion protection," *Electrochimica Acta*, vol. 77, pp. 339–347, 2012.

3. T.G. Zavalis, M. Ström, D. Persson, E. Wendel, J. Ahlström, K.B. Törne, C. Taxén, B. Rendahl, J. Voltaire, K. Eriksson, D. Thierry, and J. Tidblad, "Mechanistic Model with Empirical Pitting Onset Approach for Detailed and Efficient Virtual Analysis of Atmospheric Bimetallic Corrosion," *Materials*, vol. 16, pp. 923–946, 2023.

Application Library path: `Corrosion_Module/Atmospheric_Corrosion/act_scratched_galvanized_steel`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 In the **Select Physics** tree, select **Electrochemistry** > **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 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 `act_scratched_galvanized_steel_parameters.txt`.

GEOMETRY 1

Draw the geometry.

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 `w_sample`.

4 In the **Height** text field, type `h_sample`.

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 `w_sample`.

4 In the **Height** text field, type `h_scratch`.

5 Locate the **Position** section. From the **Base** list, choose **Center**.

6 In the **x** text field, type `w_sample/2`.

7 In the **y** text field, type `h_sample/2`.

8 Locate the **Rotation Angle** section. In the **Rotation** text field, type `45`.

Rectangle 3 (r3)

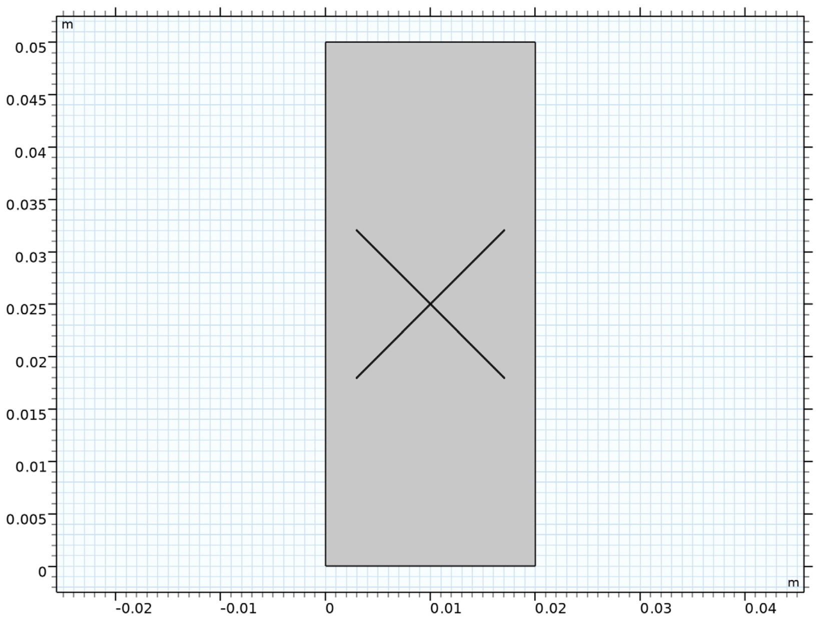
1 Right-click **Rectangle 2 (r2)** and choose **Duplicate**.

2 In the **Settings** window for **Rectangle**, locate the **Rotation Angle** section.

3 In the **Rotation** text field, type `315`.

4 Click **Build All Objects**.

Your geometry should now look like this:



Due to symmetry, only one quarter of the drawn geometry is modeled. The upper right corner is selected as model geometry.

Rectangle 4 (r4)

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 `w_sample/2`.

4 In the **Height** text field, type `h_sample`.

Rectangle 5 (r5)

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 `w_sample/2`.

4 In the **Height** text field, type `h_sample/2`.

5 Locate the **Position** section. In the **x** text field, type `w_sample/2`.

Difference 1 (dif1)

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

2 Select the objects **r1**, **r2**, and **r3** only.

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

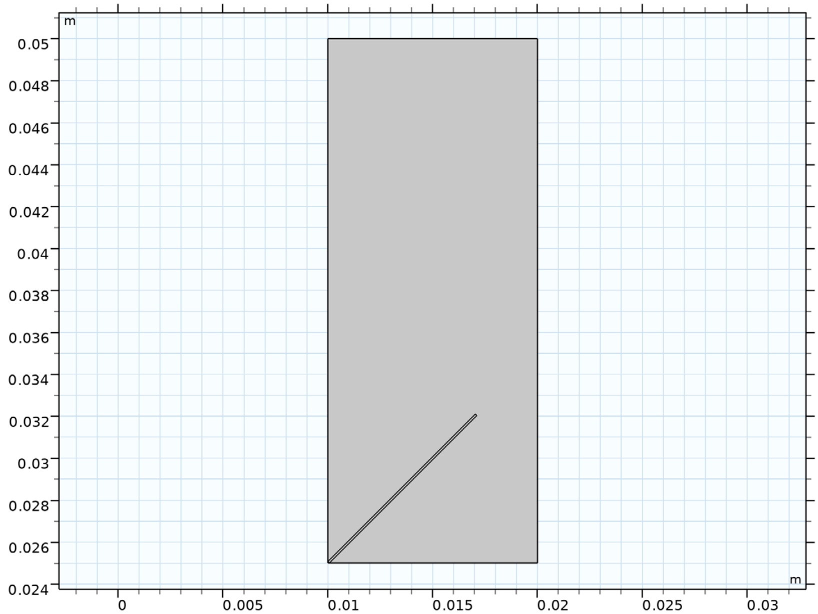
4 Click to select the **Activate Selection** toggle button for **Objects to subtract**.

5 Select the objects **r4** and **r5** only.

6 Click **Build All Objects**.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

Your model geometry should now look like this:



Make selections to help with the model setup.

DEFINITIONS

Zinc

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

2 In the **Settings** window for **Explicit**, type `Zinc` in the **Label** text field.

3 Select Domain 2 only.

Steel

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

2 In the **Settings** window for **Explicit**, type `Steel` in the **Label** text field.

3 Select Domains 1 and 3 only.

Wetted Surface

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

2 In the **Settings** window for **Explicit**, type `Wetted Surface` in the **Label** text field.

3 Locate the **Input Entities** section. Select the **All domains** checkbox.

Add some integration operators for probes and postprocessing.

