



Numerical method for time-dependent localized corrosion analysis with moving boundaries by combining the finite volume method and voxel method

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ARTICLE INFO

Article history:

Received 11 January 2012

Accepted 5 June 2012

Available online 14 June 2012

Keywords:

- A. Alloy
- B. Electrochemical calculation
- B. Modeling studies
- B. Polarization
- C. Crevice corrosion
- C. Pitting corrosion

ABSTRACT

A novel numerical method for time-dependent localized corrosion analysis is presented. Electromigration, mass diffusion, chemical reactions, and moving boundaries are considered in the numerical simulation of localized corrosion of engineering alloys in an underwater environment. Our method combines the finite volume method (FVM) and the voxel method. The FVM is adopted in the corrosion rate calculation so that the conservation of mass is satisfied. A newly developed decoupled algorithm with a projection method is introduced in the FVM to decouple the multiphysics problem into the electrostatic, mass transport, and chemical reaction analyses with electroneutrality maintained. The polarization curves for the corroding metal are used as boundary conditions for the metal surfaces to calculate the corrosion rates. The voxel method is adopted in updating the moving boundaries of cavities without remeshing and mesh-to-mesh solution mapping. Some modifications of the standard voxel method, which represents the boundaries as zigzag-shaped surfaces, are introduced to generate smooth surfaces. Our method successfully reproduces the numerical and experimental results of a capillary electrophoresis problem. Furthermore, the numerical results are qualitatively consistent with the experimental results for several examples of crevice corrosion.

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1. Introduction

Localized crevice and pitting corrosion damages the passive films of corrosion-resistant alloys, such as stainless steel and aluminum alloys, and is a major cause of damage to engineering alloys in underwater environments [1–3]. Small differences in pH, electric field, and metal alloy composition [4–7] cause large changes in localized corrosion. Localized corrosion has been studied experimentally under specific conditions [6,8–12], yet corrosion rate prediction based on those observations remains difficult. Therefore, numerical analysis for predicting corrosion rates is important from an engineering perspective.

The analysis of localized corrosion rates is a complex multiphysics problem [13–15] that involves electrostatics, mass transport, and chemical reactions. The conservation of mass and electroneutrality must be simultaneously satisfied. Moreover, the moving boundaries of the analysis domain must be taken into consideration to perform a time-dependent analysis [13,16].

Localized corrosion studies have focused mainly on the ion concentration distribution and the current density distribution over a one-dimensional domain [17,18,13,15,14,19–24]. The numerical

method used to calculate the effect of charge density on mass transport (i.e., to calculate the Poisson term [25,13]) over the localized corrosion timescale is important, because it affects the calculation efficiency. Heppner et al. have developed a computationally efficient correction algorithm that satisfies electroneutrality [25], but their method does not satisfy conservation of mass in arbitrary boundary shapes. Scheiner and Hellmich [26,27] have proposed a method that deals with the moving boundaries by using the finite volume method (FVM) and the voxel method over two-dimensional domains. However, their approach neglects the interaction between multiple ions which is necessary to consider for chemical reactions and electroneutrality, and the method does not treat cavity boundaries as smooth surfaces. Laycock et al. [28–30] have presented computer simulations of single pit propagation in stainless steel. However, their method employs the finite element method (FEM) with the remeshing and mesh-to-mesh solution mapping method; thus, the conservation of mass get broken little by little in timesteps. Moreover, the method neglects the Poisson term without any numerical correction; thus, the electroneutrality also gets broken as well. To our knowledge, there have been no studies that have successfully handled both the multiphysics calculation and the smooth moving boundaries of arbitrary cavity shapes with the conservation of mass and electroneutrality satisfied.

In the present study, a numerical method for time-dependent localized corrosion analysis is presented, which satisfies all the

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Nomenclature

| | | | |
|-----------------|--|---------------|---|
| j_{\square} | notation for variable of cell j | u_i | mobility of ion i ($= D_i/RT$) [$\text{m}^2 \text{mol}^{-1} \text{s}^{-1}$] |
| k_{\square} | notation for variable of face k | Z_i | charge number of ion i |
| \square' | notation for spatial derivative | λ_i | composition ratio of metal of ion i |
| $\hat{\square}$ | notation for normal component | K | equilibrium constant |
| Φ | electrostatic potential [V] | q | reaction rate constant |
| ϕ | smoothed electrostatic potential [V] | V | volume [m^3] |
| \mathbf{J} | current density vector [A s^{-1}] | M | volume fraction of solid metal |
| κ | electrical conductivity [$(\Omega\text{m})^{-1}$] | \mathbf{n} | unit normal vector |
| ϵ | permittivity [F m^{-1}] | A | surface area [m^2] |
| F | Faraday's constant $F = 96487$ [C mol^{-1}] | \mathcal{M} | molar mass of solid metal [kg mol^{-1}] |
| C_i | molar concentration of ion i [mol m^{-3}] | ρ | density of solid metal [kg m^{-3}] |
| \mathbf{N}_i | ionic molar flux density vector of ion i [$\text{mol m}^{-2} \text{s}^{-1}$] | Γ_m | metal boundary |
| E_i | chemical reaction rate of ion i [$\text{mol m}^{-3} \text{s}^{-1}$] | Γ_c | off-shore boundary |
| D_i | diffusion coefficient of ion i [$\text{m}^2 \text{s}^{-1}$] | | |
| R | gas constant [$\text{J K}^{-1} \text{mol}^{-1}$] | | |
| T | absolute temperature [K] | | |

