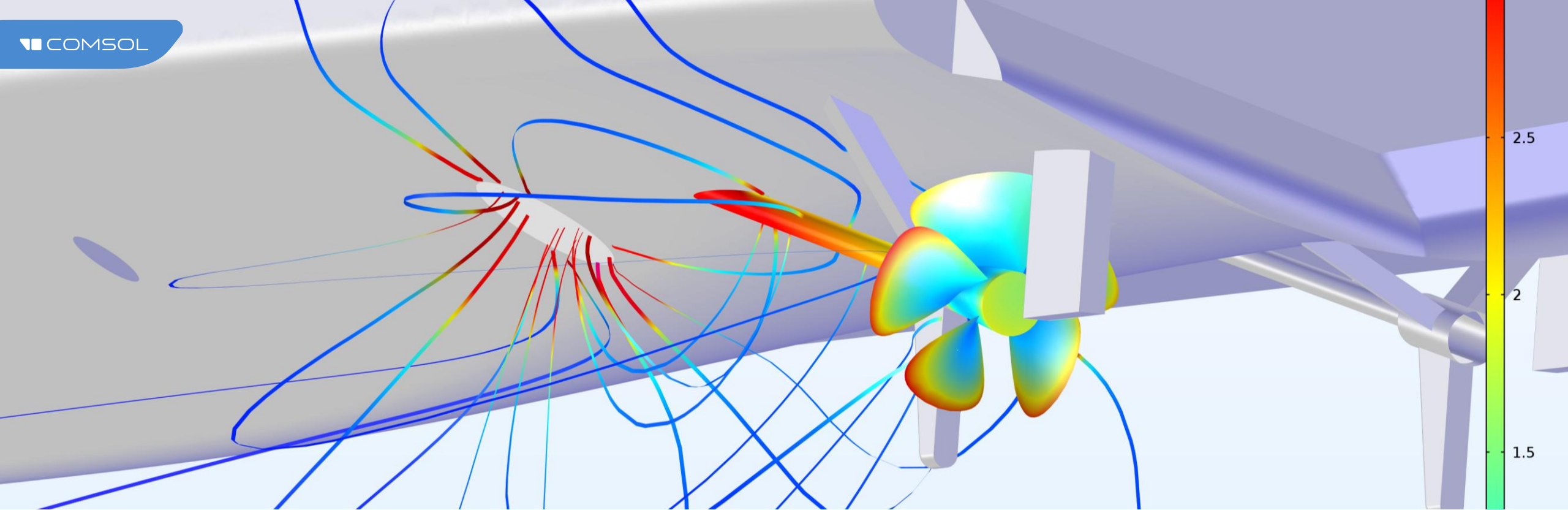
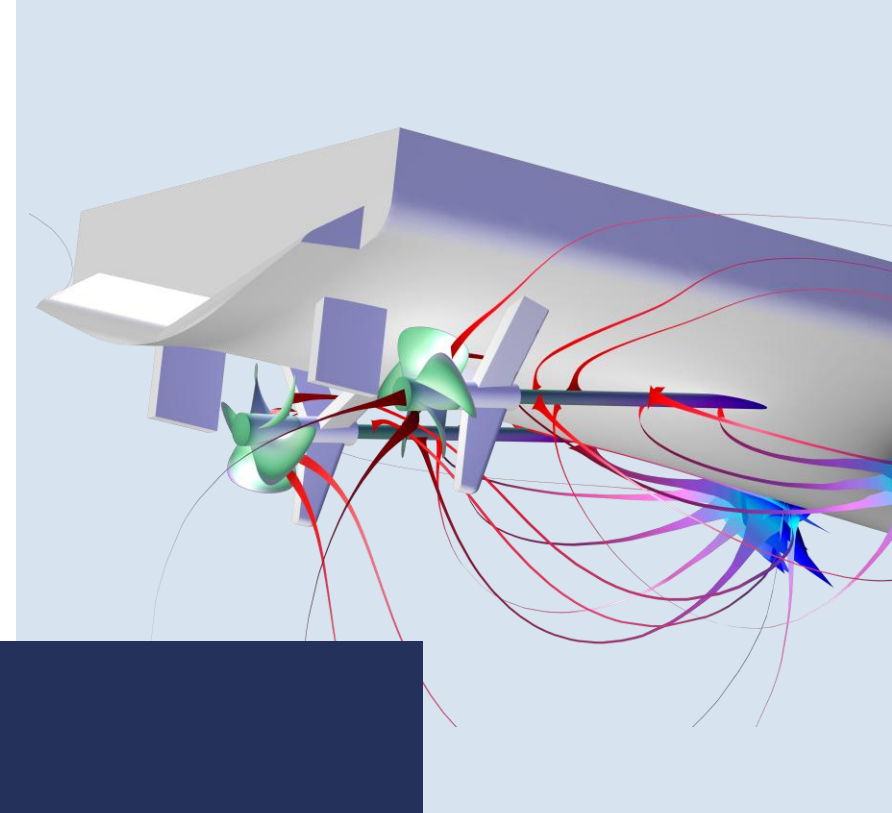
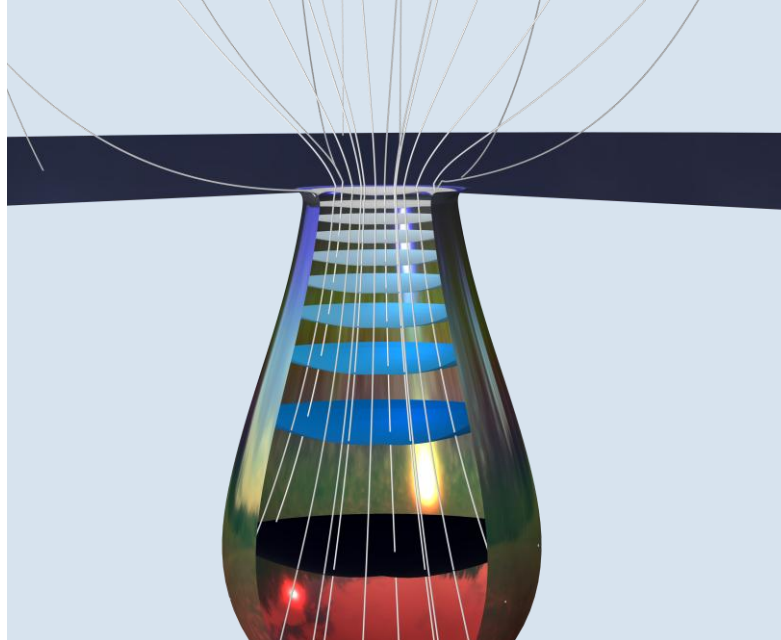
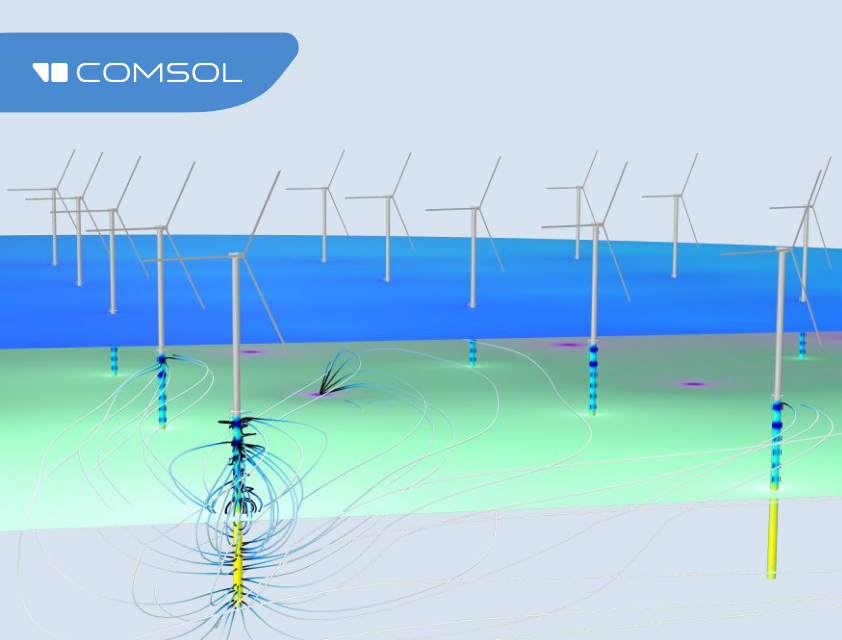




Modeling Corrosion Prediction and Protection in COMSOL Multiphysics®

Chen You

COMSOL Inc



Typical Corrosion Applications Modeled Using COMSOL Multiphysics®

Corrosion Processes

- Galvanic corrosion
- Pitting and crevice corrosion
- Atmospheric corrosion
- Stray currents

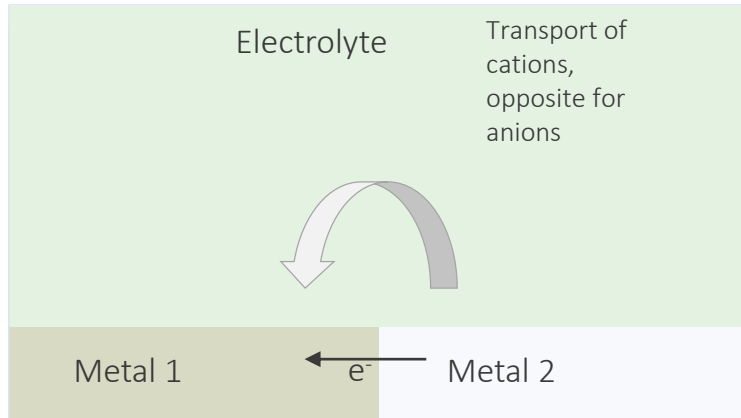
Protection Systems

- Impressed current cathodic protection (ICCP)
- Cathodic protection with sacrificial anodes (SACP)
- Anodic protection
- Internal cathodic protection in pipelines

