A Nonlocal Multiphysics Model for Local Corrosion

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Introduction

Corrosion adversely affects the performance of metal alloys that are widely used as structural materials in the automobile, naval, and aircraft industries. We have developed a simplified multiphase (solid, liquid, and porous interphase) nonlocal model for pitting corrosion in aluminum alloys.

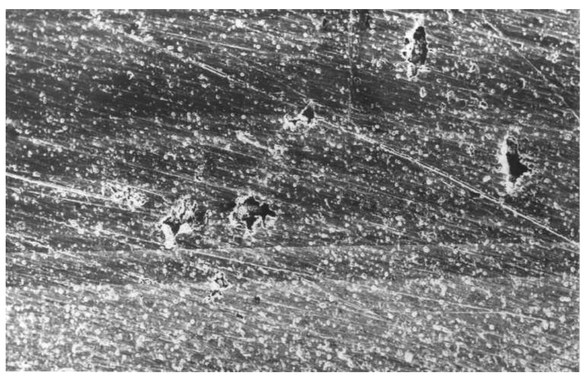


Figure: Pitting corrosion of aluminium

- Corrosion can cost nations between 2% to 5% of their Gross National Product.
- Pits often go undetected and as they grow the chance of a structural failure or cracking increases
- The damage caused by pitting corrosion can lead to catastrophic events such as oil and gas pipelines exploding.

Geometry of the system

Initially, the domain is divided into two regions

- Ω_e - the liquid *electrolyte* phase which contains dissolved species
- Ω_m - the pristine Al *metal* phase.

As the salt solution gradually infiltrates into the metal subsurface, a third region

- Ω_i - the interphase

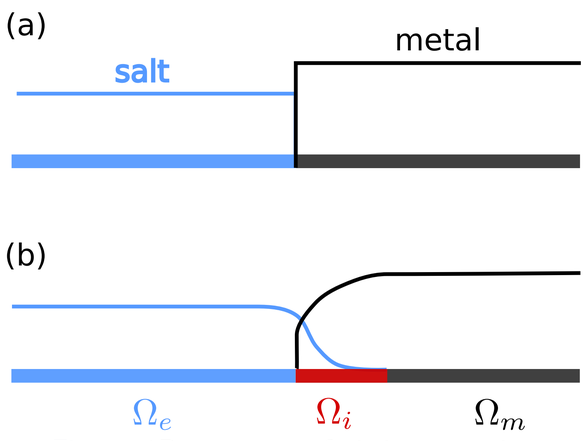


Figure: 1D geometry of pitting corrosion

The rules governing the movement of the boundaries depend on the degree of corrosion ψ.

$$\psi(x,t) = \begin{cases} 0 & \text{for } x \in \Omega_e \\ 1 - \dfrac{C_{\mathrm{Al}}(x,t)}{C^0_{\mathrm{Al}}} & \text{for } x \in \Omega_m \cup \Omega_i \end{cases} \tag{1}$$

Thus, $\psi = 0$ and $\psi = 1$ in Ω_e and Ω_m, respectively. In Ω_i, it takes intermediate values, $0 < \psi < 1$. We specify two threshold levels, ψ_m and ψ_e, that determine when an element is transformed from one phase to another.

Chemical Reaction networks

We will define the dynamics of a chemical reaction network as such. Given n chemical species and m reactions, the j^{th} reaction can be written as

$$s_{1j}C_1 + s_{2j}C_2 \ldots + s_{nj}C_n \xrightarrow{k_j} r_{1j}C_1 + r_{2j}C_2 + \ldots + r_{nj}C_n \tag{2}$$

or more succinctly as

$$\sum_{i=1}^{n} s_{ij}C_i \xrightarrow{k_j} \sum_{i=1}^{n} r_{ij}C_i. \tag{3}$$

Where C_i is the concentration of the i^{th} chemical species, and s_{ij} and r_{ij} are the the stoichiometric coefficients of reactants and products, respectively.
Applying the law of mass action we can calculate the rates for each reaction as

$$f_j([\vec{C}]) = k_j \prod_{i=1}^{n} [C_i]^{s_{ij}} \tag{4}$$

If we define a stoichiometric matrix as $S_{ij} = r_{ij} - s_{ij}$ then we can write the time evolution for our system as

$$\frac{d[C_i]}{dt} = \sum_{j=1}^{m} S_{ij} f_j([\vec{C}]) \tag{5}$$

Nonlocal Reaction Diffusion

The nonlocal reaction-diffusion model with homogeneous reactions

$$\dot{C}_j(x,t) = \int_{x-\delta}^{x+\delta} J_j(x,\hat{x},t)\, d\hat{x} + R_j(\mathbf{C}(x,t)) \tag{6}$$

with

$$J_j(x,\hat{x}) = \left(D_j \Delta C_j(x,\hat{x}) + z_j \frac{F D_j \bar{C}_j(x,\hat{x})}{RT} \Delta\phi(x,\hat{x}) \right) K(x,\hat{x}), \tag{7}$$

