Created in COMSOL Multiphysics 6.3

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.

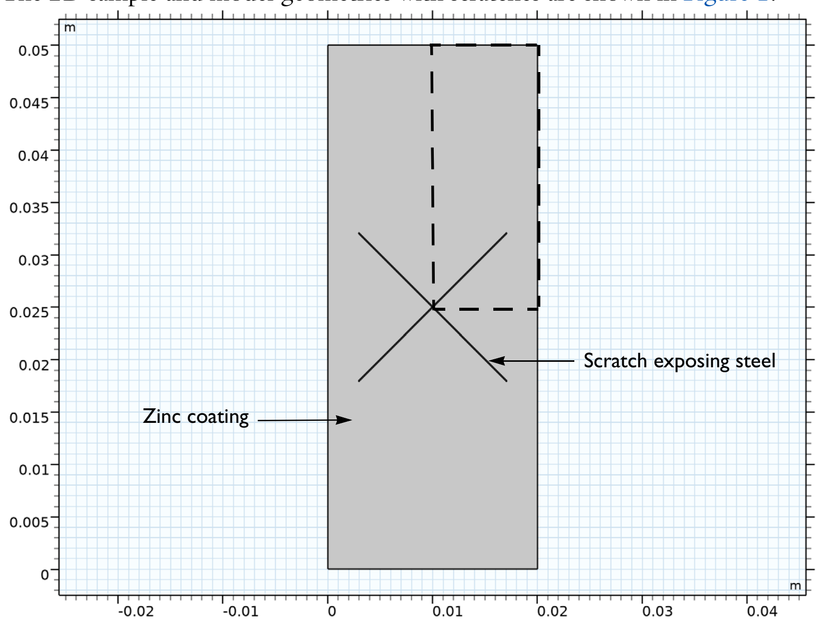


Figure 1: The galvanized steel sample geometry with 0.1 mm wide scratches exposing the steel. The model geometry is marked with dashed lines.

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.

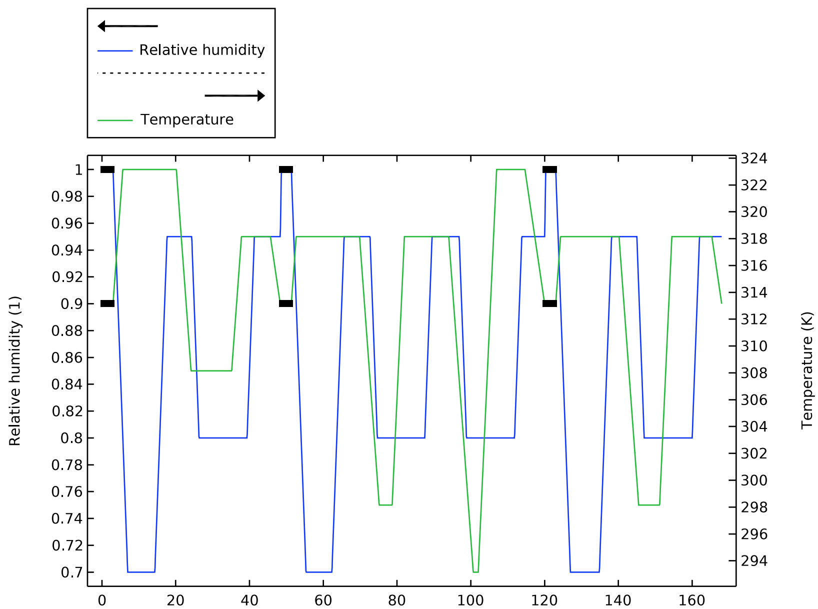


Figure 2: ACT. Solid black line indicates periods of spraying 1 wt% NaCl solution onto the sample.

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.

ELECTROPHORETIC 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)).

No conditions can be defined at atmosphere-liquid and liquid-metallic surface boundaries using the interface for the 2D model geometry. However, since the film is thin with no gradients along the film thickness all boundary conditions are converted to sources. For instance for a flux, N_m, the source, S_m, is given by

$$S_m = \frac{N_m}{L} \tag{2}$$

where L is the thickness of the liquid film.

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:

$$\mathrm{Zn(s)} \rightarrow \mathrm{Zn}^{2+} + 2\mathrm{e}^{-}$$
$$\frac{1}{2}\mathrm{O}_2 + \mathrm{H}_2\mathrm{O} + 2\mathrm{e}^{-} \rightarrow 2\mathrm{OH}^{-}$$

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 reactions are added to as volumetric currents ($\mathrm{A/m^3}$), $I_{\mathrm{v,Ox}}$ and $I_{\mathrm{v,Red}}$, using **Current Source** nodes. The added formulations are

$$I_{\mathrm{v,Ox}} = \frac{1-\theta}{L} \cdot \frac{c_{\mathrm{NaCl}}}{c_{\mathrm{NaCl,ref}}} \cdot i_{\mathrm{loc,Zn}} \cdot e^{\frac{E_a}{R_g}\left(\frac{1}{T_{\mathrm{ref}}} - \frac{1}{T}\right)} \tag{3}$$

$$I_{\mathrm{v,Red}} = \frac{1-\theta}{L} \cdot \frac{c_{\mathrm{O_2,sat}}}{c_{\mathrm{O_2,sat,ref}}} \cdot i_{\mathrm{loc,\,Fe}} \cdot e^{\frac{E_a}{R_g}\left(\frac{1}{T_{\mathrm{ref}}} - \frac{1}{T}\right)} \tag{4}$$