Modeling and Simulation

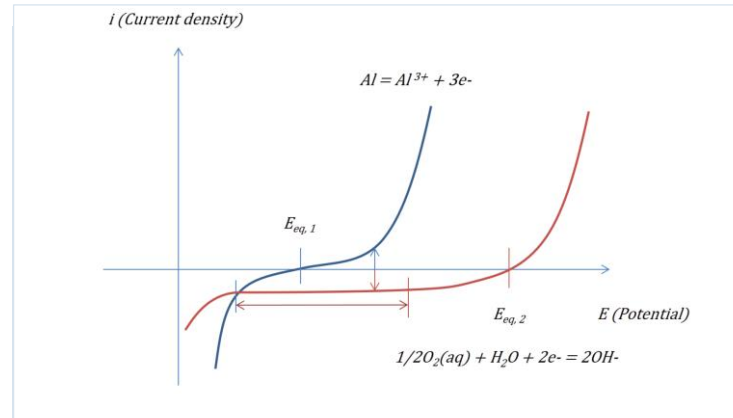
- To investigate corrosion processes for given geometries, materials, and environmental conditions
- To understand, design, and optimize corrosion protection systems

Corrosion Modeling



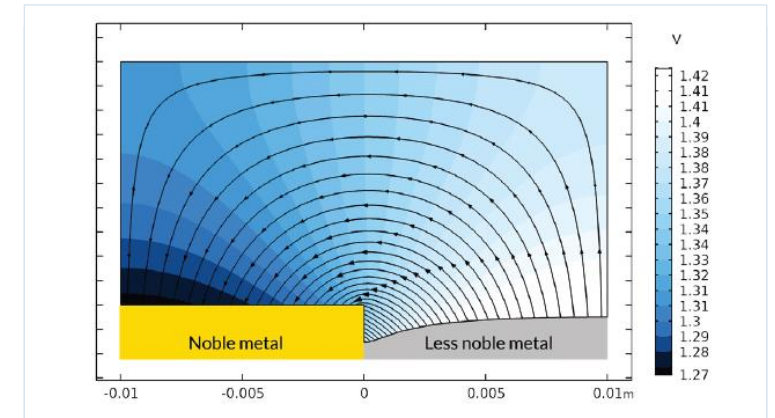
Transport of Anions and Cations in an Electrolyte

- Charge and mass transport
- Charge conservation and neutrality
- Mass conservation



Electrochemical Reactions at the Anode and Cathode

- Multiple reactions
- Polarization curves show current density as a function of the electrode potential
- Polarization expression given by, for example, Butler-Volmer and Tafel equations
- Thermodynamics for metals in electrolytes

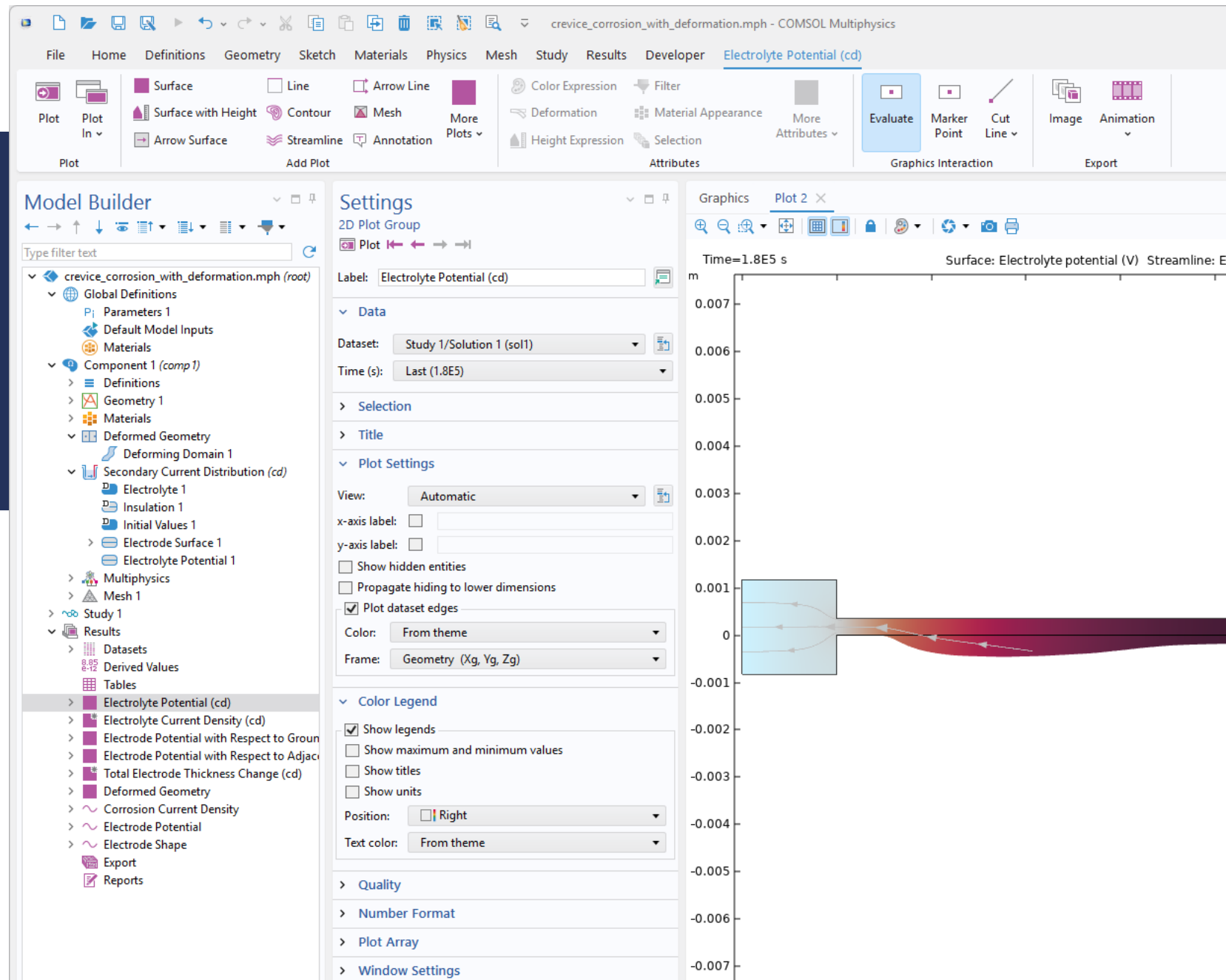


Deforming Geometry: Deposition and Dissolution

- Dissolution of metals
- Deposition of thin films and calcareous deposits
- Deforming geometries change the current and potential distribution

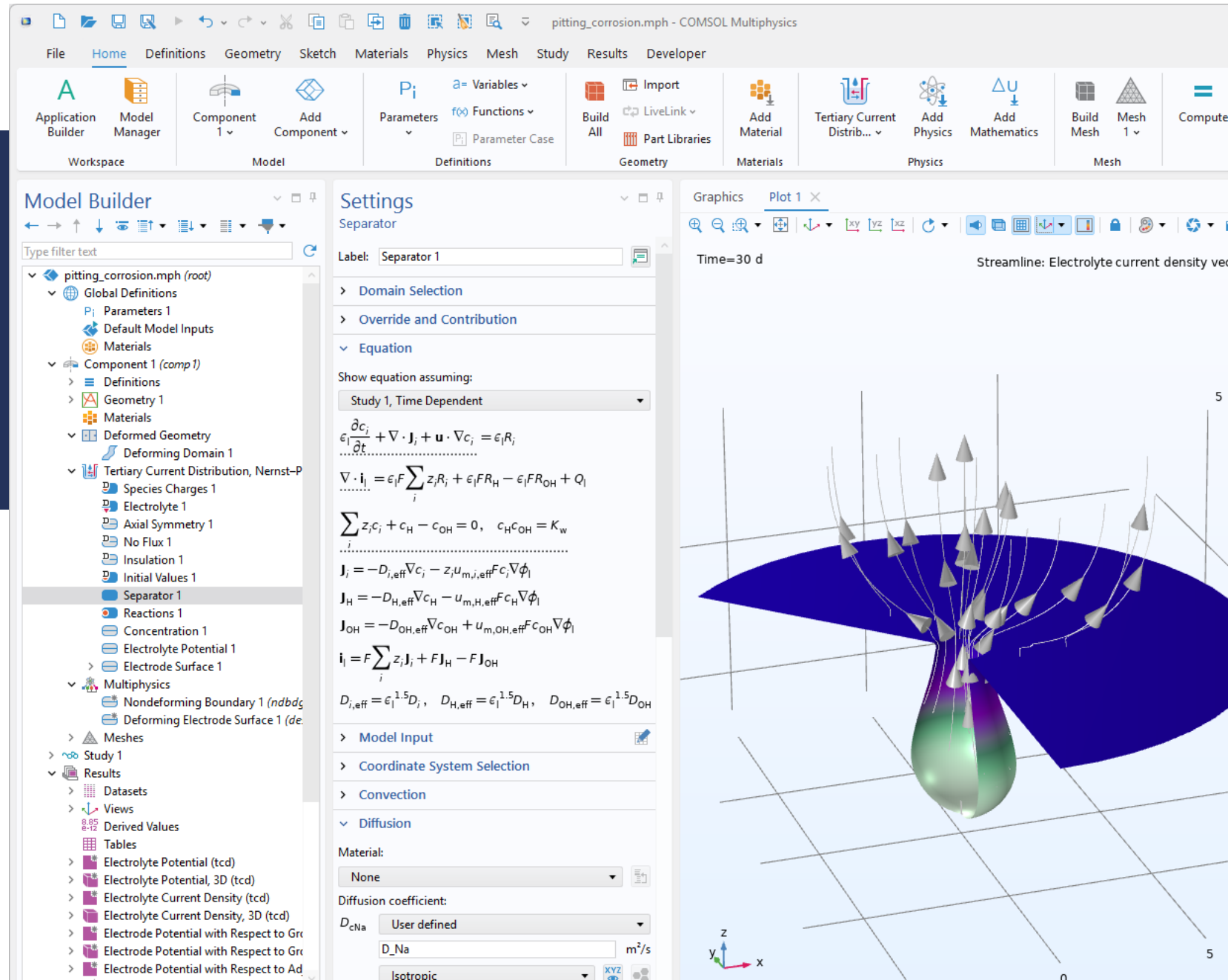
Current Distribution

- Modeling current distribution in the electrodes and electrolyte with reaction kinetics on the anodic and cathodic boundaries enables accurate description of a corroding system.



