

A Novel Physics-Weighted Adaptive Finite Element Method for Numerical Analysis and High-Accuracy Prediction of Localized Corrosion in Protective Nanocomposite Coatings

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ABSTRACT

In this work, numerical methods for the modeling of reactant transport in nanocomposite coated metallic materials are studied and a physics-weighted adaptive finite element framework is proposed to predict localized corrosion behavior. Using a one-dimensional steady-state reaction–diffusion model, we examined the effects of coating thickness and connected porosity on the metal-interface reactant flux. Numerical solutions are obtained by second-order finite-difference discretization for uniform and geometrically graded meshes and are compared with analytical reference solutions. Mesh convergence study showed that the near second-order accuracy was obtained with estimated convergence orders of 2.01 and 1.96 for uniform and graded meshes, respectively. The relative flux error was reduced from 0.7829% to 0.0030% for uniform meshes and from 5.8919% to 0.0261% for graded meshes by increasing the number of elements from 12 to 192. The parametric calculations showed that the transport of reactants decreased significantly with increasing coating thickness and decreasing porosity. The calculated flux decreased from 266.784 to 12.087 $\mu\text{mol m}^{-2} \text{s}^{-1}$ at 5% porosity with an increase in thickness from 25 to 100 μm , representing a 95.47% reduction. Reactant flux was increased approximately 77.5-fold by increasing porosity from 1% to 10% with a constant thickness of 50 μm . The results demonstrate the sensitivity of transport predictions to coating geometry, effective diffusivity and numerical discretization. On the basis of these preliminary results, a physics-weighted adaptive finite element approach is proposed to incorporate residual-based error estimation and electrochemical gradient indicators. This framework opens the way for additional coupled electrochemical simulations, numerical optimization and corrosion resistant coating design.

KEYWORDS: Adaptive Finite Element Method; Numerical Analysis; Localized Corrosion; Nanocomposite Coatings; Electrochemical Modeling; Nernst–Planck Equation; Butler–Volmer Kinetics; Adaptive Mesh Refinement; Multi-Objective Optimization

INTRODUCTION

Corrosion is a change caused by electricity and chemicals. It reduces the strength, reliability and life of metal engineering parts. Metals used in transportation, biomedical applications, marine structures, energy systems, or industrial processing equipment may develop rust when exposed to water, dissolved oxygen, chloride ions, acidic solutions, or other aggressive chemical species. Damage can be done by uniform dissolution, galvanic coupling, crevice corrosion or localized pitting. It is contingent upon the electrochemical properties of the material and the environment it is used in. Electrochemical reactions are

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highly sensitive to the local electrolyte composition, electrical potential, and surface geometry, which are not uniform and therefore make it difficult to predict the development of localized corrosion. For example, a small defect in a protective coating may allow the surrounding electrolyte to reach a metallic substrate below, thereby creating an electrochemically active region. As ions flow in and out of this region they may establish strong concentration gradients. Charge transfer reactions and geometrical confinement may increase the likelihood that something will fail at a single point.

Thus, the numerical modeling of corrosion has become an important area of research for understanding the mechanisms of electrochemical degradation and for the design of non-corrosive materials. Thermodynamic methods (e.g. first principles electrochemical phase diagrams) can tell us about the stability of a material and products that may form during corrosion. Nevertheless, the prediction of when and where localized corrosion will happen requires consideration of reaction kinetics, species transport, and interfacial phenomena [1]. Recent computer studies have shown that electrochemical phase-field models can describe the evolution of corrosion fronts and the interplay of electrochemical and mechanical processes. Martínez-Pañeda [2] described the growing application of phase-field methods for the modeling of corrosion damage such as film rupture, repassivation and the transition from reaction-controlled to diffusion-controlled dissolution. Cui et al. [3] developed an electro-chemo-mechanical model in COMSOL Multiphysics to demonstrate the significance of the electrostatic potential, the electrolyte concentration, and the interfacial kinetics in predicting the localized corrosion.

Nevertheless, it remains difficult to accurately describe corrosion numerically near microscopic defect sites. Electrochemical fields can vary greatly over very short distances, particularly where coatings are compromised and metals and electrolytes meet. Such local differences are usually eliminated by standard numerical techniques on uniformly discretized computational domains only after many elements. Instead, one can use adaptive numerical methods that concentrate the computational effort on regions where the shape of the numerical solution changes rapidly or large discretization errors are likely to occur. Thus, the development of a robust adaptive finite element framework is a good stride to improve the accuracy and usefulness of electrochemical corrosion simulations.

NANOCOMPOSITE COATINGS AND LOCALIZED CORROSION

Three types of nanostructured materials (polymeric, ceramic and inorganic) have been extensively studied as nanocomposite coatings for corrosion protection. Depending on their composition, these coatings can physically block the penetration of electrolyte, change surface wettability, enhance surface adhesion and modify electrochemical reactions at the coating/substrate interface. But protective coatings are almost never without flaws. Microcracks, interfacial discontinuities and incomplete coverage may form during preparation and service pores. While present, these defects can help transport toxic substances to the underlying metal substrate.

In computer models of these kinds of systems, the coating can be modeled as a disordered transport domain capable of moving and distributing things well, and defects can be modeled as electrolyte-filled channels or open edges. A good model must be capable of discriminating between movement in the bulk electrolyte, movement in the porous coating, and electrochemical reactions on accessible metal surfaces. Where all of these things happen, the math problem is not linear. It has many dependent variables and coefficients spread out in different places. The electric potential moves charged particles. The distribution of ions affects the conductivity of the electrolyte and the rate of the reaction. These coupled processes can produce large variations in the local area that must be accurately discretized numerically. A numerical framework that can address these differences could be useful to learn more about the effect of coating architecture on electrochemical protection.

NUMERICAL MODELING OF ELECTROCHEMICAL CORROSION

For numerical simulations of corrosion, the governing equations describing mass conservation, ion transport, charge conservation and the kinetics of electrochemical reactions are typically solved. The Nernst–Planck formulation is particularly useful to explain the results of the combined action of ionic diffusion and

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electromigration. Without fluid convection, the local concentration gradients and electric fields control the motion of charged species. Electrochemical reduction and dissolution reactions at the interface of two metals can be demonstrated using Butler-Volmer kinetics or polarization relationships calibrated from experiment. The phase-field formulations have increased the utility of these methods by adding changing metal-electrolyte interfaces. Lin et al. [4] developed a coupled phase-field approach for mechanico-electrochemical corrosion. Imanian and Amiri [5] studied corrosion damage with electrochemical phase-field modeling. Later, Amador et al. [6] developed a mathematical model for the aqueous corrosion of low-carbon steel, considering electrochemical, diffusion, and migration processes.

These studies exemplify the importance of multiphysics coupling in corrosion modeling. In contrast, adding detailed physical processes complicates the math, and can make solving problems with sharp gradients or moving interfaces much more expensive. So, this idea starts with a fixed-geometry electrochemical corrosion model that displays metal that is exposed and coatings that aren't functioning properly, but doesn't actually model the movement of the corrosion front. This approach allows the numerical discretization method to be studied on its own, before more complex interface evolution models are considered.

RESEARCH GAP AND PROPOSED INNOVATION

The main goal of this study is to find the best way to numerically solve localized electrochemical phenomena in non-uniform coating systems. Classical finite element computations can show the variations of electrolyte concentration and potential in space but are strongly dependent on the quality of the mesh and the distribution of elements. New ideas in adaptive finite element analysis have demonstrated the importance of a posteriori error estimates for the guidance of local mesh refinement. Basic error estimates for adaptive finite element calculations were given by Babuška and Rheinboldt [7]. Dörfler [8] then proposed a convergent adaptive refinement algorithm for Poisson-type problems and Zienkiewicz and Zhu [9] introduced a recovery-based approach to estimate finite element errors.

In this work we are interested in the investigation of an adaptive refinement indicator weighted based on physics, obtained by combining a well known numerical residual estimator with additional information about the variation of local concentration and current density. The proposed indicator will be validated against the traditional residual only refinement, uniform refinement and fixed fine-mesh reference calculations. The novelty is not only the application of FEM to study corrosion but also the development, validation and quantification of a corrosion sensitive mesh refinement strategy. Its novelty and efficiency will be demonstrated by mathematical analysis, numerical benchmarks and comparison with other published approaches, rather than assumed beforehand.