Integration - Zinc

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

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

3 In the **Operator name** text field, type `intop_zinc`.

4 Locate the **Source Selection** section. From the **Selection** list, choose **Zinc**.

Integration - Steel

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

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

3 In the **Operator name** text field, type `intop_steel`.

4 Locate the **Source Selection** section. From the **Selection** list, choose **Steel**.

Integration - Wetted Surface

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

2 In the **Settings** window for **Integration**, type `Integration - Wetted Surface` in the **Label** text field.

3 In the **Operator name** text field, type `intop_wet`.

4 Locate the **Source Selection** section. From the **Selection** list, choose **Wetted Surface**.

The ACT cycle is added as three separate interpolation files. The first describes the variation in RH, the second temperature, and the third spraying periods over time. Use the piecewise cubic interpolation alternative for smoother transitions.

Interpolation - Relative Humidity

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

2 In the **Settings** window for **Interpolation**, type `Interpolation - Relative Humidity` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `RH_ACT`.

4 Click **Load from File**.

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

6 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.

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

Function	Unit
RH_ACT	1

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	s

Interpolation - Temperature

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

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

3 Locate the **Definition** section. In the **Function name** text field, type `T_ACT`.

4 Click **Load from File**.

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

6 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.

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

Function	Unit
T_ACT	K

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	s

Interpolation - Spray

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

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

3 Locate the **Definition** section. In the **Function name** text field, type `spray_ACT`.

4 Click **Load from File**.

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

6 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.

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

Function	Unit
spray_ACT	1

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	s

Add zinc and iron from the **Corrosion** branch in the **Material Library**.

ADD MATERIAL

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

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

3 In the tree, select **Corrosion** > **Elements** > **Fe in 3% NaCl**.

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

5 In the tree, select **Corrosion** > **Elements** > **Zn in aerated 3.5 wt% NaCl**.

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

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

MATERIALS

Fe in 3% NaCl (mat1)

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

2 From the **Selection** list, choose **Steel**.

Zn in aerated 3.5 wt% NaCl (mat2)

1 In the **Model Builder** window, click **Zn in aerated 3.5 wt% NaCl (mat2)**.

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

3 From the **Selection** list, choose **Zinc**.

Add variables describing the system. Unknown variables warnings will be resolved as soon as the physics have been set up.

DEFINITIONS

Variables - Global

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

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

3 Locate the **Variables** section. Click **Load from File**.

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

Variables - Rates

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

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

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Wetted Surface**.

5 Locate the **Variables** section. Click **Load from File**.

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

Variables - Film

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

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

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Wetted Surface**.

5 Locate the **Variables** section. Click **Load from File**.

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

Variables - Zinc

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

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

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Zinc**.

5 Locate the **Variables** section. Click **Load from File**.

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

Variables - Steel

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

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

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Steel**.

5 Locate the **Variables** section. Click **Load from File**.

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

Start defining the transport and reactions in the **Aqueous Electrolyte Transport** interface. The **Out-of-Plane Thickness** is set to the film thickness. Leave the default active setting **Include out-of-plane thickness in time-derivative in material balances** on the interface top node untouched. In this manner, species concentrations will change with the film thickness. The approach assumes that the film is so thin that no gradients exist along the thickness of the film.

AQUEOUS ELECTROLYTE TRANSPORT (AQT)

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

2 In the **Settings** window for **Aqueous Electrolyte Transport**, locate the **Out-of-Plane Thickness** section.

3 In the d_z text field, type `d_film`.

Electrolyte 1

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

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

3 From the T list, choose **User defined**. In the associated text field, type `T_ACT(t)`.

4 Locate the **Proton and Hydroxide Ion Transport Properties** section. In the D_{H^+} text field, type `DH`.

5 In the D_{OH^-} text field, type `DOH`.

Use an **Ampholyte** node to model the hydrolysis equilibrium reactions of the aqueous zinc species.

Ampholyte - Zinc

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

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

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

4 In the k text field, type `4`.

5 In the table, enter the following settings:

Dissociation step (1)	pKa (1)
1	`-log10(K_Znstep1)`
2	`-log10(K_Znstep2)`
3	`-log10(K_Znstep3)`
4	`-log10(K_Znstep4)`

6 In the z_0 text field, type `-2`.

7 Locate the **Diffusion and Migration** section. In the D text field, type `DZn`.

Use a **Carbonic Acid** node to model the carbonic acid dissociation.

Electrolyte 1

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

Carbonic Acid 1

1 In the **Settings** window for **Carbonic Acid**, locate the **Diffusion and Migration** section.

2 In the $D_{\mathrm{CO2(aq)}}$ text field, type `DCO2aq`.

3 In the D_{H2CO3} text field, type `DH2CO3`.

4 In the D_{HCO3^-} text field, type `DHCO3`.

5 In the $D_{\mathrm{CO3}^{2-}}$ text field, type `DCO3`.

Add the NaCl as two fully dissociated species, sodium and chloride ions, with the **Fully Dissociated Species** node.

Electrolyte 1

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

Fully Dissociated Species - Na

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

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

3 In the z text field, type `1`.

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

Electrolyte 1

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

Fully Dissociated Species - Cl

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

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

3 In the z text field, type `-1`.

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

Initial Values 1

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 $\phi_{l,0}$ text field, type `V0`.

4 Locate the **Concentration** section. In the $c_{H2CO3,0}$ text field, type `cCO2aq0`.

5 In the $c_{Na,0}$ text field, type `cNaCl0`.

6 In the $c_{Cl,0}$ text field, type `cNaCl0`.

Local electrochemical reactions are incorporated using the **Highly Conductive Porous Electrode** nodes. These reactions are user-defined, with the material properties for zinc and steel being imported accordingly. Additionally, the Dissolving–Depositing Species feature is used to account for the effects of corrosion product formation as well as metal dissolution and deposition.

Highly Conductive Porous Electrode - Steel

1 In the **Physics** toolbar, click **Domains** and choose **Highly Conductive Porous Electrode**.

2 In the **Settings** window for **Highly Conductive Porous Electrode**, type `Highly Conductive Porous Electrode - Steel` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Steel**.

Leave the **Electrolyte volume fraction** as it is (1) to define that the entire domain contains electrolyte solution only.