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

The flux of zinc ions into the film from the metal dissolution is accounted for using a **Species Source** node added under the **Ampholyte** node for aqueous zinc species (see next section). The flux is defined as a source, $S_{\mathrm{Ox,Zn}}$, given by

$$S_{\mathrm{Ox,Zn}} = \frac{I_{\mathrm{v,Ox}}}{2F} \tag{5}$$

Homogeneous Reactions in Liquid Film

Carbonates originating from the atmosphere are accounted for. Two deprotonation steps are defined, starting with the deprotonation of carbonic acid equilibrium reaction:

$$\mathrm{H_2CO_3} \Leftrightarrow \mathrm{H}^{+} + \mathrm{HCO_3^{-}}$$
$$\mathrm{HCO_3^{-}} \Leftrightarrow \mathrm{H}^{+} + \mathrm{CO_3^{-}}$$

Hydrolysis of zinc ions from the dissolution of the zinc coating are considered in four steps (Ref. 2):

$$Zn^{2+} + H_2O \Leftrightarrow Zn(OH)^{+} + H^{+}$$
$$Zn(OH)^{+} + H_2O \Leftrightarrow Zn(OH)_2(aq) + H^{+}$$
$$Zn(OH)_2(aq) + H_2O \Leftrightarrow Zn(OH)_3^{-} + H^{+}$$
$$Zn(OH)_3^{-} + H_2O \Leftrightarrow Zn(OH)_4^{2-} + H^{+}$$

Two **Ampholyte** nodes are used in the model. One node defines the mass balance accounting for all forms of the aqueous zinc species (Zn^{2+}, $Zn(OH)^{+}$, $Zn(OH)_2(aq)$, $Zn(OH)_3^{-}$, and $Zn(OH)_4^{2-}$) reactions and the other does the same for the carbonate (H_2CO_3, HCO_3^{-}, and CO_3^{2-}) reactions.

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 using the **Fully Dissociated Species** node.

Corrosion Products and Passivation

Corrosion products are formed can passivate the metallic surface. This example accounts for the formation of ZnO in 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 added as a reaction source, S_{Zn}, in a **Species Source** node in the **Ampholyte** node for the zinc species. The source formulation is based on the corrosion product solubility, as follows:

$$S_{Zn} = -\frac{k_{ZnO}}{L}(c_{Zn^{2+}}c_{OH^-}^2 - K_{S,ZnO}), \text{ if prec.}; (c_{Zn^{2+}}c_{OH^-}^2 - K_{SP,ZnO}) > 0 \tag{6}$$

$$S_{Zn} = -\theta\frac{k_{ZnO}}{L}(c_{Zn^{2+}}c_{OH^-}^2 - K_{S,ZnO}), \text{ if diss.}; (c_{Zn^{2+}}c_{OH^-}^2 - K_{SP,ZnO}) < 0 \tag{7}$$

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 both electrochemical reactions (see above). The ZnO coverage degree, θ, is assumed to change according to the following expression (Ref. 3):

$$\theta = 1 - e^{-\frac{m_{\mathrm{ZnO}}}{m_{\mathrm{tot,surf}}}} \tag{8}$$

where m_{ZnO} is the precipitated molar amount of ZnO per surface area (mol/m^2) and $m_{\mathrm{tot,surf}}$ is the molar metal surface availability per surface area for ZnO precipitation.

The precipitated ZnO amount is computed locally on the surface using a **Coefficient Form PDE**.

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, $c_{\mathrm{CO2,sat}}$, depends on the partial pressure, p_{CO2}, together with temperature and the salt concentration (Ref. 1). A reaction source, $S_{\mathrm{carbonate}}$, is defined in a **Species Source** node in the **Ampholyte** node for the carbonte species. The source minimizes the difference between the carbonate concentration in the film and the saturation concentration, as follows:

$$S_{\mathrm{carbonate}} = \varepsilon\frac{k_{\mathrm{CO_2,sat}}}{L}(c_{\mathrm{CO_2,sat}}(p_{\mathrm{CO_2}}, T, c_{\mathrm{NaCl}}) - c_{\mathrm{H_2CO_3}}), \quad c_{\mathrm{CO_2(aq)}} \approx c_{\mathrm{H_2CO_3}} \tag{9}$$

In the expression, $k_{\mathrm{CO2,sat}}$ is the rate constant for the carbon dioxide (1/s). The expression assumes that the carbonic acid concentration is mainly in the form of dissolved carbon dioxide in the liquid, as the following equilibrium reaction for carbon dioxide in liquid is strongly driven toward the left (Ref. 3):

$$\mathrm{CO_2(aq) + H_2O \Leftrightarrow H_2CO_3}$$

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

Drying and Condensation

The liquid film thickness varies with drying/evaporation that in turn affects species concentration. Therefore, an expanded formulation of the accumulation term in the material balances needs to be defined, as follows:

$$\frac{1}{L} \cdot \frac{\partial(c_i L)}{\partial t} + \nabla \cdot J_i = S \tag{10}$$

or

$$\frac{\partial c_i}{\partial t} + \frac{\varepsilon c_i}{L} \cdot \frac{\partial L}{\partial t} + \nabla \cdot J_i = S \tag{11}$$

The second term on the left-hand side in the equation is defined in **Species Source** nodes for the species.