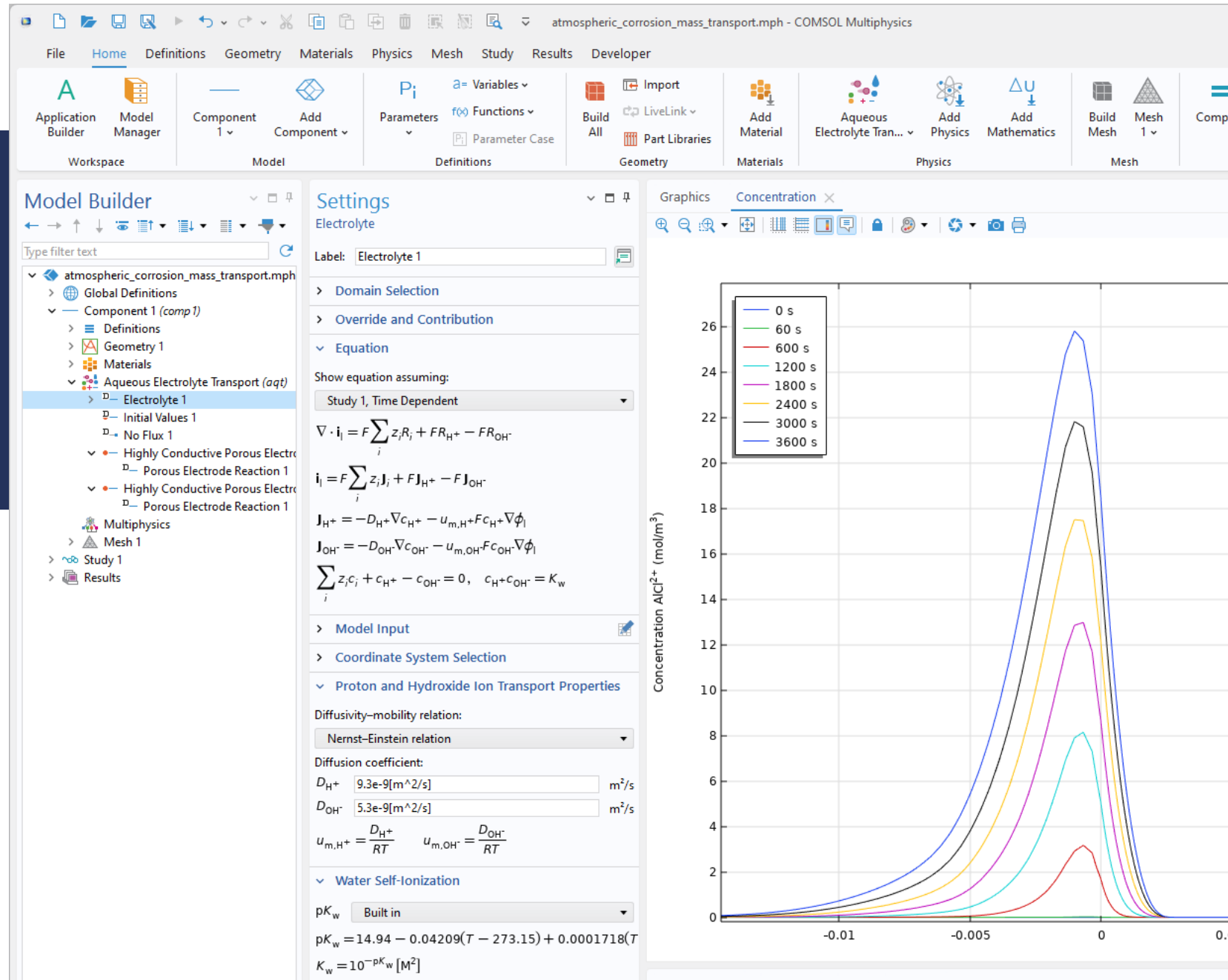
Nernst–Planck Equations

- Tertiary current distribution features the Nernst–Planck equations for an arbitrary number of species.
- In the crevice corrosion example here, a water-based electrolyte is used, which automatically adds the equilibrium reactions for water self-ionization.



Aqueous Electrolyte Transport Interface

- Defines equations for only a minimal set of concentration-dependent variables for species subject to chemical equilibria:
 - Weak acids and bases
 - Ampholytes (molecules that can act as both acid and base)
 - Arbitrary complex species
- Uses electroneutral Nernst-Planck formulation with automatic handling of self-ionization of water (autoprotolysis)
- Automatically defines consistent initial and inflow concentrations



Corrosion Material Library

270 materials, with imported
polarization curves and
equilibrium potentials from
published papers

pitting_corrosion.mph - COMSOL Multiphysics

Material Browser

Corrosion

- Electrolytes
- Elements
- Aluminum Alloys
- Copper Alloys (Bronzes)
- Iron Alloys (Steels)
 - AISI 1020 steel in 0.1 M NaHCO₃
 - AISI 1020 steel in 0.1 M NaHCO₃ and 0.2 M NaCl
 - AISI 1020 steel in 0.1 M NaHCO₃ and 0.5 M NaCl
 - AISI 1020 steel in 0.1 M NaHCO₃ and 0.8 M NaCl
 - AISI 1020 steel in 0.2 M NaCl
 - AISI 1020 steel in 0.5 M NaCl
 - AISI 1020 steel in 0.8 M NaCl
 - AISI 1020 steel in seawater at 4 C
 - AISI 1020 steel in seawater at 8 C
 - AISI 1020 steel in seawater at 20 C**
 - AISI 1030 steel in CO₂ saturated 3% NaCl and 0.01% NaHCO₃
 - AISI 1030 steel in CO₂ saturated 3% NaCl, 0.01% NaHCO₃ and 100 mg/L 2-Mercaptopyrimidine 98%
 - AISI 1030 steel in CO₂ saturated 3% NaCl, 0.01% NaHCO₃ and 100 mg/L 1-Dodecylpyridinium chloride hydrate 98%
 - AISI 1040 steel embedded in mortar and immersed in water
 - AISI 1040 steel embedded in mortar and immersed in 3.5% NaCl
 - AISI 1040 steel embedded in mortar and exposed to 98% RH
 - AISI 1040 steel embedded in mortar containing 5% NaCl and exposed to 98% RH
 - AISI 4140 steel in aerated ASTM substitute ocean water
 - AISI 4140 steel in deaerated ASTM substitute ocean water
 - AISI 4150 steel in 5% NaCl
 - AISI 4340 steel in 0.6M NaCl at pH = 8.3
 - Alloy 800 (annealed) in 1 M NaCl
 - Alloy 800 (annealed and aged) in 1 M NaCl
 - Alloy 800 (annealed) in 1 M NaCl and 0.001 M Na₂S₂O₃
 - Alloy 800 (annealed and aged) in 1 M NaCl and 0.001 M Na₂S₂O₃
 - API 5L X52 steel in simulated soil containing NaCl and CaSO₄

Material: AISI 1020 steel in seawater at 20 C

Phase:

Orientation/variation:

Properties

Property	Expression	Unit	Property group
Local current density expression	$i_{loc_exp}(E_vs_ref_exp)$	A/m ²	Local current density
E_vs_SHE	V		Local current density
$E_ref_exp_vs_SHE$	0.197 [V]	V	Local current density
$E_vs_ref_exp$	$E_vs_SHE - E_ref_exp_vs_SHE$		Local current density
Equilibrium potential	$E_{eq_vs_SHE}$	V	Equilibrium potential
Temperature derivative of e_{eq}	0 [V/K]	V/K	Equilibrium potential
Reference concentration	0 [mol/m ³]	mol/m ³	Equilibrium potential

Property reference:
Select a property in the list above to display its reference.