RESEARCH OBJECTIVES AND HYPOTHESES

The main goal of this study is to develop and validate an accurate and fast adaptive finite element framework for simulating localized electrochemical corrosion in nanocomposite coated metals. The objective of this study is to combine advanced numerical analysis with electrochemical transport modeling to predict corrosion related events in the vicinity of coating defects and exposed metal surfaces. Much focus will be on the development of a mathematical model that includes ionic species transport, electrolyte potential distribution, charge conservation and electrochemical reaction kinetics at interfaces. These governing processes will provide us with the maths we need to explore how coating properties and environmental factors influence the behavior of corrosion in particular areas.

A main goal of the study is to develop a physics-weighted adaptive mesh refinement strategy that combines common numerical error indicators with physically useful electrochemical data, namely, changes in current density and ionic concentration gradients. The accuracy, stability, conservation properties and the speed of the proposed numerical method will be examined carefully. We will compare its performance in comparison to standard uniform-mesh discretization and well-known residual-based adaptive finite element methods. To see if the addition of electrochemical refinement indicators improves numerical resolution in areas more likely to rust, while decreasing the amount of work that needs to be done on the computer.

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The study also aims to determine the influence of coating thickness, associated porosity, defect geometry, chloride content and temperature on the electrochemical and transport behavior that can be predicted. We will use numerical sensitivity analyzes to identify the factors that have a significant effect on the movement of reactants, the distribution of electrolyte potential, the density of localized currents, and the total anodic current. A constrained numerical optimization procedure will also be developed to search for coating configurations that improve performance against corrosion considering practical issues such as coating thickness, material use, and ability to manufacture the coatings.

The first hypothesis is that the combination of residual-based numerical error estimation with electrochemical concentration and current-density gradients can improve the spatial allocation of finite elements in the vicinity of localized coating defects, thus enabling more accurate predictions of corrosion-related phenomena for a similar computational cost. The second hypothesis is that coating thickness, porosity, permeability, and defect dimensions, interactively and possibly nonlinearly, influence corrosion behavior. To test these hypotheses, a verified multiphysics numerical framework will be used to identify combinations of coating parameters that yield better protective performance than an optimization based on the individual variables, through analytical benchmarks, numerical convergence studies and sensitivity analyzes, and comparisons with established computational approaches.

MATERIALS AND METHODS

RESEARCH DESIGN AND COMPUTATIONAL APPROACH

The computer and mathematical modeling will be based on adaptive finite element analysis for the proposed research. There will be a mathematical formulation, a numerical implementation, a verification, a parametric study, and a numerical optimization. Fig. 1 presents the overall computational workflow. It depicts the steps performed in order, i.e. identifying the material properties and coating geometry, formulating the governing equations mathematically, discretizing finite elements, adaptive mesh refinement, numerical verification, and design optimization.

The computational domain will be a metal substrate protected by a nanocomposite coating in contact with an electrolyte made of water and chloride. Localized coating defects will be provided for studying electrochemical activity at bare metal surfaces. In the first step, the modeling phase, as shown in Fig. 1, the properties of the material, coating thickness, porosity, defect geometry and electrochemical boundary conditions are employed to create a typical computer domain.

In the early stages of development the numerical model will be used in two dimensions to simplify computations and make verification easier. After that some 3-dimensional simulations can be run to see how the geometry of space affects things. The governing equations will be discretized by the finite element method. An adaptive mesh refinement strategy will be employed to enhance the numerical resolution in regions characterized by steep concentration gradients, sharp potential changes, and localized electrochemical activity. We will verify the numerical solution by checking its convergence, estimating its errors and comparing it with analytical benchmarks or available experimental data, as presented in Fig. 1.

Another adaptive discretization strategy in the proposed computational strategy is similar to general multiphysics modeling approaches used by Mai et al. [10], [11], and Xiao et al. [12]. New studies have also looked into corrosion that varies with temperature [13], corrosion assisted by mechanical forces in magnesium alloys [14] and degradation due to diffusion in thermal barrier coatings [15]. These studies provide us with useful physical and mathematical tools for the investigation of the effects of various protective layers. Finally, a parametric sensitivity analysis and numerical optimization will be performed to determine coating configurations that minimize predicted corrosion activity while maintaining a high degree of numerical accuracy and computer efficiency.

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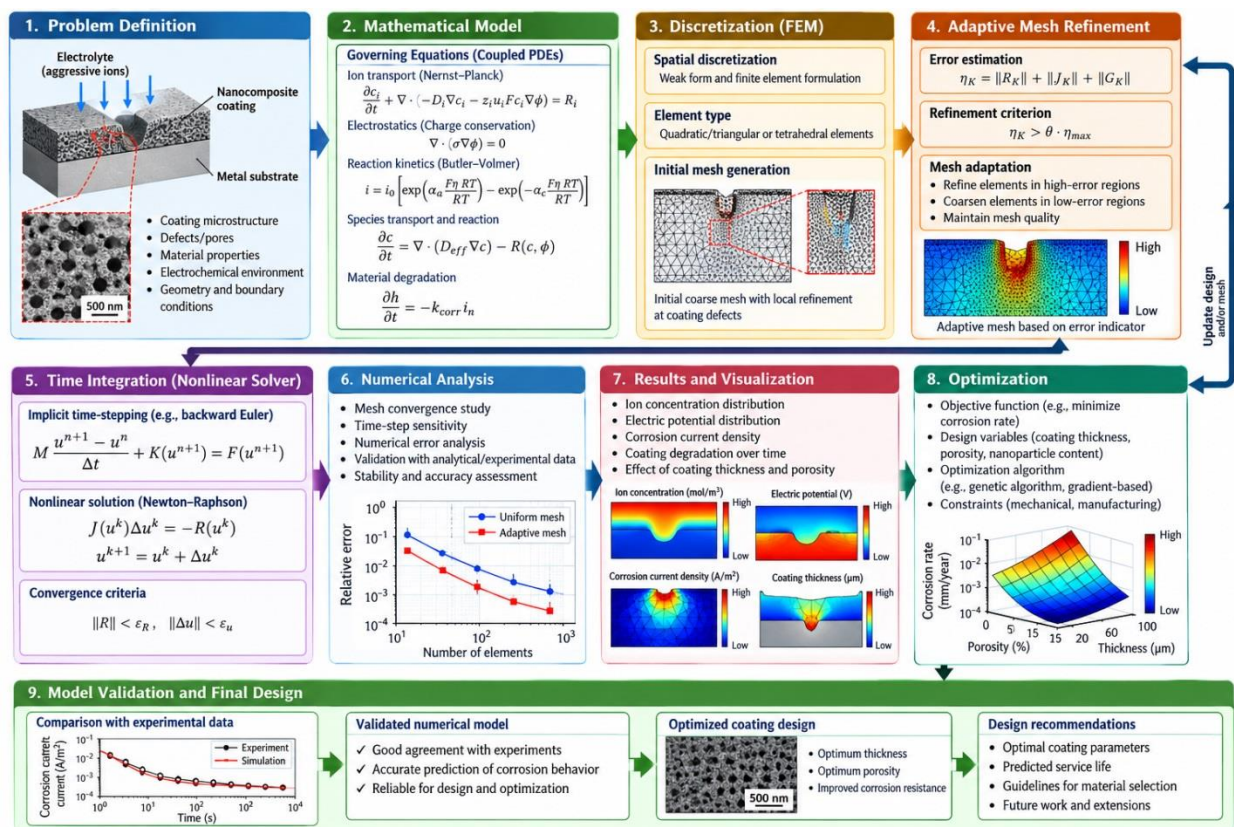


Fig. 1. Proposed computational workflow for adaptive finite element-based numerical analysis and optimization of localized corrosion in nanocomposite-coated metallic materials.

SELECTION OF MATERIALS AND COMPUTATIONAL DOMAIN

The reference metal substrate will be AISI 316L stainless steel because of its use in engineering and the ability to rust in certain areas when levels of chlorides are sufficient. Consider a general polymer-ceramic nanocomposite coating. To separate the effects of transport properties, porosity and coating geometry. The mathematical framework is expected to be general enough to be applied for other metal substrates and coating compositions.