4 Click to expand the **Dissolving–Depositing Species** section. Click **Add**.

5 In the table, enter the following settings:

Species name	Molar volume (m^3/mol)	Initial concentration (mol/m^3)
`ZnO`	`Vm_ZnO`	`0[mol/m^3]`

6 Clear the **Subtract volume change from electrolyte volume fraction** checkbox.

Porous Electrode Reaction 1

1 In the **Model Builder** window, expand the **Highly Conductive Porous Electrode - Steel** node, then click **Porous Electrode Reaction 1**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Model Input** section.

3 From the T list, choose **User defined**. In the associated text field, type `T_ACT(t)`.

4 Locate the **Stoichiometric Coefficients** section. In the ν_{OH^-} text field, type `2`.

5 Locate the **Electrode Kinetics** section. From the $i_{loc,expr}$ list, choose **User defined**. In the associated text field, type `i_red`.

Set the **Active Species Surface Area** to the inverse of the film thickness to define the **Highly Conductive Porous Electrode** as a thin liquid film.

6 Locate the **Active Specific Surface Area** section. In the a_v text field, type `1/d_film`.

Define the ZnO corrosion product formation by adding a **Reactions** subnode.

Highly Conductive Porous Electrode - Steel

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

Reaction - ZnO Corrosion Product

1 In the **Settings** window for **Reaction**, type `Reaction - ZnO Corrosion Product` in the **Label** text field.

2 Locate the **Reaction Rate** section. In the R text field, type `R_ZnO`.

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

4 In the ν_{OH^-} text field, type `-2`.

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

Species name	Stoichiometric coefficient (1)
ZnO	1

Highly Conductive Porous Electrode - Zinc

1 In the **Physics** toolbar, click **Domains** and choose **Highly Conductive Porous Electrode**.

2 In the **Settings** window for **Highly Conductive Porous Electrode**, type `Highly Conductive Porous Electrode - Zinc` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Zinc**.

4 Click to expand the **Dissolving–Depositing Species** section. Click + **Add**.

5 In the table, enter the following settings:

Species name	Molar volume (m^3/mol)	Initial concentration (mol/m^3)
Zn	Vm_Zn	0[mol/m^3]

6 Click + **Add**.

7 In the table, enter the following settings:

Species name	Molar volume (m^3/mol)	Initial concentration (mol/m^3)
ZnO	Vm_ZnO	0[mol/m^3]

8 Clear the **Subtract volume change from electrolyte volume fraction** checkbox.

Porous Electrode Reaction 1

1 In the **Model Builder** window, expand the **Highly Conductive Porous Electrode - Zinc** node, then click **Porous Electrode Reaction 1**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Model Input** section.

3 From the T list, choose **User defined**. In the associated text field, type `T_ACT(t)`.

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

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

Species name	Stoichiometric coefficient (1)
Zn	1

6 Locate the **Electrode Kinetics** section. From the $i_{loc,expr}$ list, choose **User defined**. In the associated text field, type `i_ox`.

7 Locate the **Active Specific Surface Area** section. In the a_v text field, type `1/d_film`.

Highly Conductive Porous Electrode - Zinc

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

Reaction - ZnO Corrosion Product

1 In the **Settings** window for **Reaction**, type `Reaction - ZnO Corrosion Product` in the **Label** text field.

2 Locate the **Reaction Rate** section. In the R text field, type `R_ZnO`.

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

4 In the $\nu_{OH}{}^{-}$ text field, type `-2`.

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

Species name	Stoichiometric coefficient (1)
ZnO	1

Add **Species Source** nodes to model atmospheric carbon dioxide dissolution and spraying.

Species Source - Atmospheric Carbon Dioxide Dissolution

1 In the **Physics** toolbar, click **Domains** and choose **Species Source**.

2 In the **Settings** window for **Species Source**, type `Species Source - Atmospheric Carbon Dioxide Dissolution` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Wetted Surface**.

4 Locate the **Species Sources** section. In the $R_{CO2(aq)}$ text field, type `R_CO2`.

Species Source - Spraying

1 In the **Physics** toolbar, click **Domains** and choose **Species Source**.

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

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Wetted Surface**.

4 Locate the **Species Sources** section. In the $R_{Zn(OH)4}{}^{2-}$ text field, type `RSpray_ZnOH4`.

5 In the $R_{Zn(OH)3}{}^{-}$ text field, type `RSpray_ZnOH3`.

6 In the $R_{Zn(OH)2}$ text field, type `RSpray_ZnOH2`.

7 In the $R_{ZnOH}{}^{+}$ text field, type `RSpray_ZnOH`.

8 In the $R_{Zn}{}^{2+}$ text field, type `RSpray_Zn`.

9 In the $R_{CO3}{}^{2-}$ text field, type `RSpray_CO3`.

10 In the $R_{HCO3}{}^{-}$ text field, type `RSpray_HCO3`.

11 In the R_{H2CO3} text field, type `RSpray_H2CO3`.

12 In the $R_{CO2(aq)}$ text field, type `RSpray_CO2aq`.

13 In the $R_{Na}{}^{+}$ text field, type `RSpray_Na`.

14 In the $R_{Cl}{}^{-}$ text field, type `RSpray_Cl`.

15 In the $R_{H}{}^{+}$ text field, type `RSpray_H`.

16 In the R_{OH^-} text field, type `RSpray_OH`.

DEFINITIONS

Ramp - Deliquescence Limit

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local > Ramp**.

2 In the **Settings** window for **Ramp**, type `Ramp - Deliquescence Limit` in the **Label** text field.

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

4 Locate the **Parameters** section. In the **Location** text field, type `ramp_loc`.

5 In the **Slope** text field, type `ramp_sl`.

6 Select the **Cutoff** checkbox. In the associated text field, type `ramp_co`.

7 Click to expand the **Smoothing** section.

8 Select the **Size of transition zone at start** checkbox. In the associated text field, type `ramp_sm`.

9 Select the **Size of transition zone at cutoff** checkbox. In the associated text field, type `ramp_sm`.

Add probes to monitor various behaviors during the ACT simulation and to reduce the amount of saved output data.