Inputs

Input	Variable	Unit
Electric potential	V	V
Concentration	c	mol/m ³

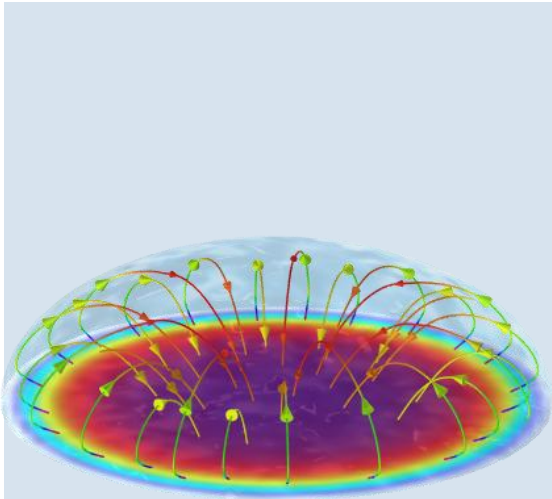
Certain materials may be proprietary, and certain material names may be trademarks of producers of such materials: www.comsol.com/trademarks

Add to Component Add To Edit

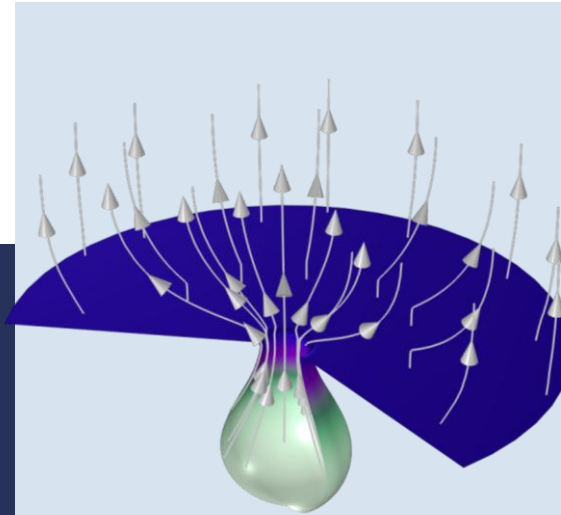
Added to model:

Remove

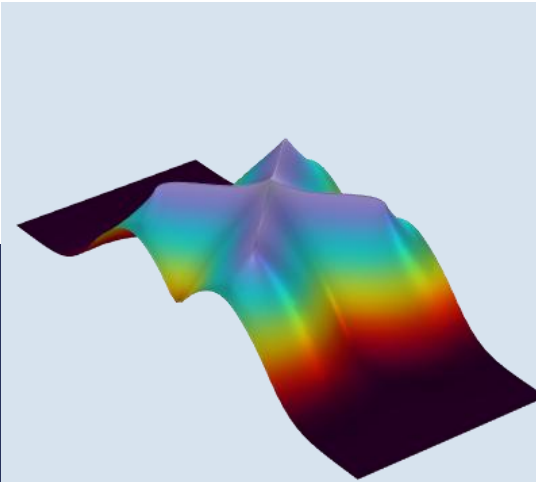
Corrosion Prediction Applications



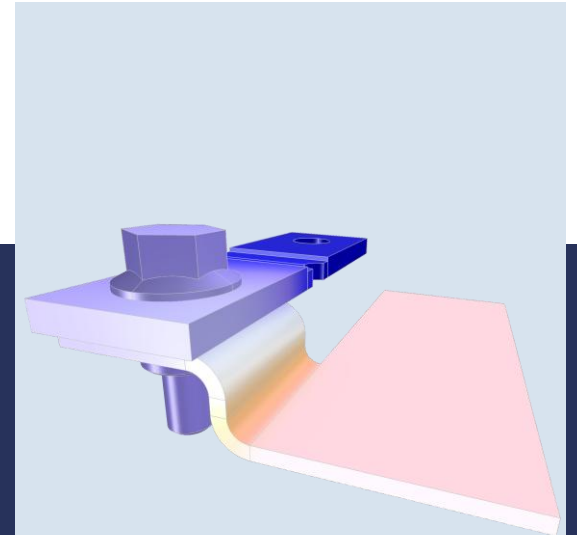
Corrosion under an Evans droplet.



Pitting corrosion.



Accelerated corrosion test (ACT) of a galvanized steel with scratch.

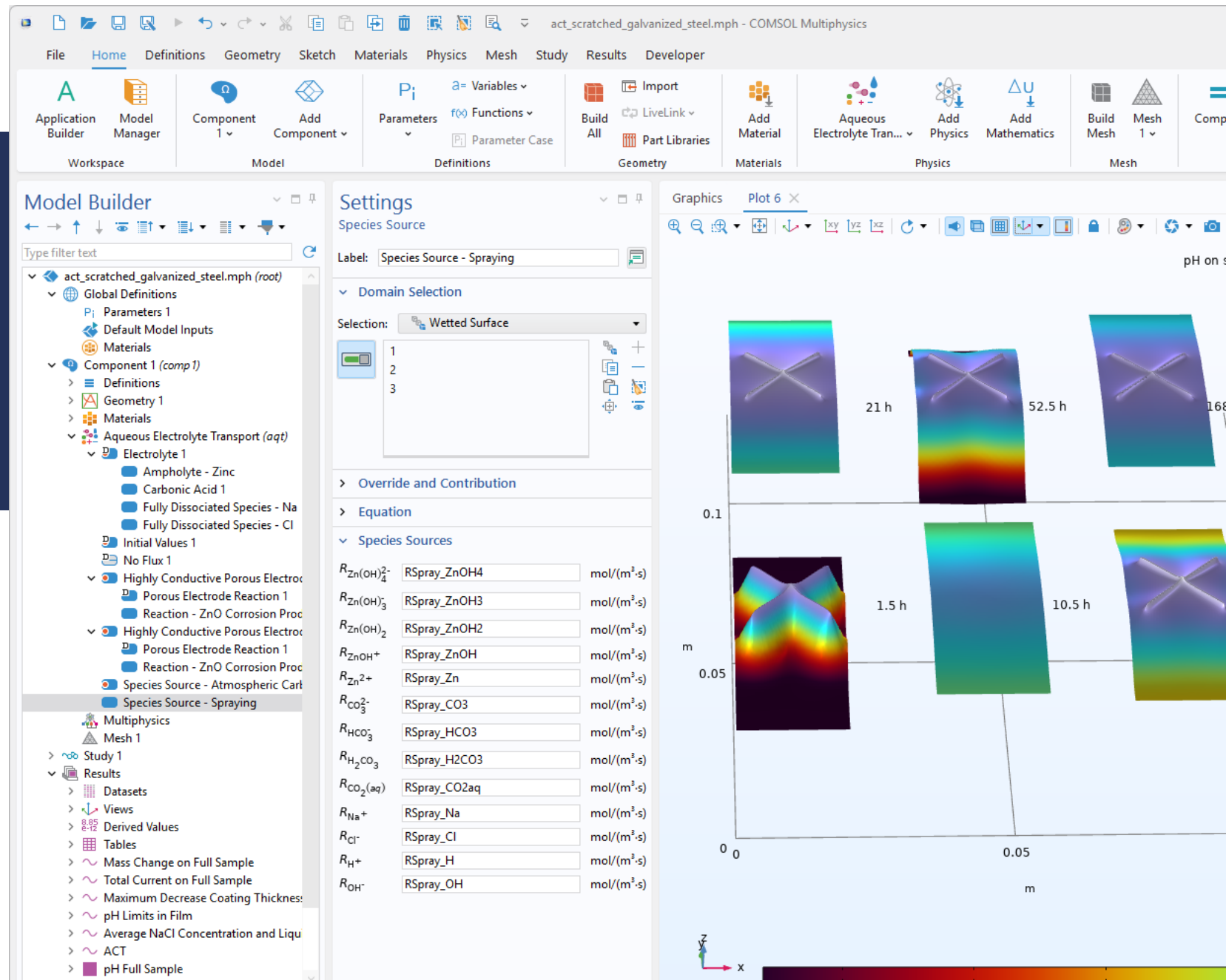


Atmospheric corrosion.

CASE STUDY

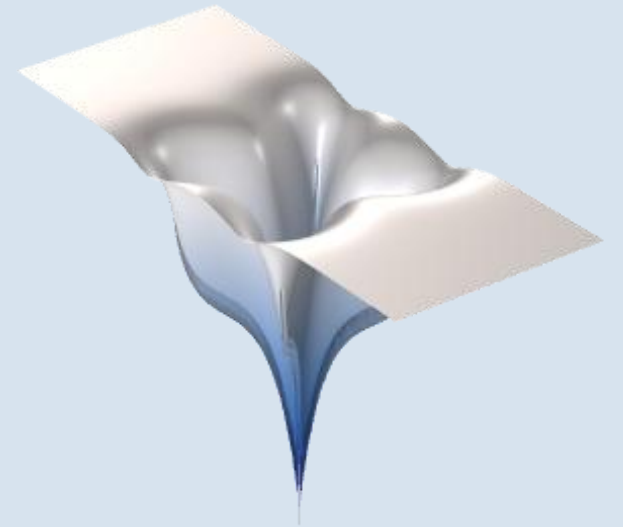
Accelerated corrosion test (ACT)

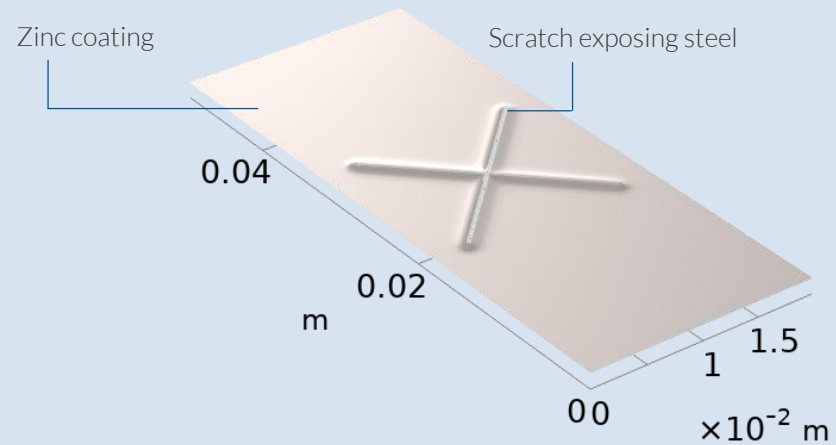
Accelerated corrosion test in a testing chamber for a scratched test plate of galvanized steel.