The main model will be formed by the bulk electrolyte domain, nanocomposite coating domain and metallic substrate boundary. Electrically connected areas of the substrate and electrochemically active surfaces will be treated separately where appropriate. The coating is described in an effective-medium approximation. The transport properties depend on the porosity and the connectivity of the coating. A few distinct geometric defects will be introduced to explore the influence of coating fracture on electrochemical activity in the region.

Recent work with finite elements to investigate corrosion in coated steel systems has demonstrated the importance of porous corrosion products, interface shape, and electrochemical boundary conditions found in experiments [16]. It is important to compare the different mathematical representations rather than to focus on a single simulation framework, as has been pointed out in a recent review of pitting corrosion models [17].

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Table 1. Proposed geometric and environmental parameters

Parameter	Symbol	Proposed range
Coating thickness	H_c	25–100 μm
Coating porosity	ε_p	0.01–0.10
Defect width	w_d	10–100 μm
Temperature	T	298.15–328.15 K
NaCl concentration	C_{NaCl}	0.1–0.6 mol/L
Electrolyte height	H_e	0.5–2 mm
Substrate width	L_s	2–10 mm
Simulation dimension	—	2D, selected 3D

The proposed ranges are design concepts only. The combinations will be checked for physical consistency before the simulation. Some material-specific properties (diffusion coefficients, exchange current densities, equilibrium potentials and effective coating conductivity) will be obtained from lab-tested systems or reliable literature sources.

GOVERNING MATHEMATICAL EQUATIONS

IONIC SPECIES CONSERVATION

The conservation equation will tell us how each type of ionic particle moves through the electrolyte:

$$\frac{\partial y}{\partial x} + \nabla \cdot J_i = R_i \quad (1)$$

where c_i represents the concentration of ionic species i , J_i is the molar flux, t is time, and R_i represents homogeneous reaction sources or sinks. Assuming a stationary electrolyte without convective flow, the Nernst–Planck flux is expressed as:

$$J_i = -D_i \nabla c_i - \frac{z_i D_i F}{RT} c_i \nabla \Phi_l \quad (2)$$

The diffusion coefficient is D_i , number of ions with charge is z_i , Faraday constant is F , universal gas constant is R , temperature is T and electrolyte potential is Φ_l . The first term is the diffusion due to concentration difference and the second term is the electromigration due to electric field. Transport through protective coatings can be very different from transport through the bulk electrolyte. This is because the microstructure of the coatings determines their ionic conductivity and water uptake. Electrochemical modeling and real experiments have been used to study different types of electrolytes and ions moving through coating systems [18, 19].

EFFECTIVE TRANSPORT PROPERTIES

The effective diffusion coefficient within the porous coating will initially be approximated using:

$$D_{i,eff} = D_i \frac{\varepsilon_p}{\tau_p} \quad (3)$$

where ε_p denotes connected porosity and τ_p represents an effective tortuosity factor.

This relationship helps to understand how the limited transport operates through a connected porous structure. The model will be able to distinguish between defects defined by their shape and those defined by uniform coating porosity, so that double counting of the same transport pathways will be avoided. Parametric variations will be used to explore the effect of pore connectivity, interfacial geometry and electrolyte accessibility. There is strong experimental or computational evidence that local transport pathways can have a large effect on the distribution of electrochemicals in systems that are not all the same [20, 21].

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CHARGE CONSERVATION

Under an electroneutral electrolyte approximation, the local ionic concentrations must satisfy:

$$\sum_i z_i c_i = 0 \quad (4)$$

The ionic current density is given by:

$$i_l = F \sum_i z_i J_i \quad (5)$$

For systems in which there is no volumetric accumulation of electrical charge, conservation of current requires:

$$\nabla \cdot i_l = 0 \quad (6)$$

Equations (1)–(6) represent a coupled set of partial differential and algebraic equations that describe the mass transport and distribution of electrochemical potential. A good electric-potential reference will be used to get rid of the random constant associated with the electrostatic potential.

ELECTROCHEMICAL REACTION KINETICS

Electrochemical reactions occurring on the exposed metallic substrate will be represented using Butler–Volmer-type kinetics:

$$i_F = i_o \left[\exp\left(\frac{\alpha_a n F \eta}{RT}\right) - \exp\left(-\frac{\alpha_c n F \eta}{RT}\right) \right] \quad (7)$$

where i_F is the Faradaic current density, i_o is the exchange current density, α_a and α_c are anodic and cathodic charge-transfer coefficients, n is the number of electrons transferred, and η is the reaction overpotential.

The overpotential is defined as:

$$H = \phi_s - \phi_l - E_{eq} \quad (8)$$

where Φ_s is the metallic potential and E_{eq} is the equilibrium potential of the corresponding reaction.

Different laws for anodic dissolution and cathodic reduction will be used if the (equilibrium) potentials or the kinetic parameters of the chemical reactions are different. We shall only consider reaction systems where it makes physical sense to use a single net Butler–Volmer expression. Stoichiometric Faraday relationships will connect species flux at reactive metal boundaries with the partial Faraday currents associated with them.

FINITE ELEMENT FORMULATION

The governing equations will be split into smaller parts by the Galerkin finite element method. Let Ω be the computational domain and Γ its boundary. Multiplying the conservation equation by a test function v and integrating over the domain, we obtain for a typical species:

$$\int_{\Omega} v \frac{\partial c_i}{\partial t} d\Omega + \int_{\Omega} v \nabla \cdot J_i d\Omega = \int_{\Omega} v R_i d\Omega \quad (9)$$

After integration by parts:

$$\int_{\Omega} v \frac{\partial c_i}{\partial t} d\Omega - \int_{\Omega} \nabla v \cdot J_i d\Omega + \int_{\Gamma} v \cdot J_i n d\Gamma = \int_{\Omega} v R_i d\Omega \quad (10)$$

where n is the outward unit normal vector.

The ionic concentrations and electrical potential will be approximated using suitable interpolation functions:

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$$c_i(x, t) \approx \sum_{j=1}^N N_j(x) c_{ij}(t) \quad (11)$$

The resulting spatially discretized system can be written in generalized form as:

$$M(U) \frac{dU}{dt} + F(U, t) = 0 \quad (12)$$

where U contains the nodal concentration and potential variables.

For short term simulations a backward differentiation method or other implicit time integration scheme is used. We will consider the Newton-type linearization for the solution of the nonlinear algebraic system. If the cause of oscillations is sharp migration driven layers, then the best stable finite element formulations will be studied. For stabilization of numerical problems that are transport-dominated an excellent starting point is the streamline-upwind/Petrov-Galerkin approach introduced by Brooks and Hughes [22].

DEVELOPMENT OF THE PROPOSED ADAPTIVE MESH REFINEMENT METHOD

The main numerical contribution of this work will be the development and testing of a physics-based adaptive mesh refinement strategy. Adaptive methods try to detect the discretization error and refine where the error indicators are large. The usefulness of adaptive finite element methods has been shown theoretically and practically by Bangerth and Rannacher [23], and adaptive error control in systems of reaction-diffusion equations has been studied by Sandboge [24]. The proposed method will incorporate more electrochemical information in the refinement process. We will first find a standard residual estimator for each finite element K:

$$\eta_{R,K}^2 = h_K^2 \|R_K\|_{L^2(K)}^2 + \frac{1}{2} \sum_{e \in \partial K} h_e \|\zeta_e\|_{L^2(e)}^2 \quad (13)$$

where R_K denotes the appropriately scaled element residual, ζ_e represents interelement flux jumps, and h_K and h_e are characteristic element and edge dimensions.

The residual estimator will then be combined with two proposed physical indicators:

$$\eta_{C,K} = \frac{h_K \|\nabla c_{c1}\|_{L^2(K)}}{C_{ref} |K|^{0.5}} \quad (14)$$

$$\eta_{I,K} = \frac{h_K \|\nabla i\|_{L^2(K)}}{I_{ref} |K|^{\frac{1}{2}}} \quad (15)$$

Here, C_{ref} and I_{ref} are fixed positive reference scales selected consistently across all compared simulations. The second expression uses the tensor norm of the current-density gradient.

The proposed combined refinement indicator is:

$$\eta_{new,K}^2 = \eta_{R,K}^2 + \lambda_C \eta_{C,K}^2 + \lambda_I \eta_{I,K}^2 \quad (16)$$

where λ_C and λ_I are nonnegative weighting coefficients.