Spraying

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

$$S_{\mathrm{NaCl}} = k_{\mathrm{spray}}(c_{i,\ \mathrm{spray}} - c_i) \tag{12}$$

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.

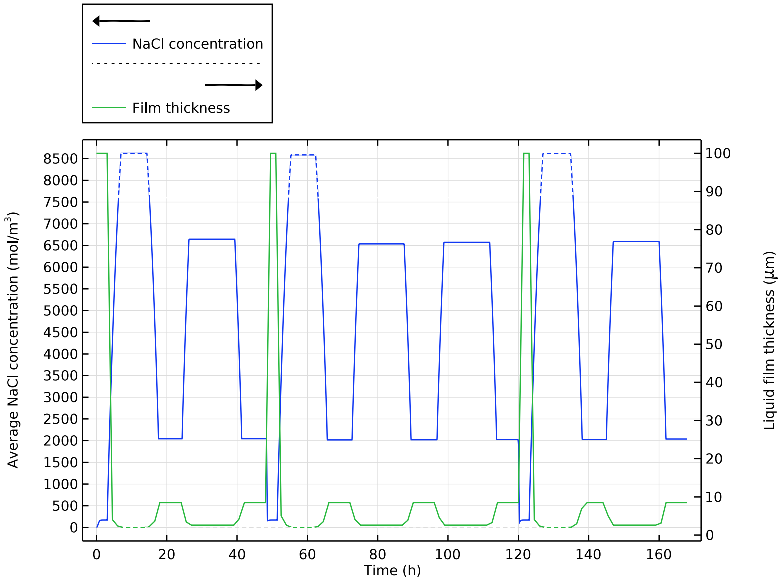


Figure 3: Salt concentration and liquid film thickness during ACT.

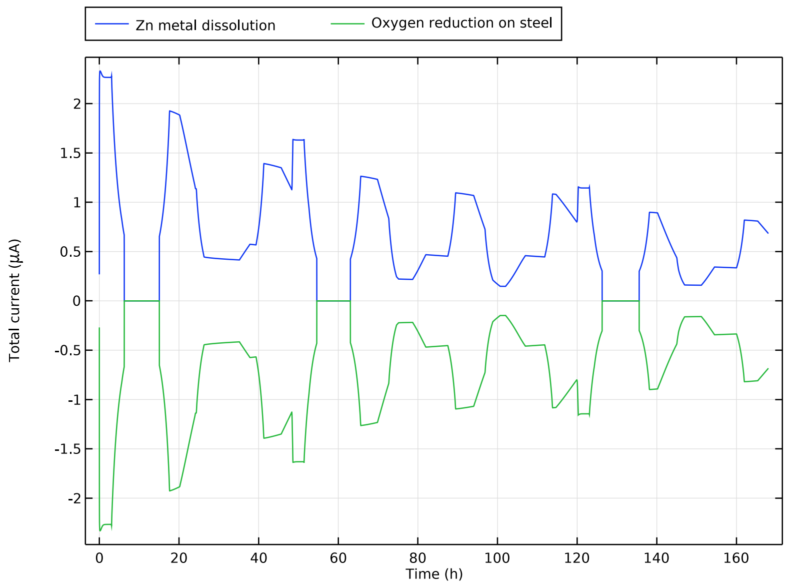


Figure 4: Total current of electrochemical reactions during ACT.

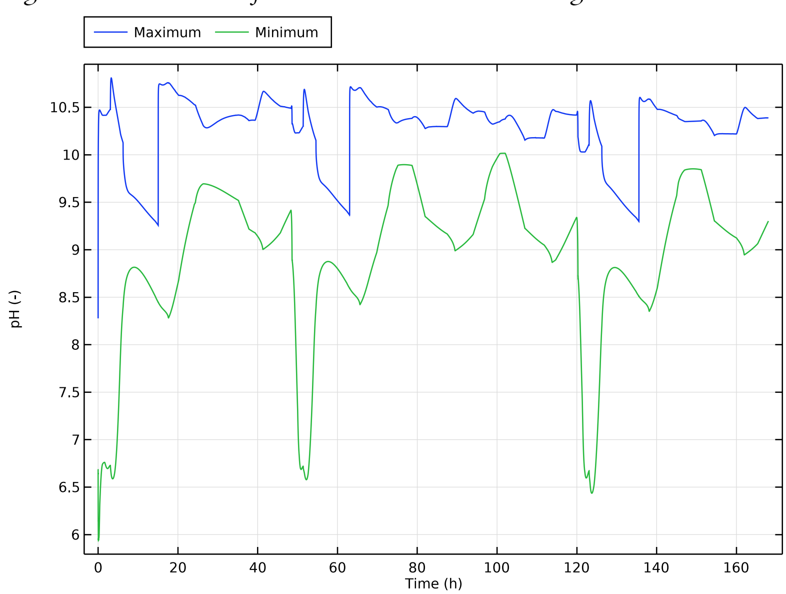


Figure 5: Maximum and minimum pH at sample during ACT.