Model Background

- An established method for benchmarking the atmospheric corrosion resistance of materials is the use of accelerated corrosion tests (ACT) performed in climate chambers
- ACTs aim at making reliable and fast predictions of the long time behavior; weeks of exposure instead of years
- Elevated temperature, repeated drying and wetting together with salt addition are conditions that typically speed up corrosion and characterize ACTs
- This example studies a thin porous film on a galvanized steel sample with crossing scratches
- The corrosion is simulated and analyzed for a dummy ACT



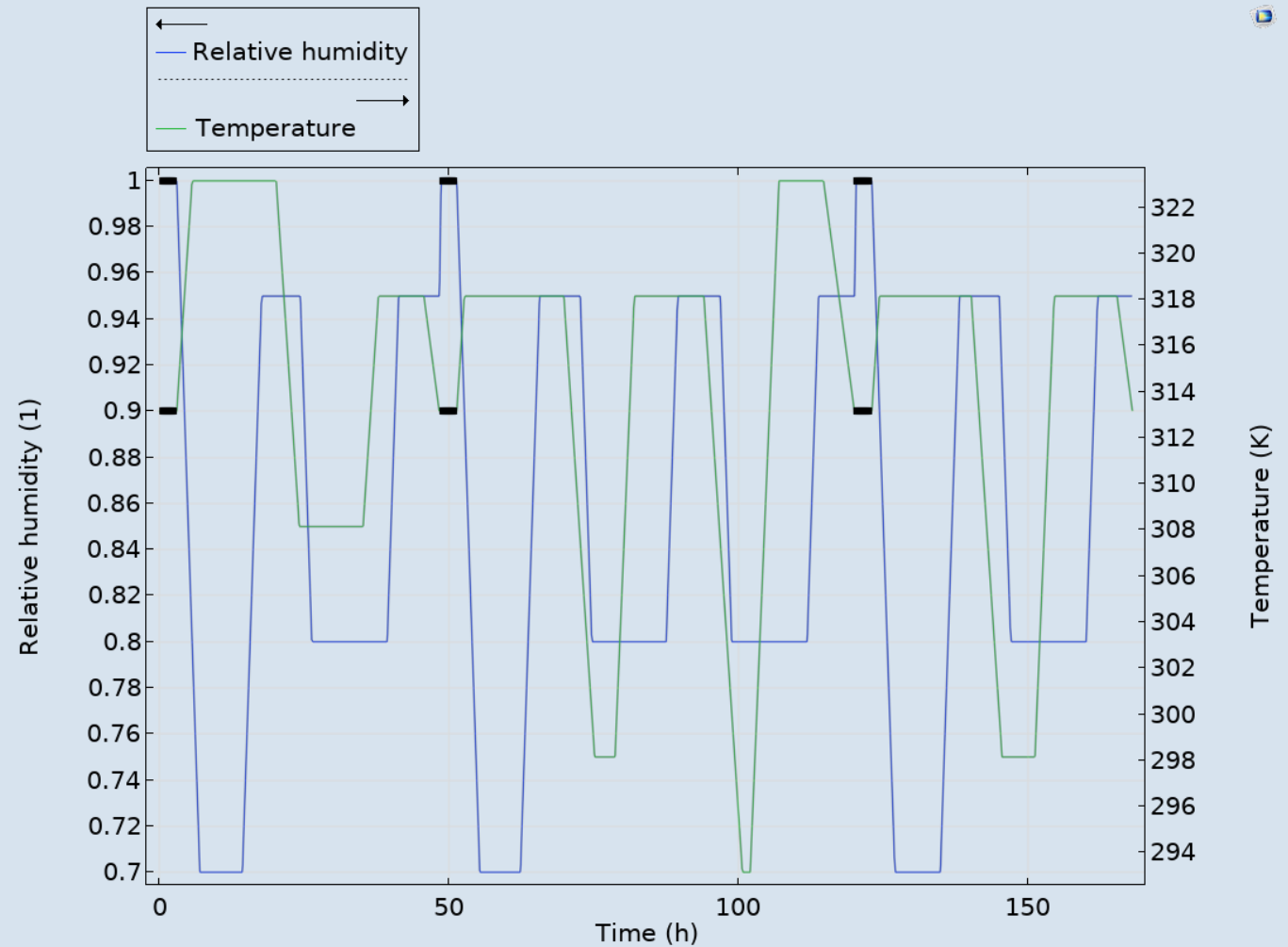


Geometry

2 x 5 cm² sample with 0.1 mm wide scratches fully penetrate the zinc coating and expose the steel

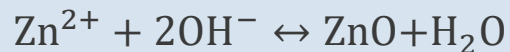
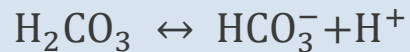
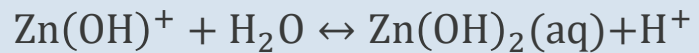
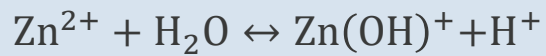
ACT Setup

- ACT running for 7 days
- Liquid film thickness depending on relative humidity (RH)
- Constant film thickness during spray and tenfold replenishment of liquid during each spraying period
- Discontinuous film below deliquescence RH for the NaCl salt
- Horizontal orientation of sample



ACT. Solid black lines indicate periods of spraying 1 wt% NaCl solution

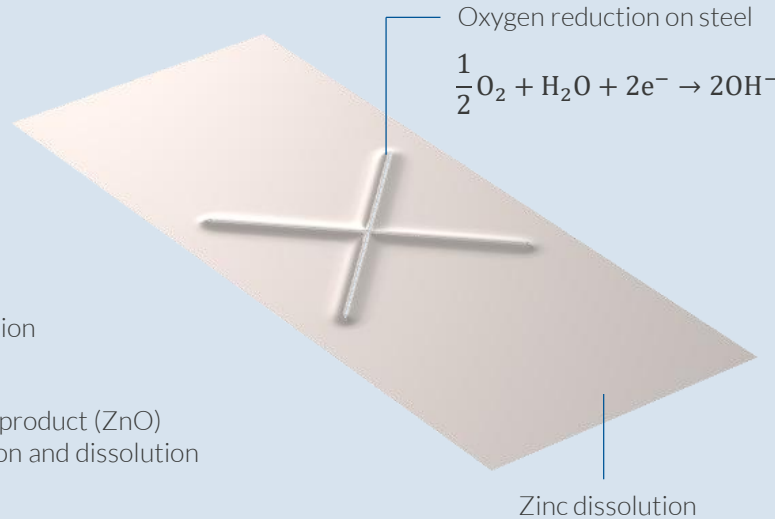
Model Setup



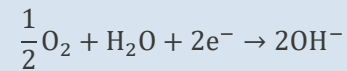
Aqueous
zinc species
hydrolysis

Carbonate
deprotonation

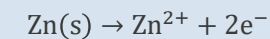
Corrosion product (ZnO)
precipitation and dissolution



Oxygen reduction on steel



Zinc dissolution



Reaction System

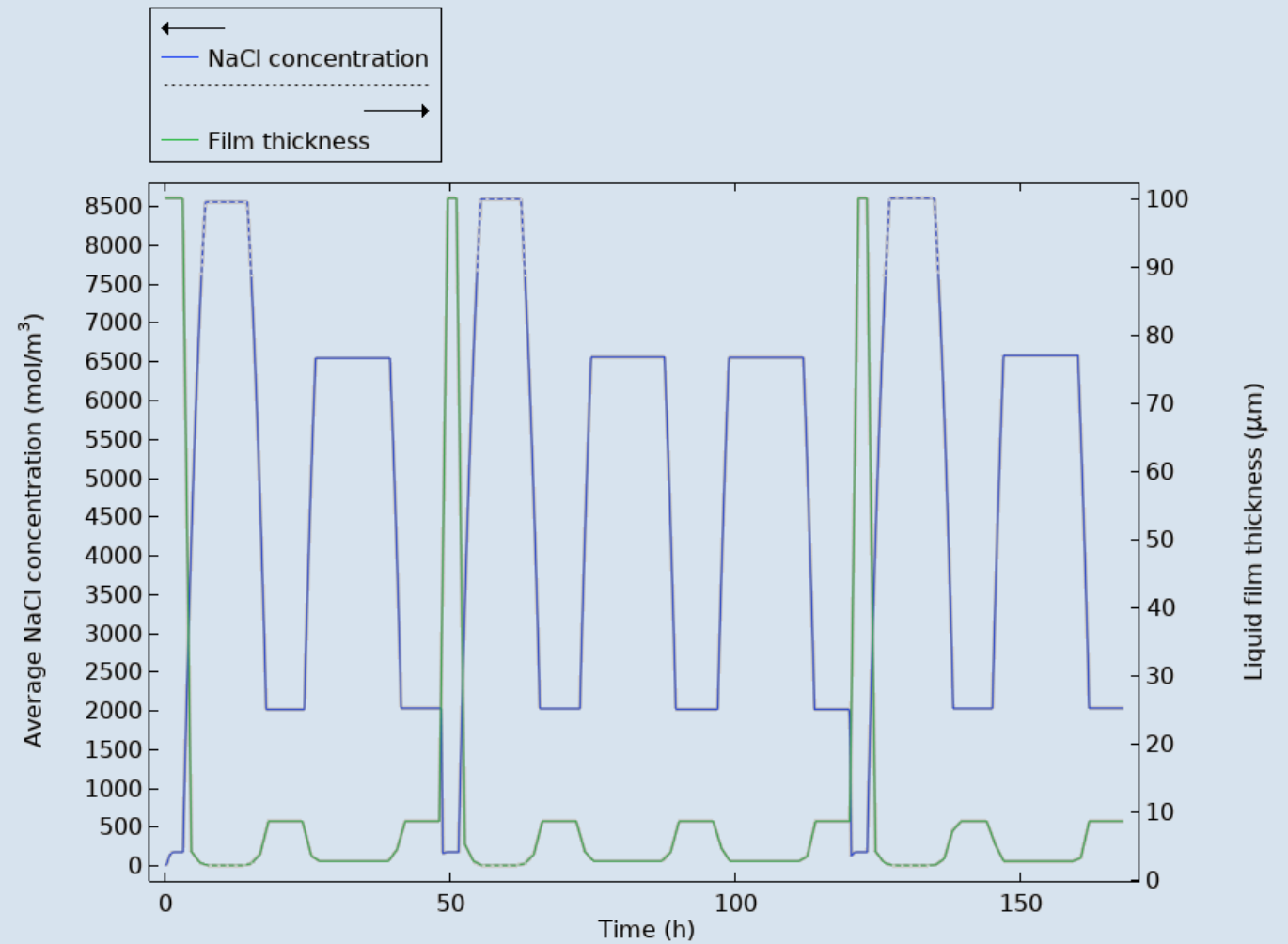
Electrochemical, homogeneous, and heterogeneous reactions accounted for