Global Variable Probe - ZnO

1 In the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe - ZnO` in the **Label** text field.

3 In the **Variable name** text field, type `var_ZnO`.

4 Locate the **Expression** section. In the **Expression** text field, type `m_ZnO`.

5 From the **Table and plot unit** list, choose **mg**.

6 Select the **Description** checkbox.

7 Click to expand the **Table and Window Settings** section. Click **+ Add Table**.

8 Click **+ Add Plot Window**.

Global Variable Probe - Zinc Metal

1 In the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe - Zinc Metal` in the **Label** text field.

3 In the **Variable name** text field, type `var_m_Zn`.

4 Locate the **Expression** section. In the **Expression** text field, type `-m_Zn`.

5 From the **Table and plot unit** list, choose **mg**.

6 Select the **Description** checkbox.

7 Locate the **Table and Window Settings** section. From the **Output table** list, choose **Table 1**.

8 From the **Plot window** list, choose **Probe Plot 1**.

Global Variable Probe - Total Zinc Metal Dissolution Current

1 In the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe - Total Zinc Metal Dissolution Current` in the **Label** text field.

3 In the **Variable name** text field, type `var_I_ox`.

4 Locate the **Expression** section. In the **Expression** text field, type `I_ox`.

5 From the **Table and plot unit** list, choose **µA**.

6 Select the **Description** checkbox.

7 Locate the **Table and Window Settings** section. Click **Add Table**.

8 Click **Add Plot Window**.

Global Variable Probe - Total Oxygen Reduction Current

1 In the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe - Total Oxygen Reduction Current` in the **Label** text field.

3 In the **Variable name** text field, type `var_I_red`.

4 Locate the **Expression** section. In the **Expression** text field, type `I_red`.

5 From the **Table and plot unit** list, choose **µA**.

6 Select the **Description** checkbox.

7 Locate the **Table and Window Settings** section. From the **Output table** list, choose **Table 2**.

8 From the **Plot window** list, choose **Probe Plot 2**.

Domain Probe - Maximum Zinc Coating Thickness Loss

1 In the **Definitions** toolbar, click **Probes** and choose **Domain Probe**.

2 In the **Settings** window for **Domain Probe**, type `Domain Probe - Maximum Zinc Coating Thickness Loss` in the **Label** text field.

3 In the **Variable name** text field, type `dom_d_Zn`.

4 Locate the **Probe Type** section. From the **Type** list, choose **Maximum**.

5 Locate the **Source Selection** section. From the **Selection** list, choose **Zinc**.

6 Locate the **Expression** section. In the **Expression** text field, type `-d_Zn`.

7 From the **Table and plot unit** list, choose **µm**.

8 Select the **Description** checkbox.

9 Click to expand the **Table and Window Settings** section. Click **Add Table**.

10 Click **Add Plot Window**.

Domain Probe - Maximum pH

1 In the **Definitions** toolbar, click **Probes** and choose **Domain Probe**.

2 In the **Settings** window for **Domain Probe**, type `Domain Probe - Maximum pH` in the **Label** text field.

3 In the **Variable name** text field, type `dom_maxpH`.

4 Locate the **Probe Type** section. From the **Type** list, choose **Maximum**.

5 Locate the **Table and Window Settings** section. Click **Add Table**.

6 Click **Add Plot Window**.

Domain Probe - Minimum pH

1 Right-click **Domain Probe - Maximum pH** and choose **Duplicate**.

2 In the **Settings** window for **Domain Probe**, type `Domain Probe - Minimum pH` in the **Label** text field.

3 In the **Variable name** text field, type `dom_minpH`.

4 Locate the **Probe Type** section. From the **Type** list, choose **Minimum**.

Domain Probe - Average NaCl Concentration in Liquid Film

1 In the **Definitions** toolbar, click **Probes** and choose **Domain Probe**.

2 In the **Settings** window for **Domain Probe**, type `Domain Probe - Average NaCl Concentration in Liquid Film` in the **Label** text field.

3 In the **Variable name** text field, type `dom_cNaCl`.

4 Locate the **Expression** section. In the **Expression** text field, type `cNaCl`.

5 Locate the **Table and Window Settings** section. Click **Add Table**.

6 Click **Add Plot Window**.

Now, adjust the solver configurations for this model.

STUDY 1

Step 1: Current Distribution Initialization

1 In the **Model Builder** window, under **Study 1** click **Step 1: Current Distribution Initialization**.
2 In the **Settings** window for **Current Distribution Initialization**, locate the **Study Settings** section.
3 From the **Current distribution type** list, choose **Secondary**.

Step 2: Time Dependent

1 In the **Model Builder** window, click **Step 2: Time Dependent**.
2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
3 From the **Time unit** list, choose **h**.
4 In the **Output times** text field, type `range(0,1.5,24*7)`.

Set the solver time-stepping to a value lower than the distinct periods of the ACT.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.
2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.
3 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.
4 From the **Times to store** list, choose **Steps taken by solver closest to output times**.
5 Click to expand the **Time Stepping** section. From the **Maximum step constraint** list, choose **Constant**.
6 In the **Home** toolbar, click **Compute**.

RESULTS

The model has solved now. Start polishing the automatically created probe plots. All figures and their description can also be found in the model documentation above.

Mass Change on Full Sample

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 1**.
2 In the **Settings** window for **1D Plot Group**, type `Mass Change on Full Sample` in the **Label** text field.
3 Click to expand the **Title** section. From the **Title type** list, choose **None**.
4 Locate the **Plot Settings** section.
5 Select the **y-axis label** checkbox. In the associated text field, type `Mass Change (mg)`.

6 Select the **Two y-axes** checkbox.

7 Select the **Secondary y-axis label** checkbox. In the associated text field, type `Relative humidity (1)`.

8 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

9 From the **Position** list, choose **Top**.

Probe Table Graph 1

1 In the **Model Builder** window, expand the **Mass Change on Full Sample** node, then click **Probe Table Graph 1**.

2 In the **Settings** window for **Table Graph**, click to expand the **Legends** section.

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

4 In the table, enter the following settings:

Legends
Total mass increase of ZnO
Total mass decrease of Zn metal

Mass Change on Full Sample

In the **Mass Change on Full Sample** toolbar, click **Global**.

Global 1

1 In the **Settings** window for **Global**, locate the **Data** section.

2 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

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

4 In the **Times (h)** text field, type `range(0,0.1,24*7)`.

5 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** checkbox.