The residual and physics-based contributions may have different mathematical units, so all terms will be nondimensionalized consistently before being added together. The proposed indicator is expected to be interpreted as a mesh marking metric, rather than as a strict a posteriori upper bound, which is assumed without any further mathematical proof.

Elements satisfying a Dörfler-type marking criterion will be selected for refinement:

$$\sum_{K \in M} \eta_{new,K}^2 \geq \theta \sum_{K \in \tau} \eta_{new,K}^2 \quad (17)$$

where M is the marked element set, τ is the full computational mesh, and $0 < \theta < 1$ is the marking parameter.

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The influence of the weights and marking parameter will be systematically examined.

In an effort to assess the influence of electrochemical gradients on the reduction of error, computational efficiency or the precision of particular quantities of interest, the proposed strategy will be compared to two other approaches, i.e. conventional residual-based refinement and uniform refinement.

INITIAL AND BOUNDARY CONDITIONS

The computing area includes the edges between the bulk and the electrolyte, the surfaces of the coating, the flaws in the coating and the electrochemically active interfaces of the metal. The electrolyte composition will be imposed, so as to set the initial ionic concentrations at the start of each simulation. The fixed reservoir concentrations can be imposed by a boundary of bulk electrolyte:

$$c_i = c_{i,\infty}$$
 (18)

At impermeable boundaries, the normal species flux will be set to zero:

$$nJ_i = 0$$
 (19)

At electrochemically active metallic boundaries, ionic fluxes will be determined from the corresponding electrochemical reactions:

$$n.J_i = -\frac{v_i i_F r}{n_r F}$$
 (20)

where v_i is the signed stoichiometric coefficient under a consistently defined reaction and normal-direction convention.

For the potentiostatic simulations, the metallic potential could be chosen. If the metal is free to corrode, then the mixed potential can be found by finding the state at which the net external current disappears. The boundary conditions of zero flux will be imposed on coating surfaces which are ideally non-permeable. Instead, regions with a porous coating will be modeled as transport domains with reduced effective transport coefficients. This distinction is important to ensure consistent boundary assignments and to guaranty mass conservation.

NUMERICAL VERIFICATION AND VALIDATION

Before physically interpreting the simulated corrosion behavior it will be checked numerically. Four main types of numerical configurations will be considered: coarse uniform meshes, fine uniform meshes, conventional residual-adaptive meshes and meshes generated by the proposed physics-weighted refinement indicator.

Table 2. Proposed numerical comparison methods

Model	Numerical approach	Purpose
M1	Uniform FEM	Baseline numerical comparison
M2	Residual-adaptive FEM	Established adaptive comparison
M3	Physics-weighted adaptive FEM	Proposed method
M4	Highly refined reference solution	Numerical benchmark

The verification process will include checks of mesh convergence, time-step convergence, nonlinear solver convergence, mass conservation, and current conservation. First we will solve a numerical benchmark for which we know the analytical answer. Then, more difficult electrochemical test cases are selected from previous researches. Comparison of experiments will not be possible until we have enough complete datasets, which should include geometry, electrolyte conditions, electrochemical polarization parameters,

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and measured quantities. Model validation and verification will be done separately. Convergence of a simulation does not guaranty the underlying physical model is an accurate description of an experiment.

NUMERICAL ERROR AND COMPUTATIONAL EFFICIENCY

The relative error for a selected output quantity (Q) will be calculated as:

$$E_Q = \frac{|Q_h - Q_{ref}|}{\max(|Q_{ref}|, Q_{scale})} \times 100 \quad (21)$$

where Q_h is the numerical approximation, Q_{ref} is the benchmark value, and Q_{scale} is a predefined small physical scale that avoids unstable normalization when the reference quantity approaches zero.

The performance of each method on the computer will be judged in terms of total degrees of freedom, solution time, peak memory need and number of nonlinear iterations.

A simple computational speedup indicator will be expressed as:

$$S = \frac{t_{uniform}}{t_{adaptive}} \quad (22)$$

where both methods must be compared at equivalent accuracy.

Instead of reporting only one speedup ratio to describe the relation between numerical error and computational resources, we will plot error versus degrees of freedom and wall-clock time. The method will also test the performance of the adaptive method for some important localized quantities such as maximum current density and total anodic current.

PARAMETER SENSITIVITY AND NUMERICAL OPTIMIZATION

Following the numerical verification, a parametric study will be performed to study the effect of the coating properties and the environment on the results. The main design variables are the thickness of the coating, the number of effective pores, the size of the defects, temperature, and chloride concentration. A constrained optimization procedure will be established to minimize an objective function associated with corrosion. A good objective is the example of the:

$$\min_p J(p) = \int_{\Gamma_\alpha} \max(i_\alpha(p), 0) d\Gamma \quad (23)$$

where p represents the vector of design parameters, Γ_α is the active anodic region, and i_α is the anodic current density.

Physical limitation of the optimization will be governed by the processing capability, transport parameters and coating size. Also multi-objective extensions could be considered:

$$\min_p [J_{corrosion}(p), J_{cost}(p)] \quad (24)$$

If the application does not permit environmental control, the optimization will distinguish between design variables including coating thickness and environmental conditions that remain constant such as chloride concentration. The sensitivity of the objective function in relation to each design parameter will be determined by finite differences or other suitable derivative-based techniques.

RESULTS AND DISCUSSION

VERIFICATION OF THE NUMERICAL MODEL

The first part of the results will show if the numerical model used is able to solve correctly the governing equations when everything is controlled. We will select a typical reaction-diffusion or electrochemical

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transport problem for which an analytical solution, a manufactured solution, or a numerical solution verified by someone else is available. The proposed model will be evaluated in terms of relative error, residual convergence and conservation properties. For the spatial discretization we will consider the convergence by:

$$E_h \propto h^p \quad (25)$$

where p is the observed order of convergence, determined from numerical results rather than assumed.

Using smooth benchmark solutions and suitable finite elements, the convergence behavior can approach the theoretical order of the approximation space you choose. But the observed behavior can be modified by localized boundary layers, irregular geometry and nonlinear coupling. The numerical analysis will then be concerned with the conditions under which the expected convergence rates hold and try to understand why things are not going as we planned.

EFFECT OF ADAPTIVE MESH REFINEMENT

We will look at how the different refinement strategies handle coating defects and large electrochemical differences by studying the spatial distribution of the finite elements. The uniform discretization strategy keeps a constant mesh density over the whole computational domain. Therefore, a large increase in the number of elements may be required to obtain a high resolution near a small defect. It is expected that the residual-based refinement is able to concentrate elements in the locations where the discretization errors are larger. The proposed physics-weighted refinement indicator may also give more weight to regions where chloride concentration is large and current density changes rapidly.

The key comparison will be to ascertain whether these additional physical indicators allow for the calculation of the amount of corrosion in a particular area, without making the calculations more complicated. The analysis will clarify the higher accuracy of the whole numerical solution in comparison with some quantities of interest. Increasing the spatial resolution of the current density distribution does not necessarily lead to a reduction of the global solution error. This difference is important in that an adaptive method that works must offer numerical benefits and not just appear denser near defects.