Corrosion Product

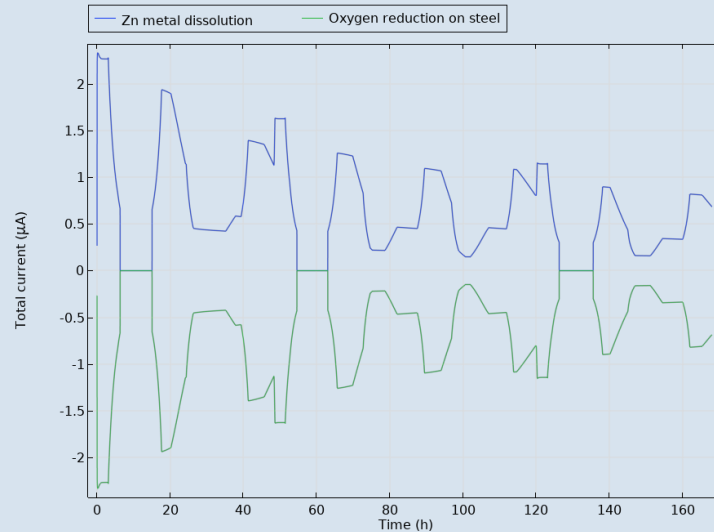
The precipitated amount of corrosion product covers the sample. The coverage acts to passivate the metals.

Results

- The salt concentration and film thickness vary considerably during the 7 days and highlight test aggressiveness

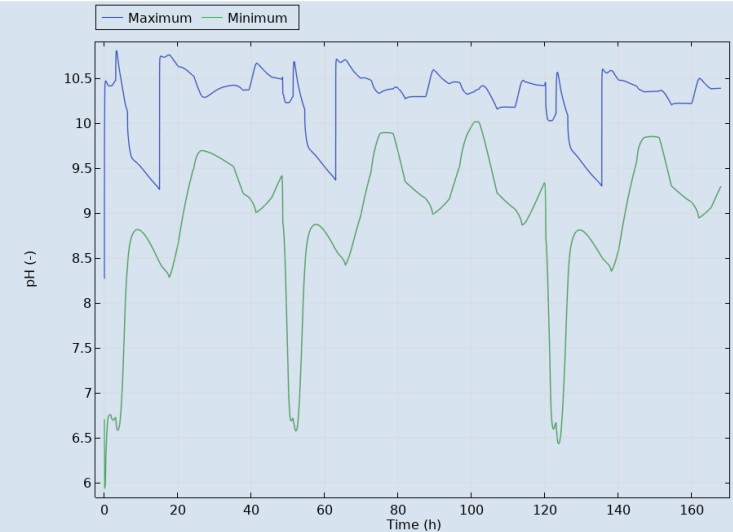


Monitored Corrosion Indicators



Electrochemical Reaction Currents

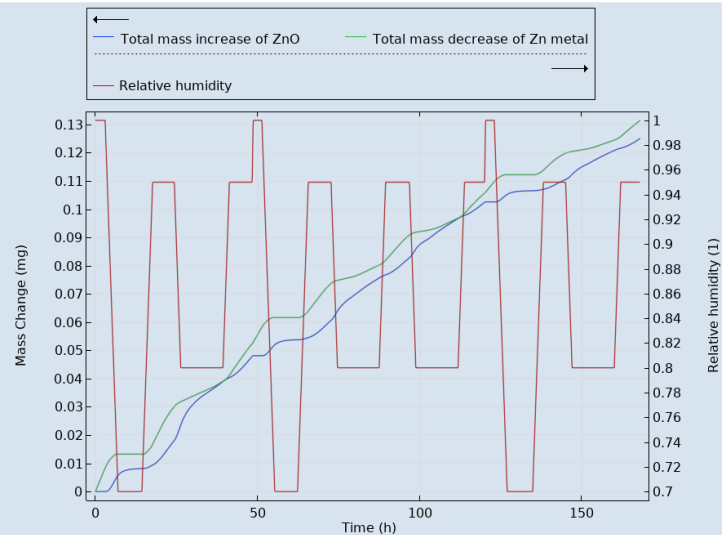
Currents are in the range of μA and decrease over time



pH

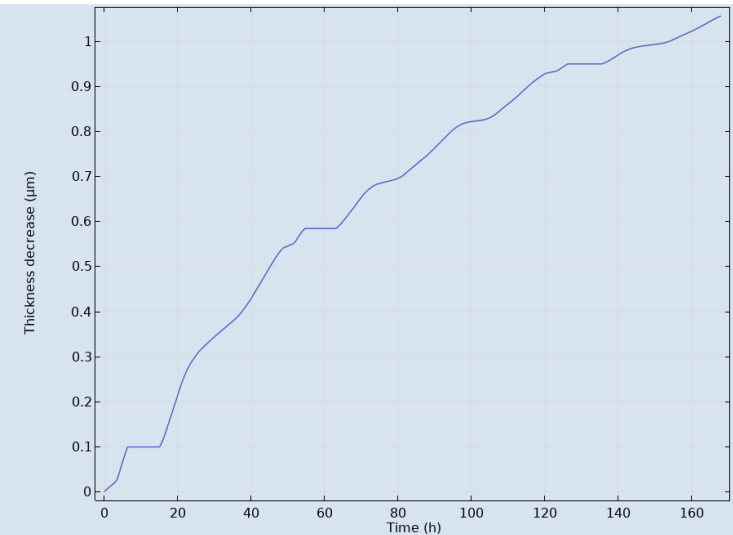
The pH variations show basic solution conditions being prominent, favoring passivating corrosion-product precipitation

Monitored Corrosion Damage



Mass Change

Zinc coating loss and corrosion product increase



Zinc Coating Thickness

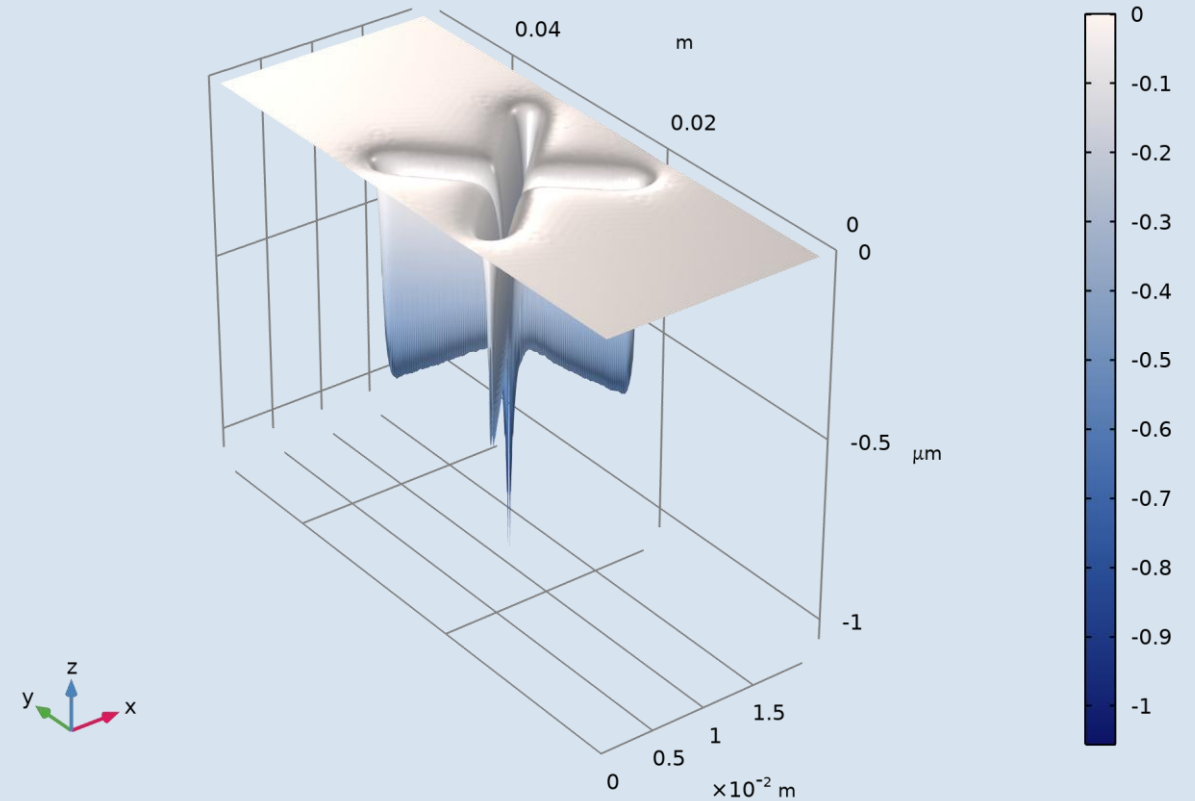
The maximum decrease in coating thickness slows down over time