6 Locate the **y-Axis Data** section. In the table, enter the following settings:

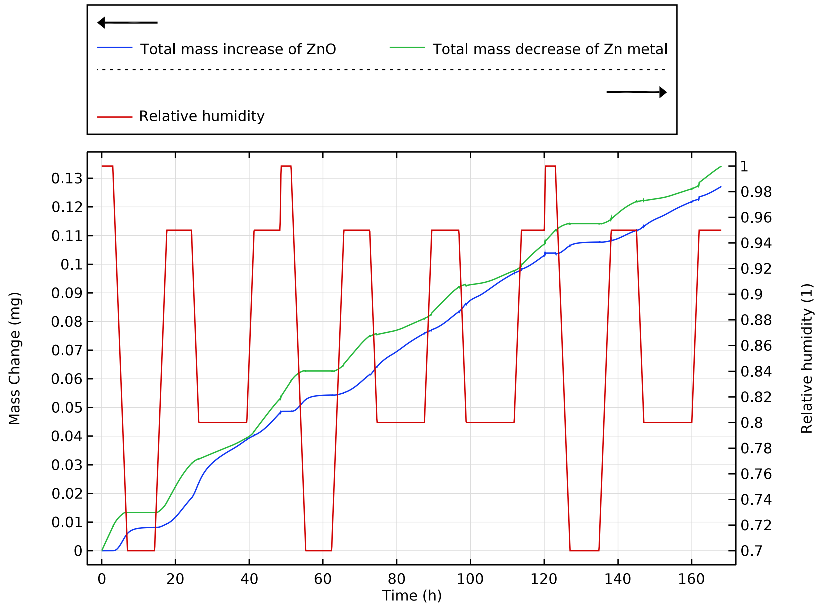
Expression	Unit	Description
RH_ACT(t)	1	Interpolation - Relative Humidity

7 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

8 In the table, enter the following settings:

Legends
Relative humidity

9 In the **Mass Change on Full Sample** toolbar, click **Plot**.



Total Current on Full Sample

1. In the **Model Builder** window, under **Results** click **Probe Plot Group 2**.
2. In the **Settings** window for **1D Plot Group**, type `Total Current on Full Sample` in the **Label** text field.
3. Locate the **Plot Settings** section.
4. Select the **y-axis label** checkbox. In the associated text field, type `Total current (\mu A)`.
5. Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.
6. From the **Position** list, choose **Top**.

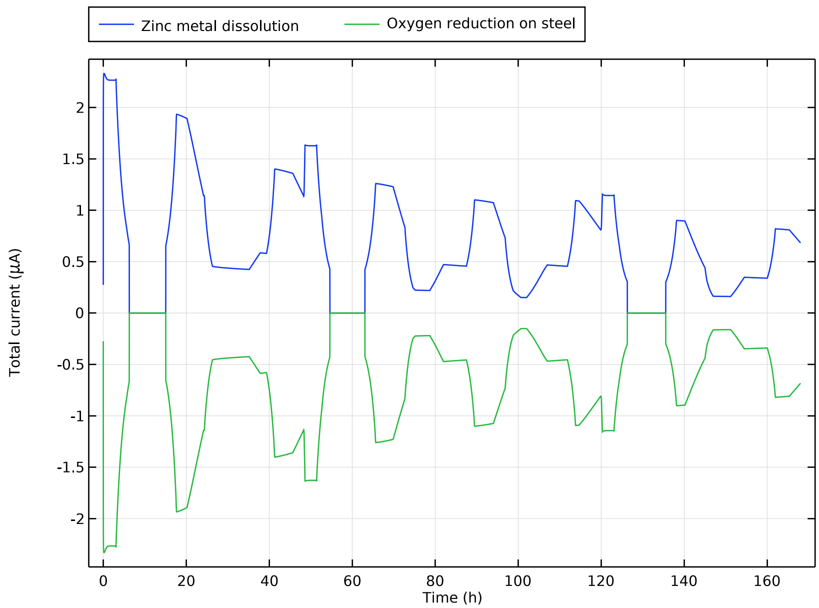
Probe Table Graph 1

1. In the **Model Builder** window, expand the **Total Current on Full Sample** node, then click **Probe Table Graph 1**.
2. In the **Settings** window for **Table Graph**, locate the **Legends** section.
3. From the **Legends** list, choose **Manual**.

4 In the table, enter the following settings:

Legends
`Zinc metal dissolution`
`Oxygen reduction on steel`

5 In the **Total Current on Full Sample** toolbar, click **Plot**.



Maximum Decrease Coating Thickness

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 3**.

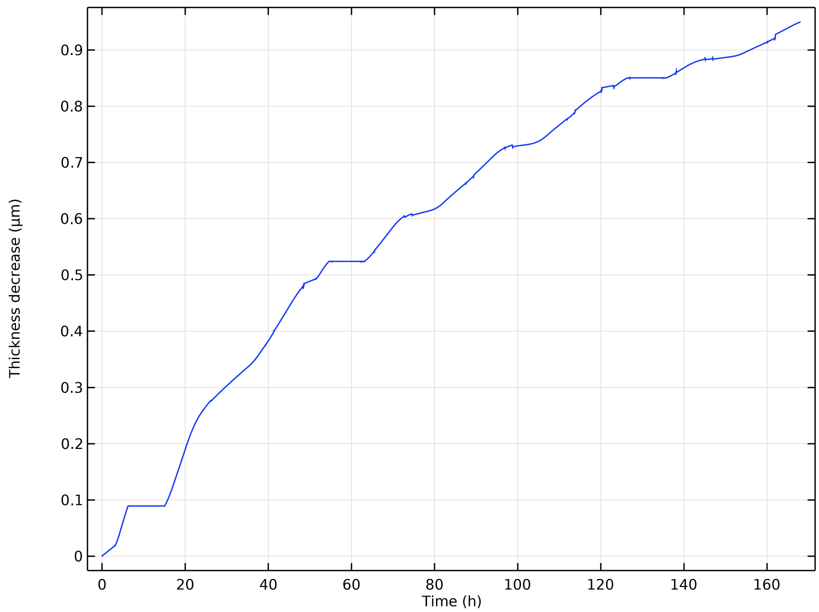
2 In the **Settings** window for **1D Plot Group**, type `Maximum Decrease Coating Thickness` in the **Label** text field.

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** checkbox. In the associated text field, type `Thickness decrease (µm)`.

5 Locate the **Legend** section. Clear the **Show legends** checkbox.

6 In the **Maximum Decrease Coating Thickness** toolbar, click **Plot**.



pH Limits in Film

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 4**.