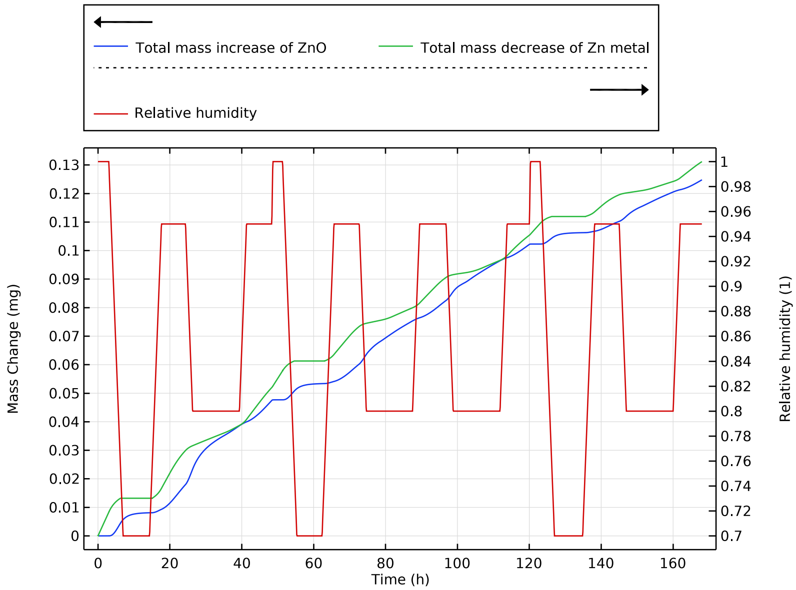


Figure 6: Mass changes over sample during ACT.

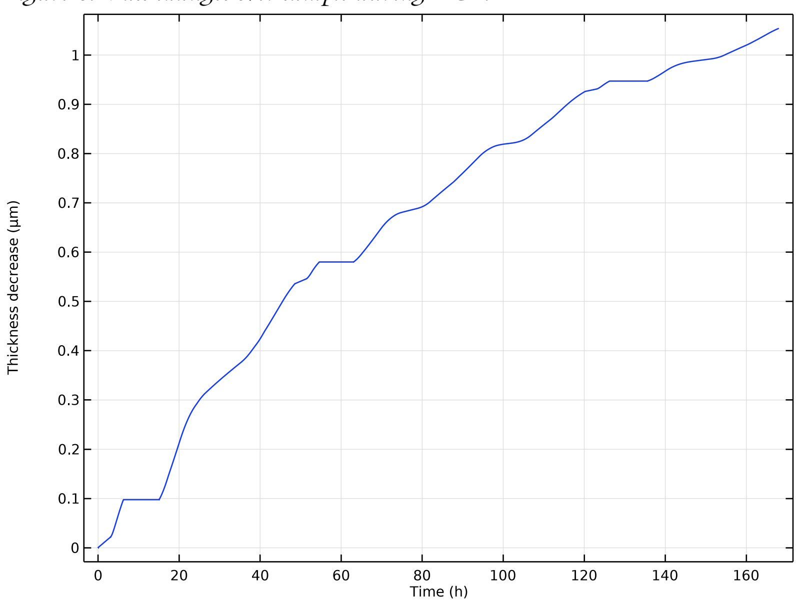


Figure 7: Maximum thickness decrease of coating during ACT.

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

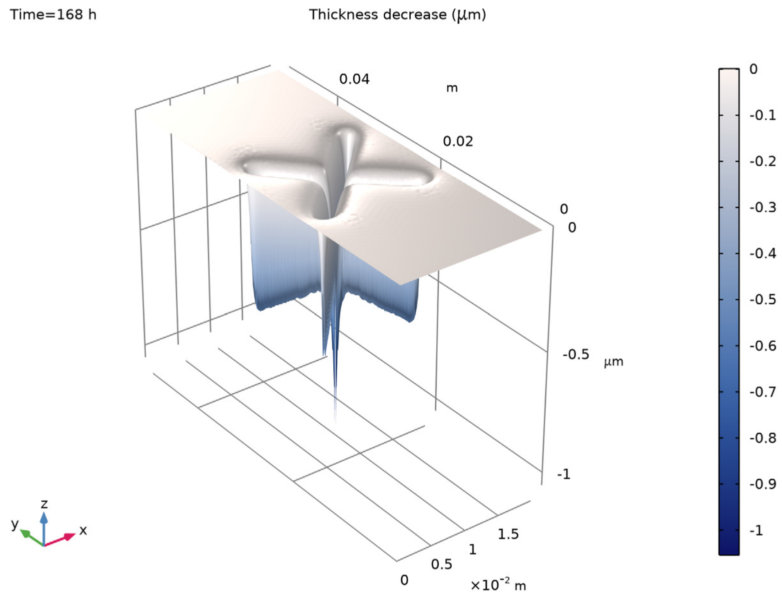


Figure 8: Local coating thickness decrease after 7 days.