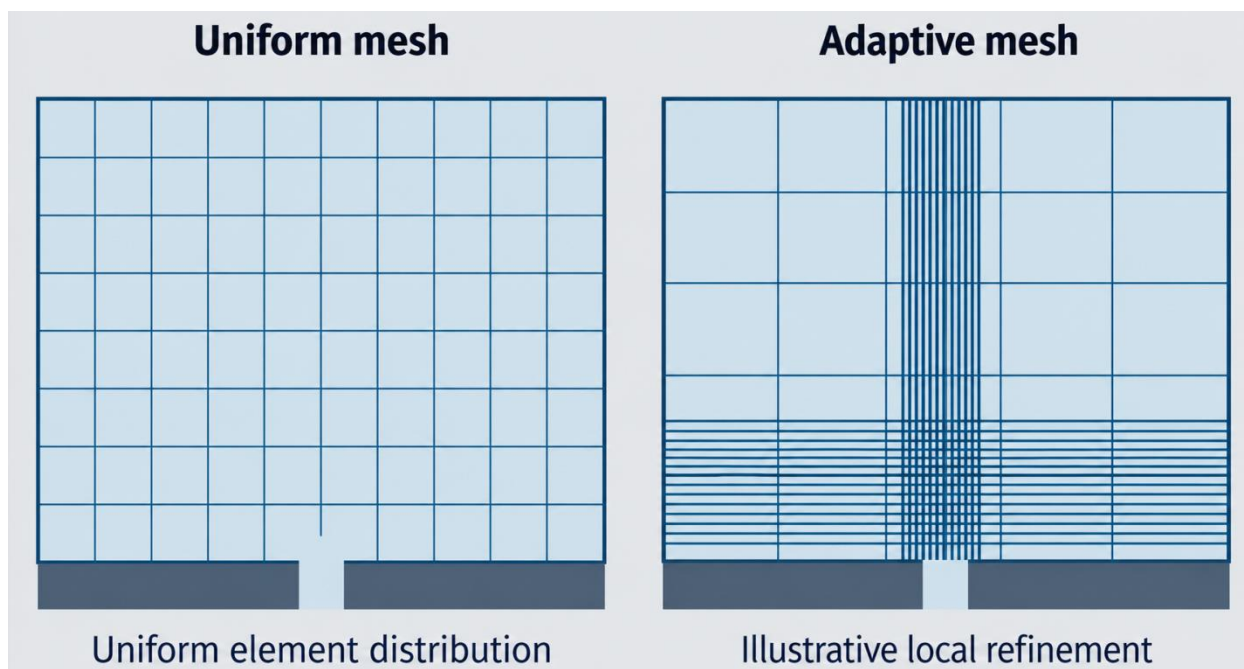


Fig. 2. Concepts of uniform finite element discretization vs. localized adaptive refinement in the vicinity of a coating defect. The picture is only a sketch and does not represent a real simulation mesh.

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NUMERICAL ERROR AND CONVERGENCE BEHAVIOR

The numerical error analysis will study the performance of the different finite element methods based on the total number of degrees of freedom. If the solution has strongly localized gradients, the adaptive refinement should be able to reach the target accuracy with fewer elements than the uniform refinement. But the computational advantage needs to be shown in numbers. In some cases the advantage of a smaller number of elements can be compensated by the additional remeshing and interpolation steps in the adaptive calculations.

So the computational analysis will consist of the time to make the mesh, the time to find a nonlinear solution, the error in interpolation and the total cost of computing. In particular we will focus on conservation errors that arise when the mesh is refined and the solution is transferred from one mesh to the next. Previous research on adaptive finite element methods and numerical error estimation has indicated the importance of accurate error indicators and proper refinement methods [7–9], [23], and [24]. One of the studies to be proposed will be to apply this numerical analysis to a coupled electrochemical corrosion problem.

Table 3. Proposed numerical verification outputs

Numerical indicator	Planned comparison	Evaluation
Concentration error	M1–M4	Relative L^2 error
Potential error	M1–M4	Relative H^1 seminorm error
Current-density error	M1–M4	Peak and integrated error
Degrees of freedom	M1–M3	Accuracy versus model size
Computational time	M1–M3	Time at matched error
Conservation residual	M1–M3	Mass and charge balance
Numerical robustness	M1–M3	Solver failures and convergence

IONIC CONCENTRATION DISTRIBUTION

The distribution of chloride ions and other electrochemically active ionic species in the electrolyte and porous nanocomposite coating is an important factor affecting the local corrosion behavior. The numerical study proposed intends to examine the effect of the size of the coating defect, the chloride content in the environment and the resistance of the ions moving through the environment on the concentration fields formed near the coating-substrate interface. Fig. 3(a–d) shows the conceptual concentration distributions for four different cases, small defects at low chloride concentration, small defects at high chloride concentration, large defects at low chloride concentration and large defects at high chloride concentration. These distributions provide a rough idea of likely transport behavior and are a starting point for more detailed finite element simulations.

A small coating defect and a low chloride concentration in the environment result in a small region of high ion concentration within the defect channel as shown in Fig. 2(a). Ions cannot reach the metal substrate. It is the nanocomposite coating around it that acts as a barrier to prevent transport. Thus, an outer layer of the coating is largely isolated from the external electrolyte, and ionic transport is concentrated around the exposed area. The fact that the concentration disturbance was only rather localized in space suggests that the size of the defect can influence how easily harmful ionic species can attach to the substrate. In contrast, the concentration profile is determined by the effective diffusion coefficient, electromigration, the boundary conditions of the electrolyte and the local electrochemical reactions.

If the shape of the defect is unchanged but the chloride concentration in the environment is increased, as in Fig. 3(b), the concentration field presents a more pronounced region of higher ionic concentration along the defect channel. There are more chloride ions outside because the concentration is higher and they may be easier to find near the metal surface. The concentration contours cross the porous coating surrounding the

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sample and penetrate inside, indicating that transport may occur through interconnected pores. But the observed spatial distribution should not be taken as direct evidence of higher corrosion current because the kinetics of anodic dissolution and the chloride concentration are not always correlated. Good predictions require linking ion transport to the appropriate laws of electrochemical reactions and, where necessary, chloride-dependent passive-film breakdown behavior.

In Fig. 3(c) the coating has a larger defect and the chloride concentration in the environment is not very high so that the effect of the defect geometry is more pronounced. The wider opening makes interface more visible comparing with Fig. 2(a) and provides a larger way for electrolytes to get through. The concentration field shown extends over a larger area in the neighborhood of the coating-substrate interface. Thus, changes of the shape of the surface can affect the distribution of the transported ionic species. While the external chloride concentration remains low, a larger defect may increase the total ion flux to the substrate by providing more space for transport. It is to be noted that a higher total flux does not necessarily correspond to a higher local concentration or higher current density everywhere on the surface. We have to check the resulting distribution with boundary conditions for coupled transport and electrochemistry.

Figure 3(d) shows the largest area of high ionic concentration. This is attributed to the influence of a large coating defect and the high concentration of chlorides in the environment. In these cases the conceptual distribution shows a large region of enhanced ionic availability near the exposed metal and along the porous coating regions adjacent to it. The larger opening means electrolytes can get in easier and the higher concentration of aggressive ions in the environment means they can get out easier. Together they may promote the growth of larger electrochemically active surface areas, particularly when the metal substrate is susceptible to chloride induced instability of the passive film. But the corrosion behavior will depend on the potential of the local electrode, the rate of reaction, the composition of the electrolyte and the movement of dissolution products. Therefore, the regions with high concentration shown in Fig. 2(d) should be regarded as possible locations with higher ionic exposure and not as confirmed locations where the metal dissolves faster.

A comparison of Fig. 3(a–d) shows that it is important to consider the size of the coating defect and the concentration of the defect in the environment together rather than as separate factors. Increasing the width of a defect changes the shape and area that can be used for ionic transport, while increasing the concentration of chloride in the environment changes the chemical conditions that are present. The interaction of the diffusion, electromigration and interfacial electrochemical reactions can result in non-linear concentration distributions. Also, the coating's porosity and tortuosity affect how well it moves things around, which in turn controls how much aggressive species can get into areas around the main defect. Previous studies of ionic transport, heterogeneous electrolyte penetration, and coating degradation have shown how important these processes are for figuring out how well corrosion-protective systems work [18], [19], [28].

From the point of view of numerical analysis, the concentration gradients presented in Fig. 3 are very important as they show how steep spatial variations can occur in the vicinity of the edges of defects, pore junctions and the coating-electrolyte interface. To be able to get the right numbers in these areas, the computational mesh may have to be tweaked in some places. Thus the proposed physics-weighted adaptive finite element method will use concentration gradient information, residual-based error estimates and changes in current density to identify regions that require higher spatial resolution. We will look at mesh convergence to see how well this strategy works, make sure there are no problems with conservation, and compare to numerical solutions that have been uniformly refined.