2 In the **Settings** window for **1D Plot Group**, type `pH Limits in Film` in the **Label** text field.

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** checkbox. In the associated text field, type `pH (-)`.

5 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

6 From the **Position** list, choose **Top**.

Probe Table Graph 1

1 In the **Model Builder** window, expand the **pH Limits in Film** node, then click **Probe Table Graph 1**.

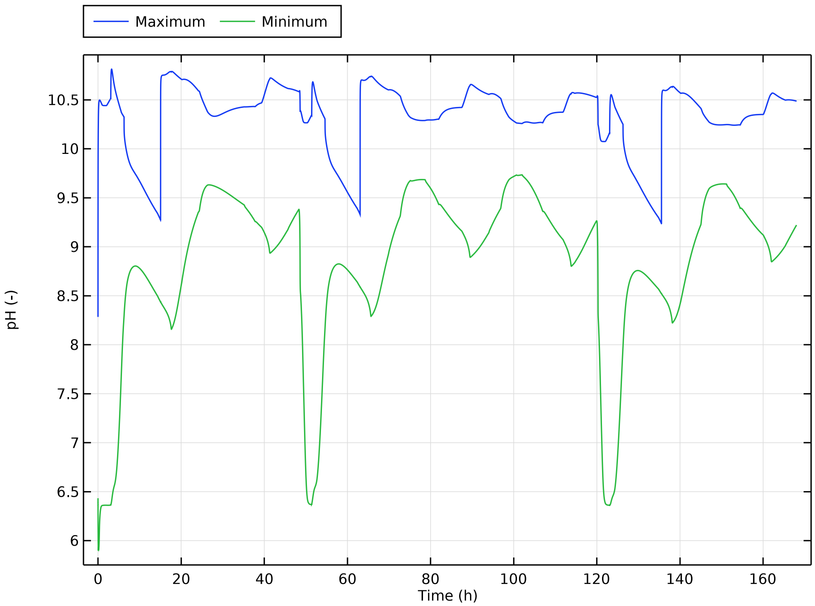
2 In the **Settings** window for **Table Graph**, locate the **Legends** section.

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

4 In the table, enter the following settings:

Legends
`Maximum`
`Minimum`

5 In the **pH Limits in Film** toolbar, click **Plot**.



Average NaCl Concentration and Liquid Film Thickness

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 5**.

2 In the **Settings** window for **1D Plot Group**, type `Average NaCl Concentration and Liquid Film Thickness` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** checkbox. In the associated text field, type `Average NaCl concentration (mol/m<sup>3</sup>)`.

6 Select the **Two y-axes** checkbox.

7 Select the **Secondary y-axis label** checkbox. In the associated text field, type `Liquid film thickness (\mu m)`.

8 Locate the **Grid** section. Clear the **Show grid** checkbox.

9 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

10 From the **Position** list, choose **Top**.

Probe Table Graph 1

1 In the **Model Builder** window, expand the **Average NaCl Concentration and Liquid Film Thickness** node, then click **Probe Table Graph 1**.

2 In the **Settings** window for **Table Graph**, locate the **Legends** section.

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

4 In the table, enter the following settings:

Legends
NaCl concentration

Probe Table Graph 1.1

1 Right-click **Probe Table Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Table Graph**, click to expand the **Preprocessing** section.

3 Find the **y-axis columns** subsection. From the **Range** list, choose **Manual**.

4 In the **y minimum** text field, type `cNaCl_deliq`.

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

6 From the **Color** list, choose **White**.

7 Locate the **Legends** section. Clear the **Show legends** checkbox.

Average NaCl Concentration and Liquid Film Thickness

In the **Average NaCl Concentration and Liquid Film Thickness** toolbar, click **Global**.

Global 1

1 In the **Settings** window for **Global**, locate the **Data** section.

2 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

3 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** checkbox.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
d_film	um	Liquid film thickness with RH

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Film thickness`

Global 2

1 Right-click **Results** > **Average NaCl Concentration and Liquid Film Thickness** > **Global 1** and choose **Duplicate**.

2 In the **Settings** window for **Global**, click to expand the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Line** list, choose **Dotted**.

4 From the **Color** list, choose **White**.

5 Locate the **Legends** section. Clear the **Show legends** checkbox.

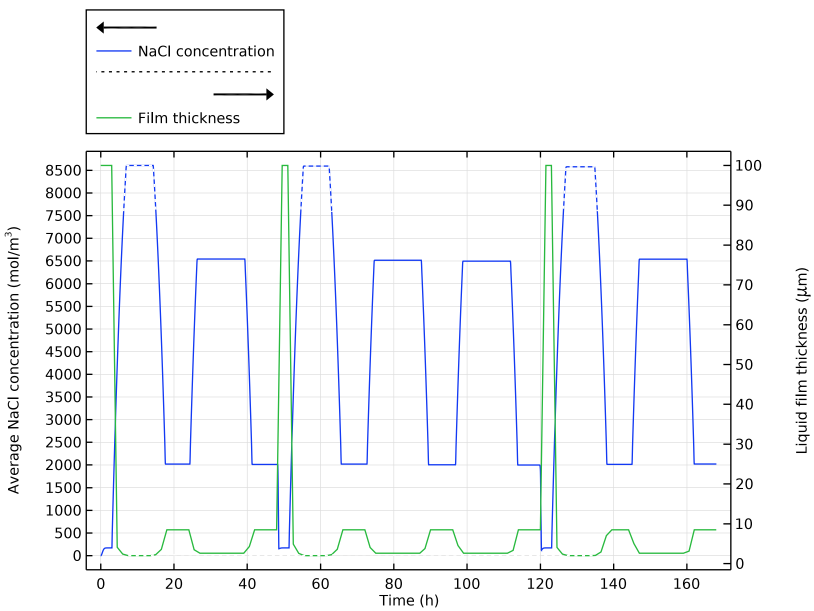
Filter 1

1 In the **Average NaCl Concentration and Liquid Film Thickness** toolbar, click **Filter**.

2 In the **Settings** window for **Filter**, locate the **Point Selection** section.

3 In the **Logical expression for inclusion** text field, type `RH_ACT(t)<RH_deliq`.

4 In the **Average NaCl Concentration and Liquid Film Thickness** toolbar, click **Plot**.



The following steps create a plot illustrating the ACT that is simulated.