The kernel $K(x,\hat{x})$ may be chosen to reflect Fickian or non-Fickian diffusion,

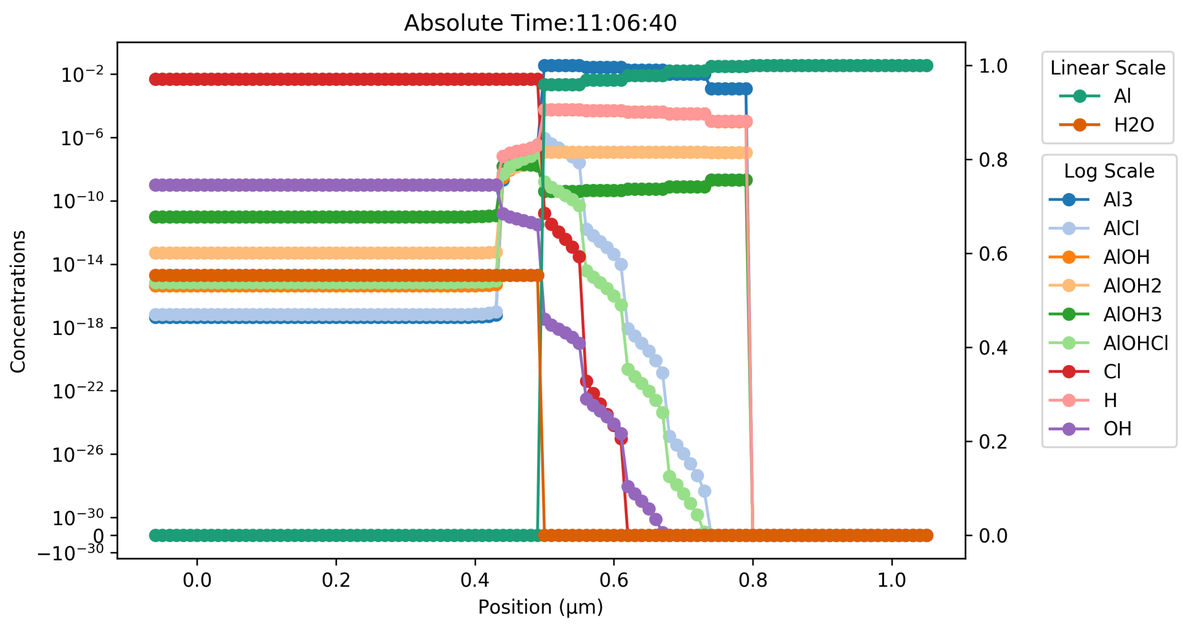
$$K(x,\hat{x}) = \frac{0.5\delta^{2s}}{|\hat{x} - x|^{1+2s}}. \tag{8}$$

A detailed chemical reaction network was used to capture the behavior of the corrosion process

$$\begin{aligned}
H_2O &\rightarrow H^+ + OH^- \\
H^+ + OH^- &\rightarrow H_2O \\
Al^{3+} + H_2O &\rightarrow AlOH^{2+} + H^+ \\
AlOH^{2+} + H^+ &\rightarrow Al^{3+} + H_2O \\
AlOH^{2+} + H_2O &\rightarrow AlOH_2^+ + H^+ \\
AlOH_2^+ + H^+ &\rightarrow AlOH^{2+} + H_2O \\
AlOH_2^+ + H_2O &\rightarrow AlOH_3 + H^+ \\
AlOH_3 + H^+ &\rightarrow AlOH_2^+ + H_2O \\
Al^{3+} + Cl^- + H_2O &\rightarrow AlCl^{2+} + H_2O \\
AlCl^{2+} + H_2O &\rightarrow Al^{3+} + Cl^- + H_2O \\
AlOH^{2+} + Cl^- + H_2O &\rightarrow AlOHCl^+ + H_2O \\
AlOHCl^+ + H_2O &\rightarrow AlOH^{2+} + Cl^- + H_2O \\
Al &\rightarrow Al^{3+}
\end{aligned}$$

- The electrolyte phase consists of 12 homogeneous reaction involving corrosion byproducts with the solution.
- A simple surface reaction is introduced which produces the aluminum ions.
- A future goal of this project is to identify and remove chemical species and reactions which don't significantly effect the profile of important species, such as the aluminum.

Initial Results



Future Work

- I am currently working on developing intermediate models maintain the corrosion profile behavior but depend on fewer reactions and species. These smaller reaction networks would run faster while minimizing deviations from the full model.

Acknowledgments

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