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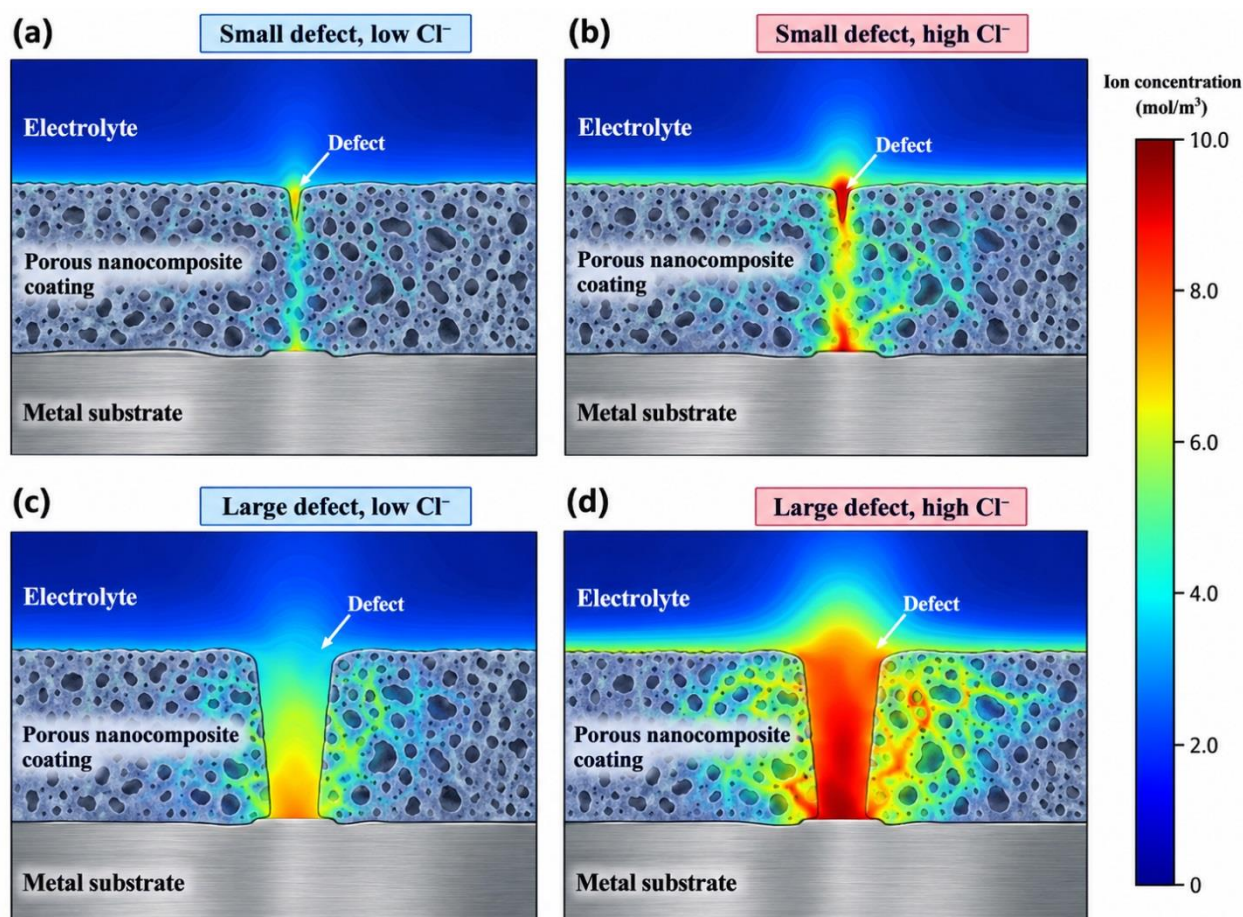


Fig. 3. Ionic concentrations in the electrolyte and porous nanocomposite coating for different defect sizes and chloride concentrations in the environment: (a) small defect and low chloride concentration; (b) small defect and high chloride concentration; (c) large defect and low chloride concentration; (d) large defect and high chloride concentration. The color contours show the concentration change of the ions near the flaws in the coating and the metal substrate.

ELECTRIC POTENTIAL AND CURRENT-DENSITY DISTRIBUTION

Determining the spatial distribution of the electrolyte potential and anodic current density is a crucial step in determining the localized electrochemical activity in metallic materials coated with nanocomposites. The effect of the shape of the coating defect on these electrochemical fields is demonstrated in Figure 4(a–d) by comparing the potential distributions and anodic current-density patterns for narrow and wide coating defects. These patterns illustrate how the geometrical discontinuities should influence the localization of the electrochemical field and offer a means to conduct a quantitative evaluation of the proposed adaptive finite element framework.

The potential contours approach each other near the opening of the defect and along its internal edges indicating locations where relatively strong electric field gradients may develop. This is due to the small channel with electrolyte solution having a limited number of ionic current pathways and the protective coating surrounding it having a high electrical resistance. Therefore, the potential distribution is no longer uniform in space, especially near the coating–electrolyte and coating–substrate interfaces. The magnitude and direction of the potential changes will be dependent on the boundary conditions, the conductivity of the electrolyte and the behavior of the electrochemical polarization.

The associated concept of an anodic current-density distribution is shown in Fig. 4(b). It can be seen from the image that the increased anodic activity is mainly located around the exposed metal at the bottom of the narrow defect, with a stronger localization around the edges of the defect. This behavior suggests that the present concentration could be due to geometrical confinement and variation of the resistance of the

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electrolyte. The small width of the defect can limit the total area of exposed metal while creating uneven current densities along the accessible surface. However, defect sizes alone do not tell you what the maximum local current density is because the electrochemical response also depends on the reaction rate, electrode potential, ionic transport and the number of available cathodic reaction sites.

As the defect width increases, the disturbance of the electrolyte potential has a wider range in the coating discontinuity, as shown in Fig. 4(c). The wider opening allows a wider transport path of electrolyte than the narrow-defect configuration in Fig. 4(a). This changes the geometric distribution of the ionic current. The curves of potential crossing the defect and the adjacent region of the electrolyte show that the electrochemical effect extends over a larger area with the increase of the defect size. However, the resultant electric field intensity may not grow uniformly, since larger flaws can decrease the solution resistance and move the ionic current to cover a larger interfacial region. The size of a defect is therefore likely to be related to the local potential gradients but also to the electrochemical boundary conditions and the conductivity of the electrolyte and the coating.

The anodic current density distribution associated with the large defect is shown in Fig. 4(d). In this configuration the considered current-density field extends over a larger surface of exposed metal, being enhanced near the coating edges. The larger defect increases the distance between the metal and the electrolyte which could result in a higher integrated anodic current under similar electrochemical conditions. However, the local peak current density may not increase to the same extent because the electrochemical current can be spread over the larger surface. The increase at the edges of the defects indicates that geometrical breaks might be the places where the current concentration is most likely to occur. Still, numerical calculations are needed to find the exact spatial distribution.

The effect of defect width on the distribution of the electrolyte potential can be seen by comparing Fig. 4(a) and Fig. 4(c), while Fig. 4(b) and Fig. 4(d) show the effect of the difference in defect width on the patterns of localized anodic current density. Electrochemical fields can be very localized with narrow defects, whereas wider defects spread the electrochemical response over a larger interfacial area. The electrolyte potential is a field variable in the conducting electrolyte, and the Faradaic anodic current density is imposed at electrochemically active metallic surfaces. The current-density contours of Fig. 4 should not be regarded as volumetric distributions of Faradaic current within the electrolyte and coating, but rather as schematic representations of interfacial anodic activity.

The discretization of finite elements has large numerical problems due to the large differences in potentials and the variation of local current density in the vicinity of coating defects. Very concentrated electrical fields can arise from sharp, idealized defect corners, which can result in mesh-dependent predictions of the highest current density. To address this, the proposed numerical scheme will employ adaptive mesh refinement in regions with steep potential gradients, large variations of the current density and high numerical residuals and will incorporate finite-radius defect geometries when physically appropriate. We will observe the convergence analysis of the resulting mesh distributions to determine if the proposed physics-weighted refinement strategy improves the numerical accuracy and computational efficiency compared to standard adaptive discretization methods that are uniform and residual-based.

In the quantitative assessment, the maximum anodic current density and the integrated anodic current will be considered separately. The model will be used to determine the total electrochemical dissolution activity by integrating the positive anodic current density over the metal surface under study, thus obtaining an integrated anodic current. This difference is very important in the case of defects of different widths, because a larger exposed area might make the total anodic current higher but not the maximum local current density. The numerical predictions will also be compared with previous studies on galvanic corrosion, evolution of corrosion defects and electrochemical modeling of metal systems [20, 33 and 35].