ACT

1 In the **Results** toolbar, click **1D Plot Group**.
2 In the **Settings** window for **1D Plot Group**, type ACT in the **Label** text field.
3 Locate the **Title** section. From the **Title type** list, choose **None**.
4 Locate the **Data** section. From the **Time selection** list, choose **Interpolated**.
5 In the **Times (h)** text field, type range(0,0.1,24*7).
6 Locate the **Plot Settings** section. Select the **x-axis label** checkbox.
7 Select the **y-axis label** checkbox. In the associated text field, type Relative humidity (1).
8 Select the **Two y-axes** checkbox.
9 Select the **Secondary y-axis label** checkbox. In the associated text field, type Temperature (K).
10 Locate the **Grid** section. Clear the **Show grid** checkbox.
11 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.
12 From the **Position** list, choose **Top**.

Global 1

1 In the **ACT** toolbar, click **Global**.
2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
3 In the table, enter the following settings:

Expression	Unit	Description
RH_ACT(t)	1	Interpolation - Relative Humidity

4 Locate the **Legends** section. From the **Legends** list, choose **Manual**.
5 In the table, enter the following settings:

Legends
Relative humidity

Global 2

1 Right-click **Global 1** and choose **Duplicate**.
2 In the **Settings** window for **Global**, locate the **Coloring and Style** section.
3 Find the **Line style** subsection. From the **Line** list, choose **None**.
4 From the **Color** list, choose **Black**.
5 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.

6 Locate the **Legends** section. Clear the **Show legends** checkbox.

Filter 1

1 In the **ACT** toolbar, click **Filter**.

2 In the **Settings** window for **Filter**, locate the **Point Selection** section.

3 In the **Logical expression for inclusion** text field, type `spray_ACT(t)>0.5`.

Global 1, Global 2

1 In the **Model Builder** window, under **Results** > **ACT**, Ctrl-click to select **Global 1** and **Global 2**.

2 Right-click and choose **Duplicate**.

Global 3

1 In the **Settings** window for **Global**, locate the **y-Axis** section.

2 Select the **Plot on secondary y-axis** checkbox.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
T_ACT(t)	K	Interpolation - Temperature

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

Legends
Temperature

Global 4

1 In the **Model Builder** window, click **Global 4**.

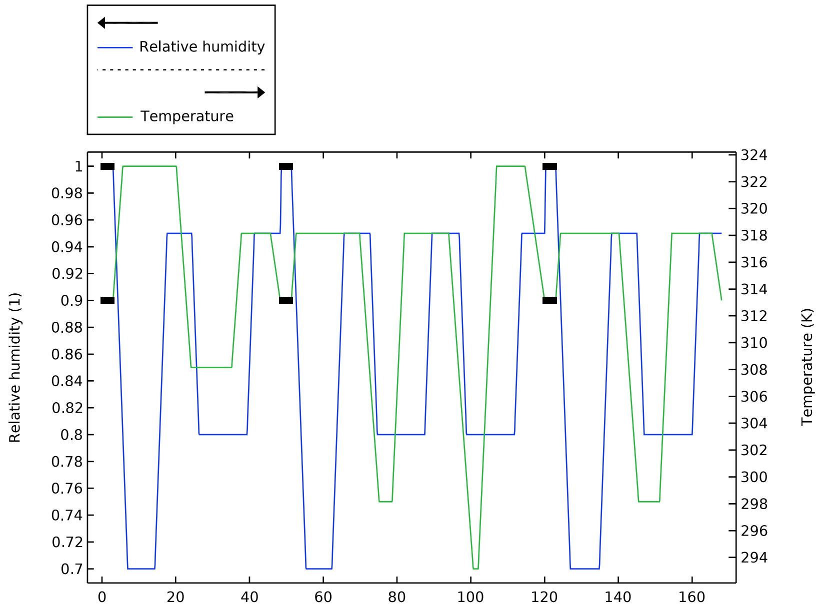
2 In the **Settings** window for **Global**, locate the **y-Axis** section.

3 Select the **Plot on secondary y-axis** checkbox.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
T_ACT(t)	K	Interpolation - Temperature

5 In the **ACT** toolbar, click **Plot**.



The following steps create 2D plots for better display of local variations at the surface. Use a **Sector 2D** dataset that can visualize the results over the whole sample surface.

Sector 2D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Sector 2D**.

2 In the **Settings** window for **Sector 2D**, locate the **Axis Data** section.

3 In the **X** text field, type `w_sample/2`.

4 In the **Y** text field, type `h_sample/2`.

5 Locate the **Symmetry** section. In the **Number of sectors** text field, type `4`.

6 From the **Transformation** list, choose **Rotation and reflection**.

pH Full Sample

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **None**.

4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `pH on sample at different times`.

6 Clear the **Parameter indicator** text field.

7 Locate the **Color Legend** section. From the **Position** list, choose **Bottom**.

8 Click to expand the **Plot Array** section. From the **Array type** list, choose **Square**.

Surface 1

1 In the **pH Full Sample** toolbar, click **Surface with Height**.

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

3 From the **Dataset** list, choose **Sector 2D 1**.

4 From the **Time (h)** list, choose **1.5319**.

5 Click to expand the **Range** section. Select the **Manual color range** checkbox.

6 In the **Minimum** text field, type `6.7`.

7 In the **Maximum** text field, type `10.7`.

8 Locate the **Coloring and Style** section. From the **Color table** list, choose **PrismDark**.

9 From the **Color table transformation** list, choose **Reverse**.

Height Expression 1

1 In the **Model Builder** window, expand the **Surface 1** node, then click **Height Expression 1**.

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

3 Clear the **Show height axis** checkbox.

Surface 2

1 In the **Model Builder** window, under **Results** > **pH Full Sample** right-click **Surface 1** and choose **Duplicate**.

