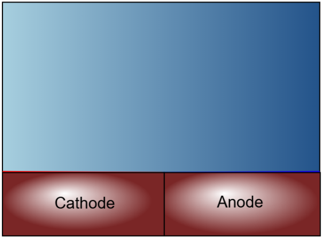
Friedrich-Alexander-Universität
DYNAMICS, CONTROL, MACHINE LEARNING AND NUMERICS

SCHAEFFLER

Analytical and Numerical Aspects of Corrosion Modeling

24.03.2025

Corrosion



- How does the metal degrade over time?

Full model

- System coupled PDEs on the domain Ω corresponding to the liquid

$$\begin{cases} -\Delta\phi = F\sum_{i=1}^{N} z_i c_i \\ \frac{\partial c_i}{\partial t} - \nabla\cdot\left(D_i\nabla c_i - \frac{z_i D_i e}{k_B T} c_i \nabla\phi\right) = 0, \quad i = 1, \cdots, N \end{cases}$$

  - ⋆ c_i: concentration of species i
  - ⋆ ϕ: electric potential of the liquid

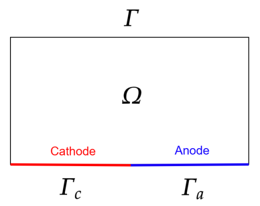
- Electroneutrality assumption:

$$\sum_{i=1}^{N} z_i c_i = 0$$

- System of PDEs with ϕ uncoupled from c_i:

$$\begin{cases} -\Delta\phi = 0 \\ \frac{\partial c_i}{\partial t} - \nabla\cdot\left(D_i\nabla c_i - \frac{z_i D_i e}{k_B T} c_i \nabla\phi\right) = 0, \quad i = 1, \cdots, N \end{cases}$$

- Example domain Ω with boundary $\partial\Omega = \Gamma_c \cup \Gamma_a \cup \Gamma$



- Boundary conditions for ϕ:

$$\begin{cases} -\Delta\phi = 0 & \text{in} \quad \Omega \\ \partial_\nu \phi = 0 & \text{on} \quad \Gamma \\ \partial_\nu \phi = -\frac{i_c(\phi)}{\kappa} & \text{on} \quad \Gamma_c \\ \partial_\nu \phi = -\frac{i_a(\phi)}{\kappa} & \text{on} \quad \Gamma_a \end{cases}$$

- Bottom BCs:

$$\begin{cases} i_a(\phi) & = A_1 \left(e^{C(B_1+\phi)} - e^{-C(B_1+\phi)} \right), \\ i_c(\phi) & = A_2 \left(e^{-C(B_2-\phi)} - e^{C(B_2-\phi)} \right), \end{cases}$$

Well-posedness of static problem

- Variational formulation:

$$\min_{\phi \in H^1(\Omega)} \frac{1}{2} \int_\Omega |\nabla \phi|^2 \, dx + \int_{\Gamma_c} \frac{I_c(\phi(s))}{\kappa} \, ds + \int_{\Gamma_a} \frac{I_a(\phi(s))}{\kappa} \, ds$$

  - ⋆ I_c, I_a primitives of i_c, i_a respectively
  - ⋆ Existence and uniqueness by standard arguments of Calculus of Variations

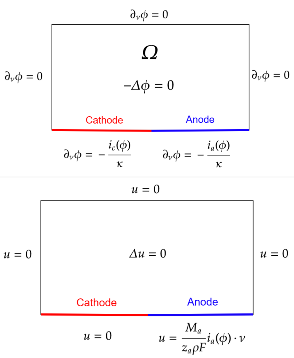
- Regularity:

$$\phi \in H^{3/2}(\Omega)$$

  - ⋆ Argument by Trudinger's embedding [1] (critical case of Sobolev's embedding: $W^{1,p}$ with $d = p = 2$)

[1] Trudinger, N. S. (1967), "On imbeddings into Orlicz spaces and some applications", J. Math. Mech., 17: 473–483.

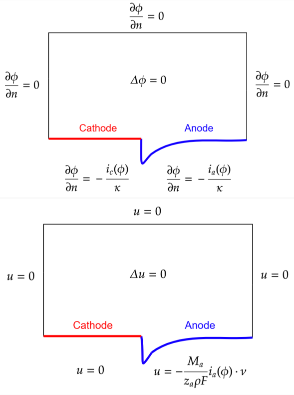
Time discretization

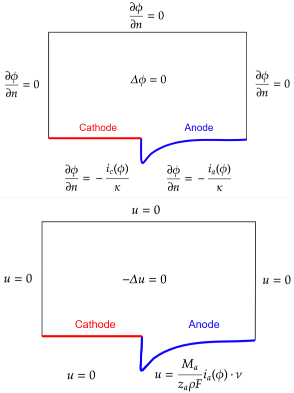


$$\Longrightarrow$$

$$x_{new} = x + \Delta t\, u(x)$$

$$x \in \Omega$$

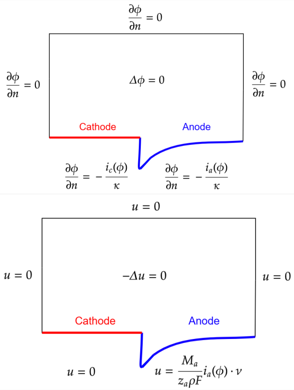




$$\Longrightarrow$$

$$x_{new} = x + \Delta t \, u(x, t_i)$$

$$x \in \Omega(t_i)$$



Full model

Time discretization: $\{t_i\}_{i=1}^{N} \subset [0, T]$.