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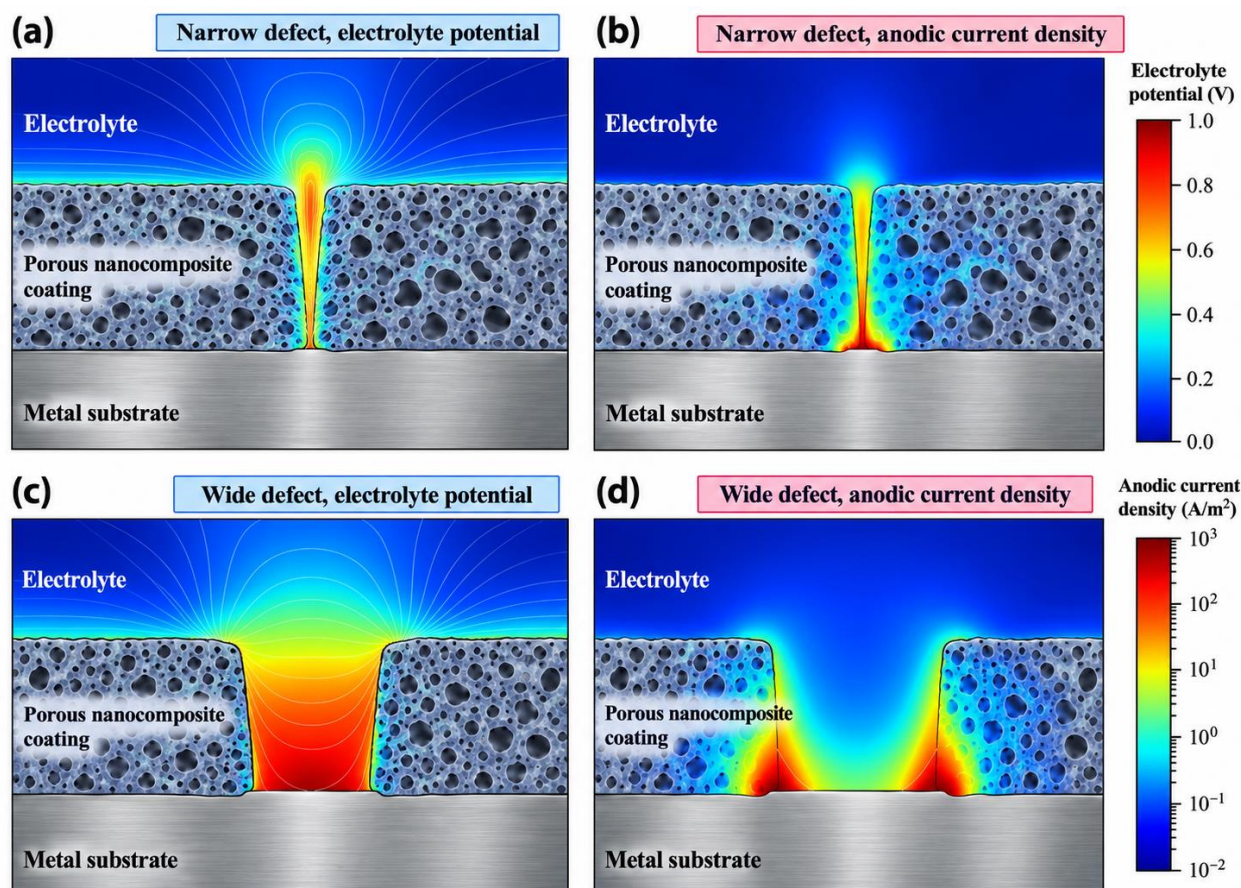


Fig. 4. Conceptual electrolyte potential contours and anodic current-density distributions for different coating defect geometries: (a) electrolyte potential around a narrow defect, (b) localized anodic current-density distribution associated with a narrow defect, (c) electrolyte potential around a wide defect, and (d) anodic current-density distribution associated with a wide defect. The illustrations highlight the influence of defect geometry on potential gradients and localized electrochemical activity within nanocomposite-coated metallic systems.

INFLUENCE OF COATING THICKNESS AND POROSITY

In the mathematical design of nanocomposite coatings it is important to consider the influence of the thickness and porosity of the coating on the electrochemical protection of metal substrates. These factors change the diffusion pathways, the effective transport resistance and the electrolyte penetration characteristics and consequently change the ease with which aggressive ionic species attach to the metal underneath. The suggested relationships between coating thickness, porosity, integrated anodic current and effective ionic transport are demonstrated by use of three-dimensional surface models and the corresponding two-dimensional contour plots (Fig. 5(a–d)). These ideas on distributions allow us to observe effects of coating geometry and microstructural features on the movement processes related to corrosion.

This is shown in figure 1. The anodic current shown in Fig. 5(a) decreases with increasing coating thickness and especially at very low thickness. This behavior is in line with the expectation that thicker protective layers increase the effective diffusion path length and hinder aggressive electrolyte species from reaching the metallic substrate. The relatively short transport pathway in thinner coatings may facilitate ion reaching and hence more anodic activity where the metal is exposed to electricity. The additional transport resistance may increase the difficulty of the reactive species to reach the interface between the coating and the substrate with the increase of the coating thickness. But the relationship between coating thickness and corrosion current is not always direct. It is dependent on the permeability of the coating, the shape of the defects, the conductivity of the electrolyte and the electrochemical reactions on the surface of the metal.

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Figure 5(a) also shows the effect of the porosity of the coating. Under the assumed transport-controlled conditions, a higher porosity corresponds to a higher anodic current. This is the expected behavior, due to the formation of interconnected pore pathways that facilitate the electrolyte passage through the coating. Increasing porosity may reduce the effective resistance to ionic transport and may allow more aggressive species to reach electrochemically active regions of the metallic substrate. However, the correlation between porosity and corrosion is influenced by the connectivity, distribution and tortuosity of the pores, and not only by the total number of pores. Hence, two coatings with the same percentage of pores can have very different electrochemical properties if the internal pore structures are very different.

The effective ionic transport coefficient depends on the coating thickness and porosity as shown in Fig. 5(b). The concept of the surface indicates that the ions have higher mobility when the coatings are thinner and there are more pores. The increase of connected pore fraction may physically increase the effective diffusion coefficient with more pathways for ion transport. However, in general, the higher the coating thickness, the higher the total transport resistance, because ionic species have to move or diffuse over a longer path. It is of mathematical importance to differentiate between these two effects: coating thickness affects the overall permeance or transport resistance, while the intrinsic effective diffusion coefficient of a homogeneous coating is a function of its microstructure and material properties. The quantity in Fig. 5(b) that depends on thickness should be seen as an apparent transport performance indicator, not a material-specific diffusion coefficient, unless the numerical formulation takes into account the thickness-dependent changes in microstructure explicitly.

Alternatively, one could look at the two dimensional contour plot shown in Fig. 5(c) which reveals the effect of coating thickness and porosity on the integrated anodic current. The shapes show that relatively thin coatings with a high degree of connected porosity have the highest anodic activity. Those coatings that are thicker and of lower ionic permeability are less anodically active. The curved contour patterns indicate that the coating thickness and porosity may not interact linearly. That is, the value of one parameter influences the other parameter. For instance, if the coating has a moderate transport resistance, increasing the coating thickness may predict a stronger decrease in anodic activity; however, if the coating has continuous defects that allow direct access of the electrolyte to the metallic substrate, increasing the thickness may not be as effective.

The contour representation of the ionic transport associated with it is shown in Fig. 5(d). The distribution shown underlines the importance of the control of the connected porosity and the transport resistance in the design of a protective coating. In the lower-transport region, the coatings are thicker and the pores are less connected. In the higher-transport region, the coatings are thinner and the transport pathways are more accessible. This qualitative relationship justifies the use of numerical sensitivity analysis to identify combinations of coating thickness and porosity that impede the passage of electrolytes. However, the actual value of the effective diffusion coefficient has to be evaluated using the appropriate microstructural transport model, such as a porosity-tortuosity relationship, rather than merely by looking at the color contours.