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.

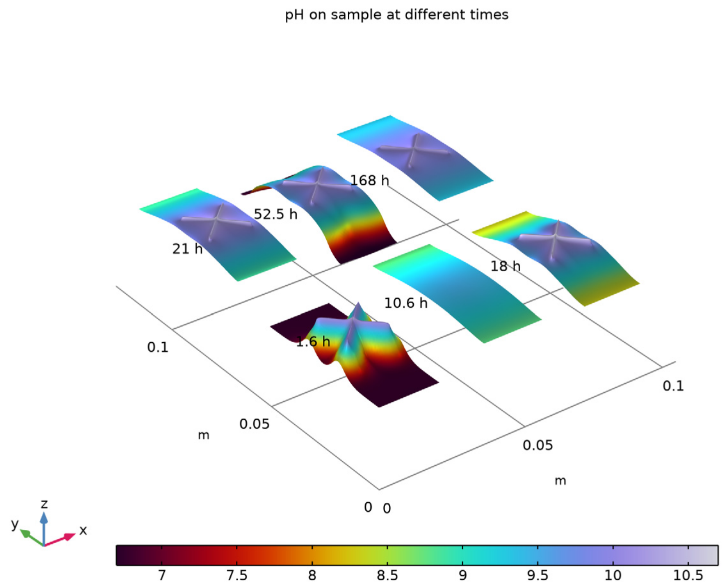


Figure 9: Local pH at the sample surface at different times during the ACT.

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

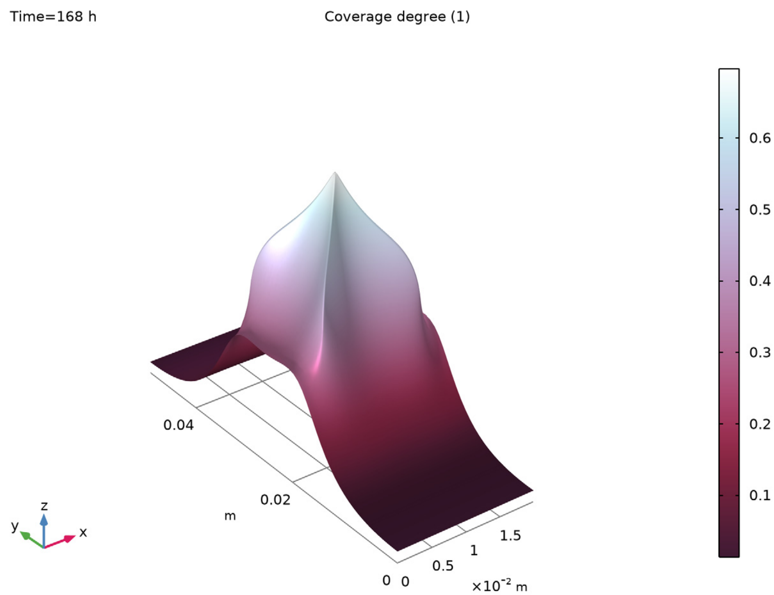


Figure 10: Local degree of coverage after 7 days.

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 **Chemical Species Transport** > **Electrophoretic Transport (el)**.
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 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**.

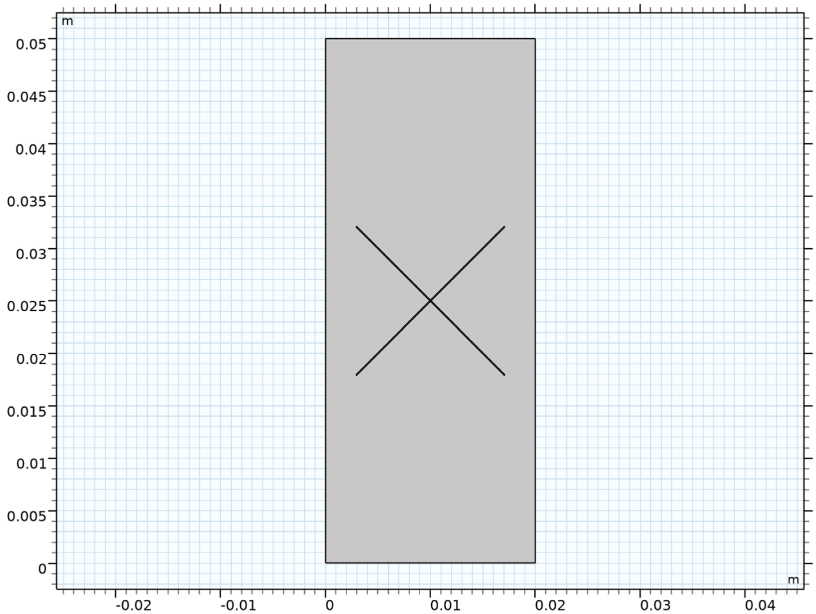
6 In the **x** text field, type `w_sample/2`.