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

3 From the **Time (h)** list, choose **10.518**.

4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

Surface 3

1 Right-click **Surface 2** and choose **Duplicate**.

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

3 From the **Time (h)** list, choose **18.055**.

Surface 4

1 Right-click **Surface 3** and choose **Duplicate**.

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

3 From the **Time (h)** list, choose **21.055**.

Surface 5

1 Right-click **Surface 4** and choose **Duplicate**.

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

3 From the **Time (h)** list, choose **52.563**.

Surface 6

1 Right-click **Surface 5** and choose **Duplicate**.

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

3 From the **Time (h)** list, choose **Last (168)**.

4 Click the **Zoom Extents** button in the **Graphics** toolbar.

Annotation 1

1 In the **Model Builder** window, right-click **pH Full Sample** and choose **Annotation**.

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

3 From the **Dataset** list, choose **Sector 2D 1**.

4 From the **Time (h)** list, choose **1.5319**.

5 Locate the **Annotation** section. In the **Text** text field, type `eval(t,h) h`.

6 Click to expand the **Advanced** section. Clear the **Show trailing zeros** checkbox.

7 In the **Precision** text field, type `2`.

8 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

9 From the **Anchor point** list, choose **Upper right**.

10 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

11 In the **Row index** text field, type `1`.

12 In the **Column index** text field, type `1`.

Annotation 2

1 Right-click **Annotation 1** and choose **Duplicate**.

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

3 From the **Time (h)** list, choose **10.518**.

4 Locate the **Advanced** section. In the **Precision** text field, type `3`.

5 Locate the **Plot Array** section. In the **Column index** text field, type `2`.

Annotation 3

1 Right-click **Annotation 2** and choose **Duplicate**.

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

3 From the **Time (h)** list, choose **18.055**.

4 Locate the **Plot Array** section. In the **Column index** text field, type 3.

Annotation 4

1 Right-click **Annotation 3** and choose **Duplicate**.

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

3 From the **Time (h)** list, choose **21.055**.

4 Locate the **Plot Array** section. In the **Row index** text field, type 2.

5 In the **Column index** text field, type 1.

Annotation 5

1 Right-click **Annotation 4** and choose **Duplicate**.

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

3 From the **Time (h)** list, choose **52.563**.

4 Locate the **Plot Array** section. In the **Column index** text field, type 2.

Annotation 6

1 Right-click **Annotation 5** and choose **Duplicate**.

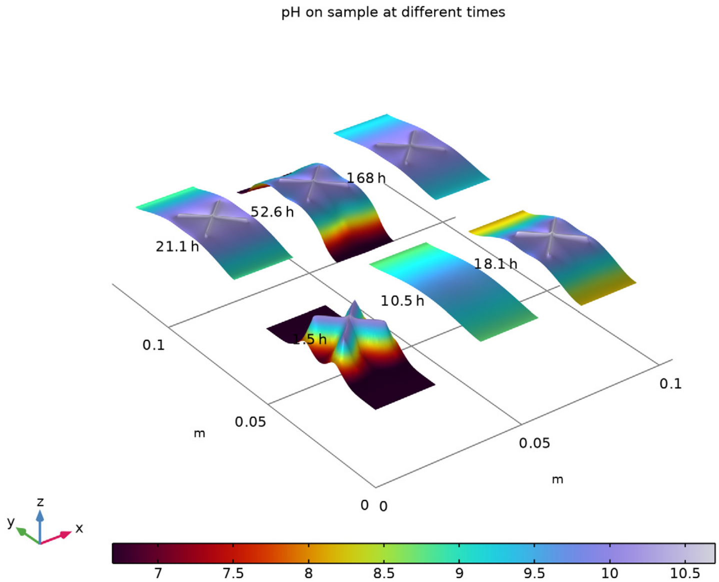
2 In the **Settings** window for **Annotation**, locate the **Data** section.

3 From the **Time (h)** list, choose **Last (168)**.

4 Locate the **Plot Array** section. In the **Column index** text field, type 3.

5 In the **pH Full Sample** toolbar, click **Plot**.

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



Coating Thickness Decrease

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Sector 2D 1**.

4 Locate the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `Thickness decrease (\mu m)`.

6 In the **Parameter indicator** text field, type `Time = eval(t,h) h`.

7 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

Surface 1

1 In the **Coating Thickness Decrease** toolbar, click **Surface with Height**.

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

3 In the **Expression** text field, type `d_Zn`.

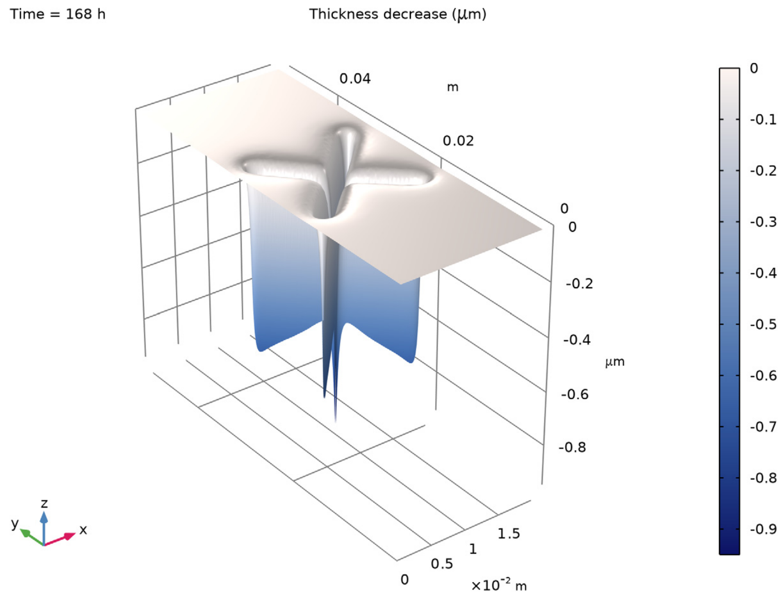
4 From the **Unit** list, choose **µm**.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prionace**.

6 From the **Color table transformation** list, choose **Reverse**.

7 In the **Coating Thickness Decrease** toolbar, click **Plot**.

8 Click the **Zoom Extents** button in the **Graphics** toolbar.



Corrosion Product Coverage Degree

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Sector 2D 1**.

4 Locate the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `Coverage degree (1)`.

6 In the **Parameter indicator** text field, type `Time = eval(t,h) h`.

7 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

Surface 1

1 In the **Corrosion Product Coverage Degree** toolbar, click **Surface with Height**.

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

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

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

5 From the **Color table transformation** list, choose **Reverse**.

Height Expression 1

1 In the **Model Builder** window, expand the **Surface 1** node, then click **Height Expression 1**.

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

3 Clear the **Show height axis** checkbox.

4 In the **Corrosion Product Coverage Degree** toolbar, click **Plot**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.