requirements listed above. Our method combines the FVM and voxel method to handle the multiphysics calculation and the moving boundaries, respectively. The FVM is adopted to satisfy the conservation of mass, and electroneutrality is satisfied by using a newly developed decoupled algorithm with a projection method. The voxel method is used in conjunction with FVM to update the moving boundaries without remeshing and mesh-to-mesh solution mapping. Some modifications of the standard voxel method, which represents the boundaries as zigzag-shaped surfaces, are introduced to generate smooth surfaces.

A brief explanation of the mechanism of localized corrosion is given in Section 2. The equations and boundary conditions used in the mathematical model of localized corrosion are shown in Section 3. The numerical procedure of the proposed method is explained in detail in Section 4. Examples of the analysis, including verification and validation, are shown in Section 5, and the conclusion is presented in Section 6.

2. Mechanism of localized corrosion

The mechanism of localized corrosion, such as crevice corrosion and pitting corrosion, [31,4,32] consists of an initiation step and a propagation step (Fig. 1).

The following general corrosion reactions occur over the entire surface of the metal during the initiation step:

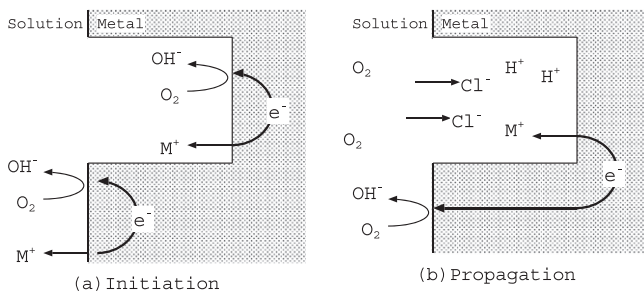
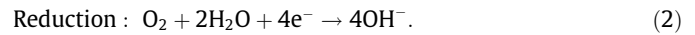
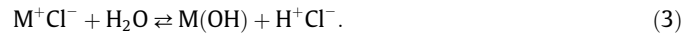


Fig. 1. Mechanism of crevice corrosion. (a) General corrosion reactions occur over the entire surface of the metal. The restricted mass convection in the cavity means O_2 is quickly depleted. (b) The localized corrosion reactions occur in the cavity, and Cl^- ions electromigrate towards the M^+ ions in the cavity. The increase in the concentration of M^+ and Cl^- ions increases the concentration of $\text{M}(\text{OH})$ and H^+ , thereby accelerating the corrosion.



The mass convection in the cavity is restricted, which results in oxygen reduction. An oxygen concentration cell forms between the inside and outside of the cavity and accelerates the internal metal dissolution until the oxygen is depleted.

During the propagation step, chloride ions electromigrate toward the dissolved metal ions in the cavity. The increase in the concentration of the chloride ions and metal ions causes an increase in hydrogen ions through the following reaction:



The hydrogen concentration cell which forms between the inside and outside of the cavity becomes the main factor in the localized corrosion.

The initial step is brief; thus, it does not significantly influence the corrosion behavior, [31] and can be neglected in the numerical analysis.

3. Governing equations and boundary conditions

In this study, electromigration, mass diffusion, chemical reactions, and moving boundaries are taken into consideration. An outline of a typical analysis domain is shown in Fig. 2. The equations for modeling the corrosion around a cavity with a constant shape [13] can be written as

$$\nabla^2 \Phi = \frac{F}{\epsilon} \sum_{i \in I} Z_i C_i, \quad (4)$$

$$\frac{\partial C_i}{\partial t} = -\nabla \cdot \mathbf{N}_i + E_i, \quad (5)$$

$$\mathbf{N}_i = -z_i u_i C_i F \nabla \Phi - D_i \nabla C_i, \quad (6)$$

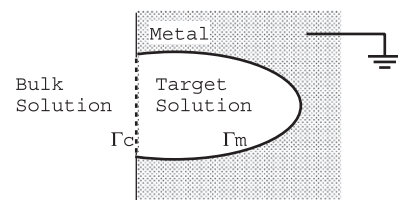


Fig. 2. Diagram of a typical analysis domain in this study. Γ_m represents the metal boundary and Γ_c represents the off-shore boundary.

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