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

8 Locate the **Rotation Angle** section. In the **Rotation** text field, type `315`.

9 Click **Build All Objects**.

Your geometry should now look like this:



Due to symmetry, 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.

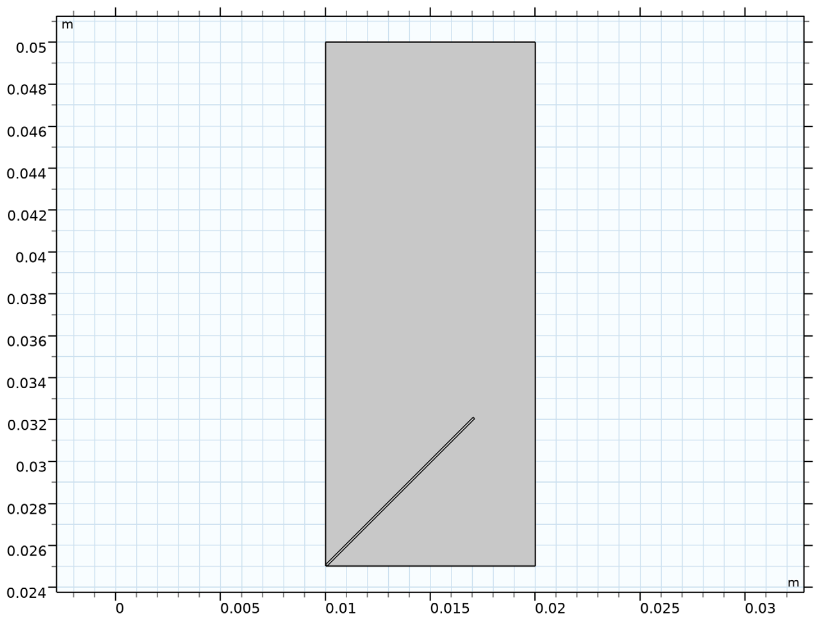
4 Click to select the **Activate Selection** toggle button for **Objects to subtract**.

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 facilitate 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 - Zn

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

2 In the **Settings** window for **Integration**, type `intop_zinc` in the **Operator name** text field.

3 In the **Label** text field, type `Integration - Zn`.

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 - Zn

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

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

3 From the **Geometric entity level** list, choose **Domain**.

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

5 In the **Label** text field, type `Variables - Zn`.

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

7 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**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

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

5 In the **Label** text field, type `Variables - Steel`.

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

7 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 **Electrophoretic Transport** interface that was added.

ELECTROPHORETIC TRANSPORT (EL)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electrophoretic Transport (el)**.

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

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

Solvent 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Electrophoretic Transport (el)** click **Solvent 1**.

2 In the **Settings** window for **Solvent**, 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 **Diffusion and Migration** section. From the **Specify** list, choose **Diffusivity**.

5 In the D_H text field, type `DH`.

6 In the D_{OH} text field, type `DOH`.

Initial Potential 1

1 In the **Model Builder** window, click **Initial Potential 1**.

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

3 In the *phil* text field, type `V0`.

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

Ampholyte - Hydrolysis Zn species

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

2 In the **Settings** window for **Ampholyte**, type `Ampholyte - Hydrolysis Zn species` 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. From the **Specify** list, choose **Diffusivity**.

8 In the D text field, type `DZn`.

The **Species Source** subnodes are available once advanced physics options are enabled. Use these to add corrosion product precipitation and spraying together with drying and condensation of the liquid film.

9 Click the **Show More Options** button in the **Model Builder** toolbar.

10 In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics > Advanced Physics Options**.

11 Click **OK**.

Species Source - ZnO Corrosion Product

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

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

3 Locate the **Species Source** section. In the S text field, type `-r_ZnO`.

Ampholyte - Hydrolysis Zn species

In the **Model Builder** window, click **Ampholyte - Hydrolysis Zn species**.

Species Source - Zn Dissolution

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

2 In the **Settings** window for **Species Source**, locate the **Domain Selection** section.

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

4 Locate the **Species Source** section. In the S text field, type `N_ox`.

5 In the **Label** text field, type `Species Source - Zn Dissolution`.

Ampholyte - Hydrolysis Zn species

In the **Model Builder** window, click **Ampholyte - Hydrolysis Zn species**.

Species Source - Zn Removal with Spraying

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

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

3 Locate the **Species Source** section. In the S text field, type `rSpray_Zn`.

Ampholyte - Hydrolysis Zn species

In the **Model Builder** window, click **Ampholyte - Hydrolysis Zn species**.

Species Source - Drying and Condensation

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

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

3 Locate the **Species Source** section. In the S text field, type `rDry_Zn`.

Use an additional **Ampholyte** node to model the carbonate deprotonation equilibrium reactions.

Ampholyte - Deprotonation Carbonate Species

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

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

3 Locate the **Ampholyte** section. In the **Species name** text field, type `CO3`.

4 In the table, enter the following settings:

Dissociation step (1)	pKa (1)
1	`-log10(K_CO3step1)`
2	`-log10(K_CO3step2)`

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

6 Locate the **Diffusion and Migration** section. From the **Diffusivity-mobility settings** list, choose **Individual**.