1. Solve for $\phi(\cdot, t_i)$:

$$\begin{cases} -\Delta\phi(\cdot, t_i) = 0 & \text{in} \quad \Omega(t_i), \\ \partial_\nu \phi(\cdot, t_i) = 0 & \text{on} \quad \Gamma_1(t_i), \Gamma_2(t_i), \Gamma_3(t_i) \\ \partial_\nu \phi(\cdot, t_i) = -\frac{i_c(\phi(\cdot, t_i))}{\kappa} & \text{on} \quad \Gamma_4(t_i), \\ \partial_\nu \phi(\cdot, t_i) = -\frac{i_a(\phi(\cdot, t_i))}{\kappa} & \text{on} \quad \Gamma_5(t_i). \end{cases}$$

2. Solve for $u(\cdot, t_i)$:

$$\begin{cases} -\Delta u(\cdot, t_i) = 0 & \text{in} \quad \Omega(t_i), \\ u(\cdot, t_i) = 0 & \text{on} \quad \Gamma_1(t_i), \Gamma_2(t_i), \Gamma_3(t_i), \Gamma_4(t_i) \\ u(\cdot, t_i) = \frac{M_a}{z_a \rho F} i_a(\phi(\cdot, t_i)) \cdot \nu(\cdot, t_i) & \text{on} \quad \Gamma_5(t_i). \end{cases}$$

3. Displace the old domain $\Omega(t_i)$ into the new domain $\Omega(t_{i+1})$:

$$\overline{\Omega}(t_{i+1}) = \overline{\Omega}(t_i) + u\left(\overline{\Omega}(t_i); t_i\right).$$

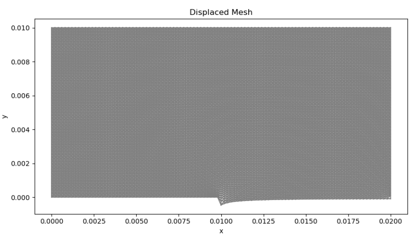
Finite Element Approximation

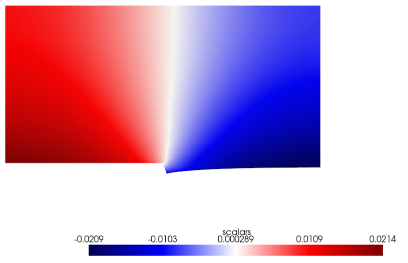
- Let $\phi \sim \sum_j \lambda_j \varphi_j^h$ where $\{\varphi_j^h\}$ is a basis of the FEM subspace $V_h \subset H^1(\Omega(t_i))$ and h is the maximum diameter of the mesh elements
- Minimization of convex energy functional through gradient descent:

$$\min_{\{\lambda_j\}_j \subset \mathbb{R}} \frac{1}{2} \int_{\Omega(t_i)} \left| \sum_j \lambda_j \nabla \varphi_j^h \right|^2 dx + \int_{\Gamma_c(t_i)} \frac{I_c(\sum_j \lambda_j \varphi_j^h)}{\kappa} ds + \int_{\Gamma_a(t_i)} \frac{I_a(\sum_j \lambda_j \varphi_j^h)}{\kappa} ds$$

- Regularity $\phi \in H^{3/2}(\Omega) \implies$ Convergence of FEM in $H^1(\Omega)$ with convergence rate $O(h^{1/2})$ if Ω is smooth

Numerical simulations

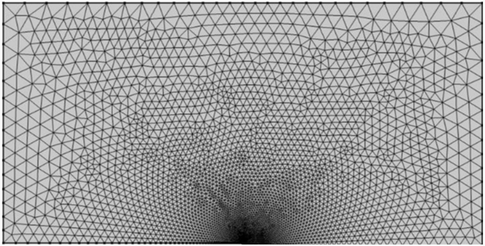




FEM simulation of corrosion between Magnesium and Steel after 90 hours under salt water - mesh (left) and colour plot of ϕ (right)

Open problems

- Convergence of FEM in non-smooth domains to $u \in H^{1/2-\epsilon}$
- More realistic boundary conditions on the electrolyte $\Longrightarrow$ Thin-film modeling of the electrolyte
- Adaptive remeshing techniques near the intersection between cathode an anode



Thank you for your attention!