Corrosion Damage

- After 7 days the zinc coating has mainly been consumed near the scratches
- Most damage is expected near the sample center

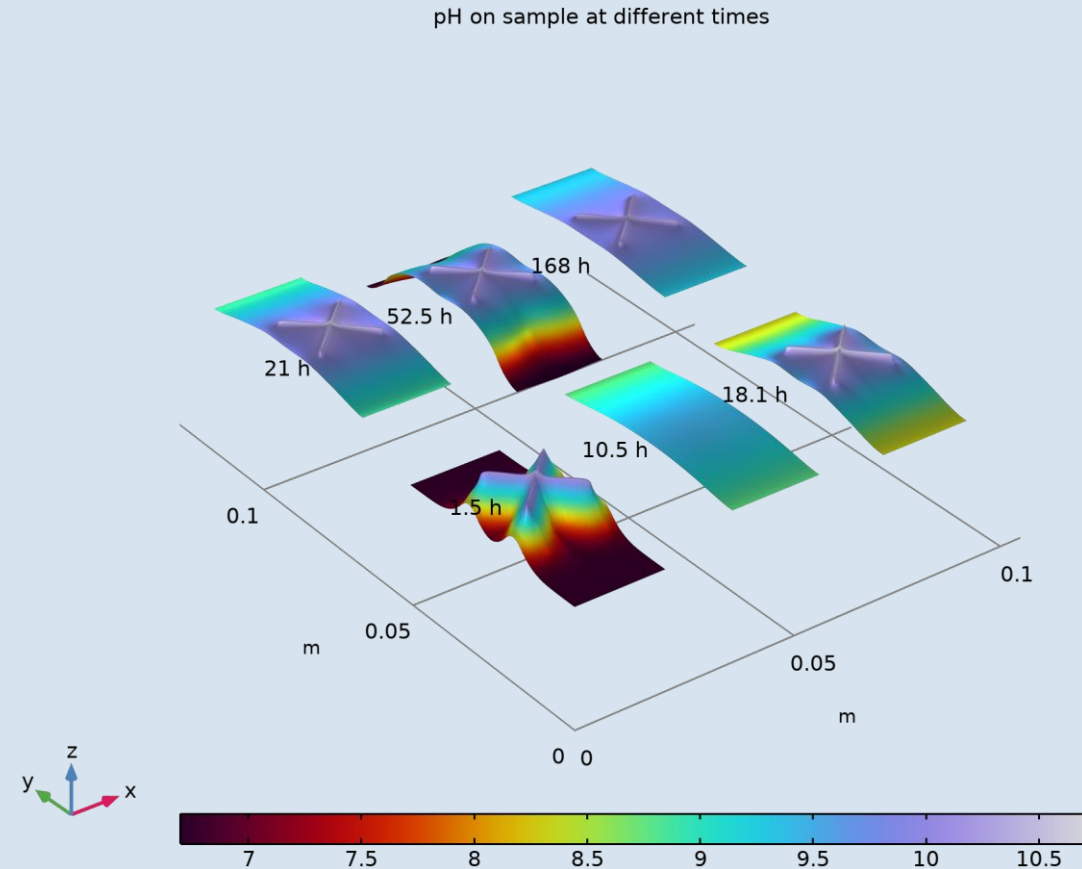
Time=168 h

Thickness decrease (μm)



pH

- The oxygen reduction reaction in the scratch raises the pH
- Acidifying reactions, such as zinc-ion hydrolysis, lowers the pH further away from the scratches

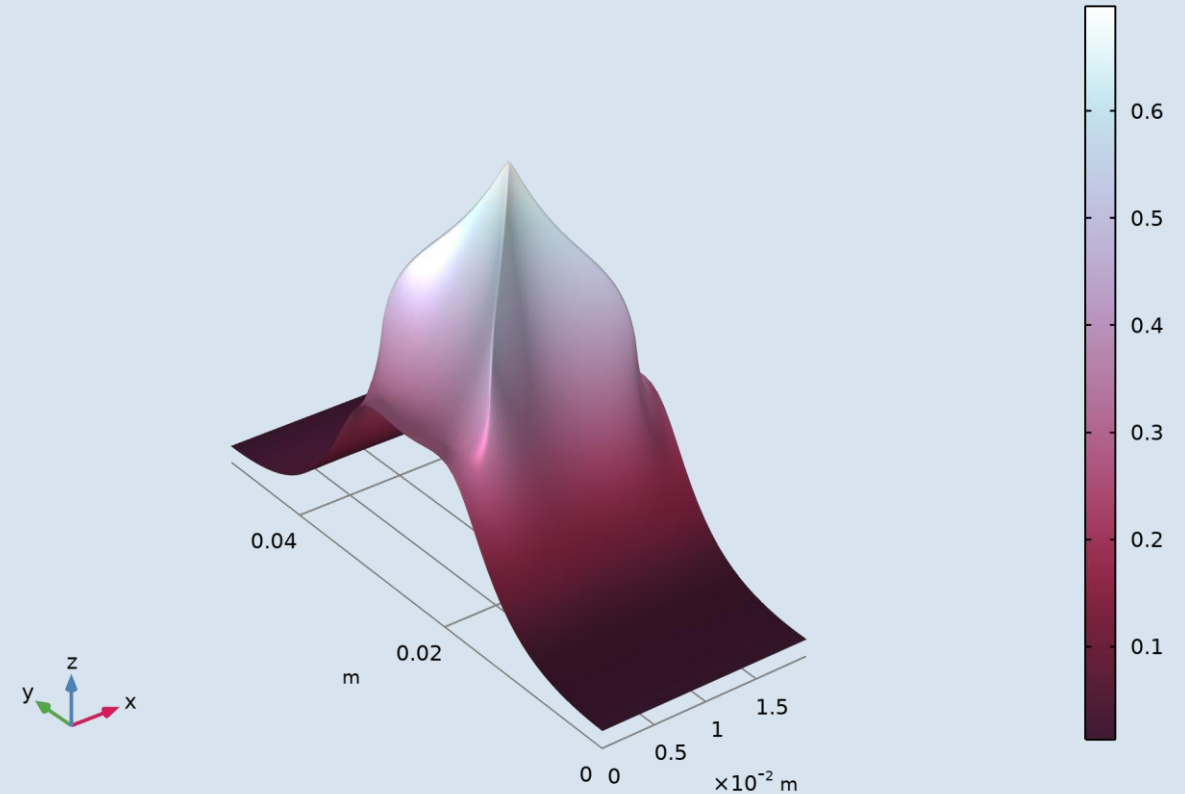


Coverage and Passivity

- Considerable increase in coverage during the ACT
- Passivating effect of coverage is manifested in the decrease in corrosion rate