7 In the table, enter the following settings:

Index (1)	Charge number (1)	Diffusivity (m^2/s)	Mobility (s*mol/kg)
0	-2	`DCO3`	`el.D1_CO3/R_const/T_ACT(t)`
1	-1	`DHCO3`	`el.D2_CO3/R_const/T_ACT(t)`
2	0	`DH2CO3`	`el.D3_CO3/R_const/T_ACT(t)`

Species Source - Carbonates from Atmosphere

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

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

3 Locate the **Species Source** section. In the S text field, type `r_CO3`.

Ampholyte - Deprotonation Carbonate Species

In the **Model Builder** window, click **Ampholyte - Deprotonation Carbonate Species**.

Species Source - Carbonate Removal with Spraying

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

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

3 Locate the **Species Source** section. In the S text field, type `rSpray_CO3`.

Ampholyte - Deprotonation Carbonate Species

In the **Model Builder** window, click **Ampholyte - Deprotonation Carbonate Species**.

Species Source - Drying and Condensation

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

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

3 Locate the **Species Source** section. In the S text field, type `rDry_CO3`.

Initial Concentration 1

1 In the **Model Builder** window, click **Initial Concentration 1**.

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

3 In the c text field, type `cCO30`.

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

Fully Dissociated Species - Na

1 In the **Physics** toolbar, click **Domains** 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 `1`.

5 Locate the **Diffusion and Migration** section. From the **Specify** list, choose **Diffusivity**.

6 In the D text field, type `DNa`.

Species Source - Spray

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

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

3 Locate the **Species Source** section. In the S text field, type `rSpray_Na`.

Fully Dissociated Species - Na

In the **Model Builder** window, click **Fully Dissociated Species - Na**.

Species Source - Drying and Condensation

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

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

3 Locate the **Species Source** section. In the S text field, type `rDry_Na`.

Initial Concentration 1

1 In the **Model Builder** window, click **Initial Concentration 1**.

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

3 In the c text field, type cNaCl0.

Fully Dissociated Species - Cl

1 In the **Physics** toolbar, click **Domains** 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 -1.

5 Locate the **Diffusion and Migration** section. From the **Specify** list, choose **Diffusivity**.

6 In the D text field, type DCl.

Species Source - Spray

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

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

3 Locate the **Species Source** section. In the S text field, type rSpray_Cl.

Fully Dissociated Species - Cl

In the **Model Builder** window, click **Fully Dissociated Species - Cl**.

Species Source - Drying and Condensation

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

2 In the **Settings** window for **Species Source**, type Species Source - Drying and Condensation in the **Label** text field.

3 Locate the **Species Source** section. In the S text field, type rDry_Cl.

Current Source 1

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

Initial Concentration 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Electrophoretic Transport (el)** > **Fully Dissociated Species - Cl** click **Initial Concentration 1**.

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

3 In the c text field, type cNaCl0.

Local electrochemical reactions are added using **Current Source** nodes. The reactions are defined in the imported Zn and steel variables.

Current Source - Oxygen Reduction

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Electrophoretic Transport (el)** click **Current Source 1**.

2 In the **Settings** window for **Current Source**, type `Current Source - Oxygen Reduction` in the **Label** text field.

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

4 Locate the **Electrolyte Current Source** section. In the Q_1 text field, type `Q_red`.

Current Source - Zn Metal Dissolution

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

2 In the **Settings** window for **Current Source**, type `Current Source - Zn Metal Dissolution` in the **Label** text field.

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

4 Locate the **Electrolyte Current Source** section. In the Q_1 text field, type `Q_ox`.

Add a **Coefficient Form PDE** interface and define dissolving and depositing species; zinc metal dissolution and ZnO dissolution/deposition.

ADD PHYSICS

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

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

3 In the tree, select **Mathematics** > **PDE Interfaces** > **Coefficient Form PDE (c)**.

4 Click the **Add to Component 1** button in the window toolbar.

5 In the **Physics** toolbar, click **Add Physics** to close the **Add Physics** window.

DISSOLVING AND DEPOSITING SPECIES

1 In the **Settings** window for **Coefficient Form PDE**, type `Dissolving and Depositing Species` in the **Label** text field.

2 Locate the **Units** section. Click **Select Dependent Variable Quantity**.

3 In the **Physical Quantity** dialog, select **Transport** > **Surface site concentration (mol/m^2)** in the tree.

4 Click **OK**.

5 In the **Settings** window for **Coefficient Form PDE**, locate the **Units** section.

6 Click **Select Source Term Quantity**.

7 In the **Physical Quantity** dialog, select **Transport** > **Molar flux (mol/(m^2*s))** in the tree.

8 Click **OK**.

9 In the **Settings** window for **Coefficient Form PDE**, click to expand the **Dependent Variables** section.

10 In the **Dependent variables (mol/m²)** table, enter the following settings:

mZn

11 Click **Add Dependent Variable**.

12 In the **Dependent variables (mol/m²)** table, enter the following settings:

mZn
mZnO

Zn

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Dissolving and Depositing Species (c)** click **Coefficient Form PDE 1**.

2 In the **Settings** window for **Coefficient Form PDE**, type `Zn` in the **Label** text field.

3 Locate the **Diffusion Coefficient** section. In the *c* text-field array, type `0` in the first column of the first row.

4 In the *c* text-field array, type `0` in the second column of the second row.

5 Locate the **Source Term** section. In the *f* text-field array, type `N_ox*d_film` on the first row.

6 In the *f* text-field array, type `r_ZnO*d_film` on the second row.

Steel

1 In the **Physics** toolbar, click **Domains** and choose **Coefficient Form PDE**.

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

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

4 Locate the **Diffusion Coefficient** section. In the *c* text-field array, type `0` in the first column of the first row.

5 In the *c* text-field array, type `0` in the second column of the second row.

6 Locate the **Source Term** section. In the *f* text-field array, type `0` on the first row.

7 In the *f* text-field array, type `r_ZnO*d_film` on the second row.

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 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 - Zn 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 - Zn 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 Zn 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 Zn 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**.

Variables - Film, Variables - Global, Variables - Rates, Variables - Steel, Variables - Zn

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Definitions**, Ctrl-click to select **Variables - Global**, **Variables - Rates**, **Variables - Film**, **Variables - Zn**, and **Variables - Steel**.

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

Group - Variables

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

Interpolation - Relative Humidity (RH_ACT), Interpolation - Spray (spray_ACT), Interpolation - Temperature (T_ACT)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Definitions**, Ctrl-click to select **Interpolation - Relative Humidity (RH_ACT)**, **Interpolation - Temperature (T_ACT)**, and **Interpolation - Spray (spray_ACT)**.

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

Group - Interpolations

In the **Settings** window for **Group**, type `Group - Interpolations` in the **Label** text field.

Domain Probe - Average NaCl Concentration in Liquid Film (dom_cNaCl), Domain Probe - Maximum Zn Coating Thickness Loss (dom_d_Zn), Domain Probe - Maximum pH (dom_maxpH), Domain Probe - Minimum pH (dom_minpH), Global Variable Probe - Total Oxygen Reduction Current (var_I_red), Global Variable Probe - Total Zinc Metal Dissolution Current (var_I_ox), Global Variable Probe - Zn Metal (var_m_Zn), Global Variable Probe - ZnO (var_ZnO)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Definitions**, Ctrl-click to select **Global Variable Probe - ZnO (var_ZnO)**, **Global Variable Probe - Zn Metal (var_m_Zn)**, **Global Variable Probe - Total Zinc Metal Dissolution Current (var_I_ox)**, **Global Variable Probe - Total Oxygen Reduction Current (var_I_red)**, **Domain Probe - Maximum Zn Coating Thickness Loss (dom_d_Zn)**, **Domain Probe - Maximum pH (dom_maxpH)**, **Domain Probe - Minimum pH (dom_minpH)**, and **Domain Probe - Average NaCl Concentration in Liquid Film (dom_cNaCl)**.

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

Group - Probes

In the **Settings** window for **Group**, type `Group - Probes` in the **Label** text field.

Integration - Steel (intop_steel), Integration - Wetted Surface (intop_wet), Integration - Zn (intop_zinc)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Definitions**, Ctrl-click to select **Integration - Zn (intop_zinc)**, **Integration - Steel (intop_steel)**, and **Integration - Wetted Surface (intop_wet)**.

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

Group - Integrations

In the **Settings** window for **Group**, type `Group - Integrations` in the **Label** text field.

Set the solver time-stepping to a value lower than the distinct periods of the ACT. In this case, 0.1 h is well below 3 h.

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 **Physics and Variables Selection** section.

3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Dissolving and Depositing Species (c)**.

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 Click **Range**.

5 In the **Range** dialog, type `1.5` in the **Step** text field.

6 In the **Stop** text field, type `24*7`.

7 Click **Replace**.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, under **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** 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

Start polishing the probe plots. All of these are found in the model documentation.

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 **Manual**.

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
`Zn 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**.

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**.

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

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. Select the **Enable** checkbox.

9 From the **Array shape** 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 **1.5543**.

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 **10.572**.

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 **18.023**.

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 **21.018**.

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 **52.522**.

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 **1.5543**.

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 **10.572**.

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 **18.023**.

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 **21.018**.

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 **52.522**.

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 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 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.

Finally, tidy some of the default plots or remove the ones considered redundant.

Dissolving and Depositing Species, Electrolyte Conductivity (el), Electrolyte Potential (el), Molar Concentration - CO3 (el), Molar Concentration - Cl (el), Molar Concentration - Na (el), Molar Concentration - Zn (el), pH (el)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **pH (el)**, **Electrolyte Conductivity (el)**, **Electrolyte Potential (el)**, **Molar Concentration - Zn (el)**, **Molar Concentration - CO3 (el)**, **Molar Concentration - Na (el)**, **Molar Concentration - Cl (el)**, and **Dissolving and Depositing Species**.

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