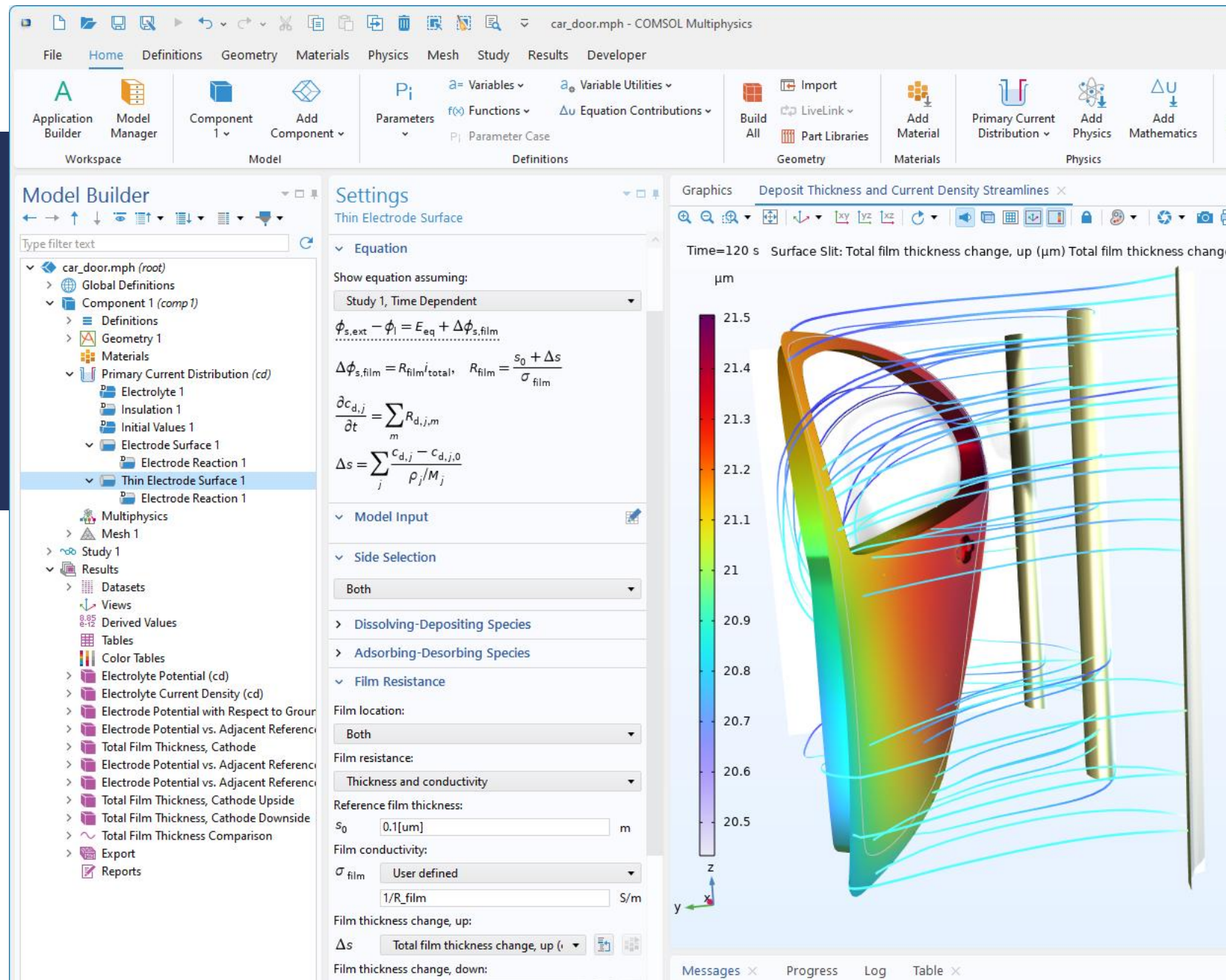
Time=168 h

Coverage degree (1)



Electrocoating of a Car Door

- Thin deposits described with thickness variable
- Deposit conductivity and thickness influence current density distribution
- The electrode can be a geometry boundary or a shell surface (thin electrode surface)

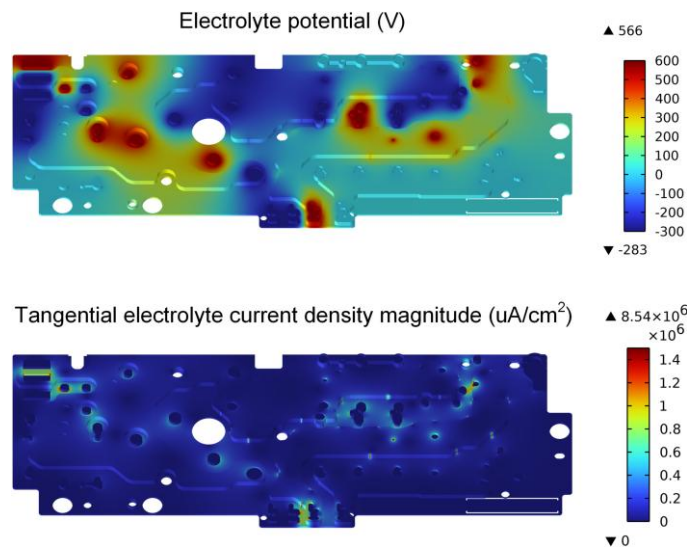


INNOVATION AT
CELCORR (DTU)

Automotive Corrosion Analysis

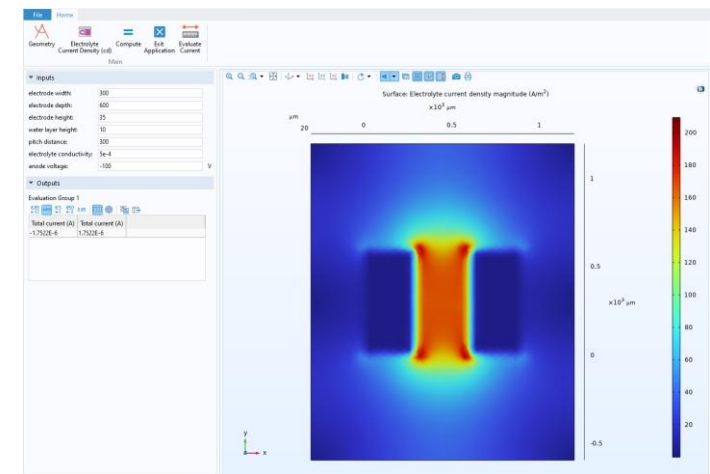
Identifying the root cause of
electronics failures with
simulation apps

Condensation on electronic surfaces caused by humidity can lead to corrosion, which can result in stray leak current and dendrite shorting during electrochemical migration. As the interest for high-voltage electronics increases, the risks associated with their sudden failure must be considered.

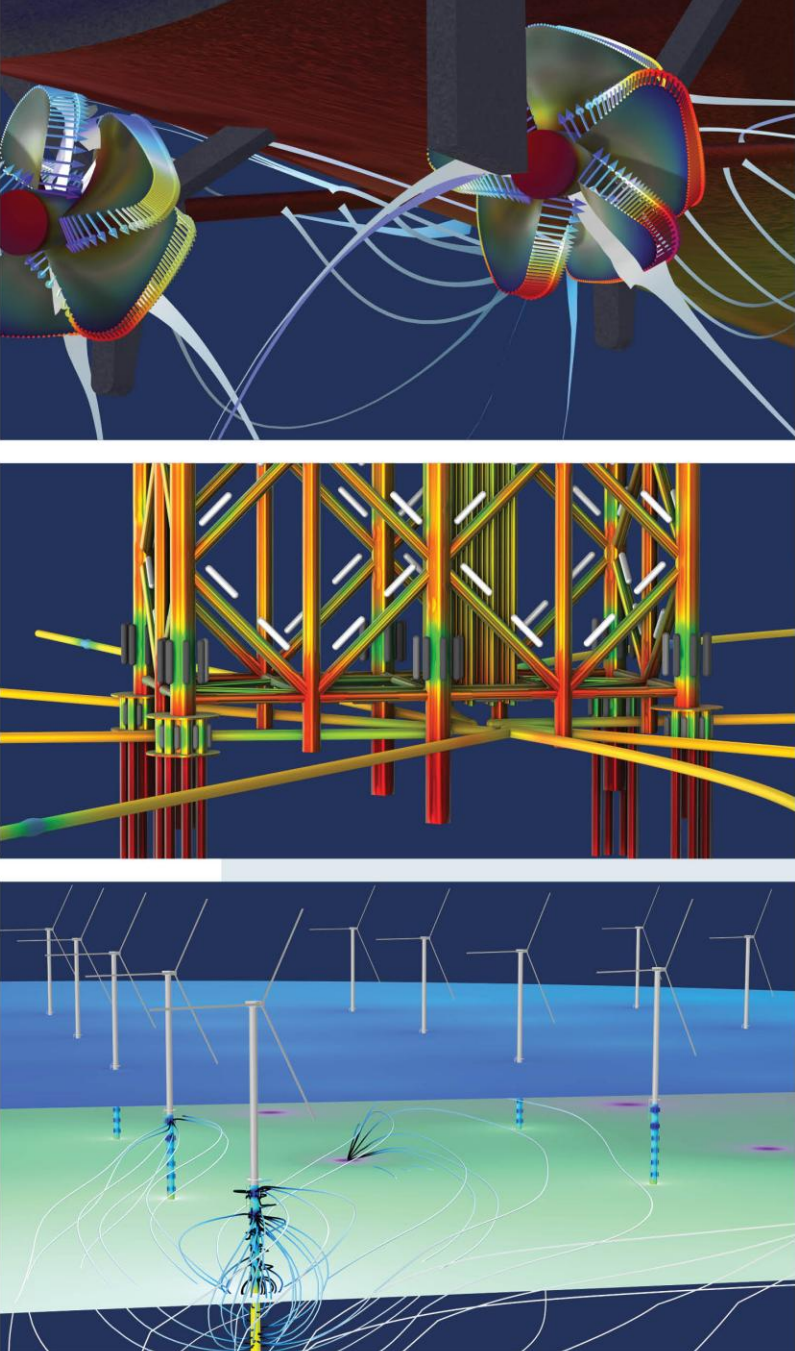


The model uses a simple PCB geometry with a water film layer added on top to represent humidity. By varying the layout, geometry, electrode spacing, water film thickness, and water film conductivity, the electrochemical leak current can be computed to indicate whether the PCB will be affected.

The simulation apps are designed to show how the distance between the electrodes and the thickness of the moisture layer affect the leak current through the water film. By analyzing multiple design elements and parameters, users can determine the relative benefits of certain design elements on humidity robustness.



“The apps we have built have really helped” because they give electronics engineers a “plug-and-play” approach for studying how design parameters influence performance under humid conditions.” — *Dr. Anish Rao Lakkaraju, postdoctoral researcher at CELCORR.*



Corrosion Protection Modeling

comsol.com/feature/corrosion-protection-innovation

Modeling and simulation helps engineers understand how corrosion will impact a particular structure and enables them to optimize the corrosion protection system design accordingly, thereby increasing structural integrity and longevity.

REAL-WORLD EXAMPLES

- Automotive Components
- Materials Science
- Nuclear Waste Storage
- Multimaterial Assemblies