The expected effect of the coating parameters on the electrochemical performance can be seen in Fig. 5(a) and Fig. 5(c). The expected effect of the coating parameters on the transport of ions can be seen in Fig. 5(b) and Fig. 5(d). These processes are interrelated, but they deal with different physical quantities. The mobility of charged particles through the coating is controlled by ionic transport. Electrochemical oxidation reactions at accessible metal surfaces cause anodic current. Thus, higher ionic permeability could facilitate corrosion if transport is limited. But, it is not the only factor in the determination of the rate of corrosion. A proper evaluation requires the coupling of ionic transport equations with charge conservation, electrochemical reaction kinetics and proper boundary conditions.

There is a significant opportunity to identify optimal combinations of coating parameters and to explore non-linear variations in corrosion-related outputs with coating thickness and porosity. We will use an adaptive finite element framework to analyze the spatial distribution of the concentration, electrolyte potential, and current density for different coating parameters. We will pay particular attention to the

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development of steep concentration gradients near coating defects and the metal–electrolyte interface, where localized mesh refinement might be needed to ensure numerical accuracy. We will verify the numerical results by convergence tests, conservation residuals, and comparisons to solutions obtained with uniform refinement.

The optimization process will also search for coating configurations that reduce the integrated anodic current, while still meeting practical constraints on coating thickness, material use and the ability to make the coatings. The thickness may not be as protective when the main cause of corrosion is direct electrolyte pathways. The test will be able to distinguish between intact porous coatings and coatings with through flaws. This difference is important to avoid too optimistic predictions of corrosion protection based on average coating properties alone.

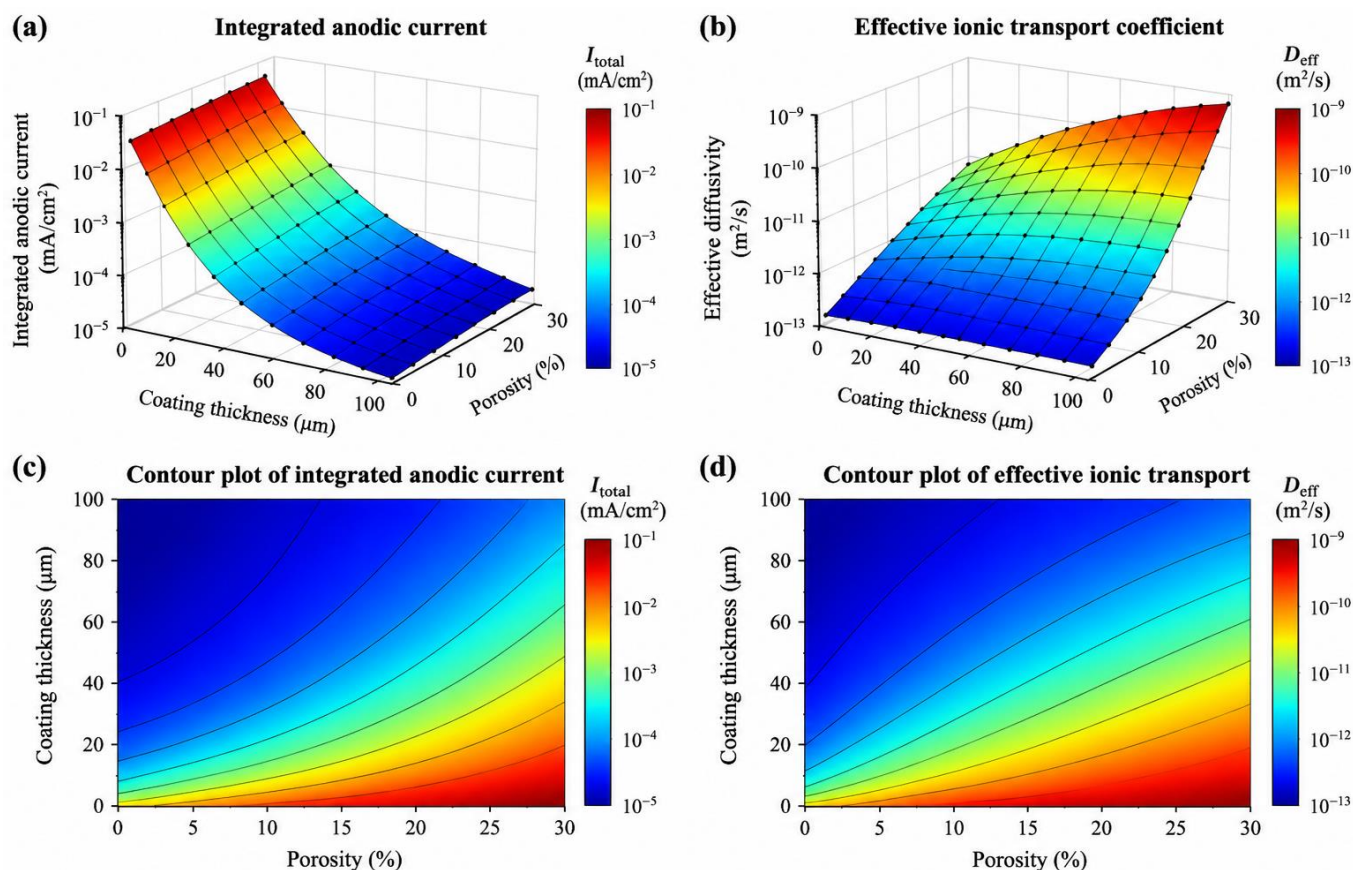


Fig. 5. Conceptual dependence of corrosion-related electrochemical behavior on coating thickness and porosity: (a) three-dimensional surface representation of integrated anodic current, (b) three-dimensional representation of apparent ionic transport performance, (c) corresponding contour distribution of anodic current, and (d) contour distribution of apparent ionic transport performance. The illustrations highlight the anticipated combined effects of coating thickness and porosity on electrolyte penetration and corrosion-related behavior.

INFLUENCE OF DEFECT GEOMETRY AND TEMPERATURE

The impact of coating defect geometry and ambient temperature on localized corrosion should be taken into account to evaluate the corrosion protection efficiency of nanocomposite coated metals. The temperature affects the ionic diffusion, the electrolyte conductivity and the rate of electrochemical reactions. The defect width affects the electrolyte accessibility and the exposed substrate to electricity. Figure 6(a–d) represents the relationships which are believed to exist between these parameters and shows the variation in total anodic current, highest anodic current density, rate of corrosion and depth of penetration of aggressive ion.

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As shown in Fig. 6(a), increasing the width of the defect can increase the integrated anodic current by allowing the electrolyte to reach to a larger metal surface. Narrow defects prevent the direct penetration of the electrolyte to the metal, while wider defects favor ion migration and electrochemical reactions at the metal-electrolyte interface. Increasing the temperature further can improve the anodic activity even more due to the acceleration of reaction kinetics and ionic transport. But the resulting current flow depends on the combined action of anodic and cathodic reactions, the resistance of the electrolyte and the limits of transport.

The highest anodic current-density distribution as seen in Fig. 6(b) provides us with more information on the severity of corrosion in some areas. The maximum current density represents the area with the highest electrochemical activity, compared to the integrated anodic current. The larger defects may increase the total anodic current but not necessarily the maximum current density to the same extent. Small defects can concentrate current at geometric breaks, whereas larger openings can spread the current over a larger surface. Thus both parameters have to be looked at separately to be able to tell the difference between the severity of the localized corrosion and the overall dissolution activity.

The corrosion rate curves in Fig. 6(c) imply that larger defects and higher temperature may accelerate corrosion when anodic dissolution is more dominant. Faraday's law can be used to determine corrosion penetration rates, provided the reaction stoichiometry, the density of the material and the current efficiency are correctly set, but this law can only be used for simulated anodic current densities. However, one needs to distinguish between maximum local penetration rates and area-averaged corrosion rates since the localized corrosion is not the same everywhere. Thus the numerical predictions will rely on the calculated electrochemical fields rather than on the conceptual contours themselves.

Figure 6(d) illustrates the effect of temperature and defect geometry on aggressive ions penetration. Larger defects may facilitate electrolyte ingress, while an elevation in temperature may assist movement through interconnected pores and open regions. However, the depth of penetration is a function of the effective diffusion coefficient, the length of exposure, and the chosen concentration threshold. Therefore, accurate predictions of the depth of penetration require transient transport calculations with well-defined boundary conditions. The ionic transport will be considered as a temperature dependent process using the Arrhenius-type relation

$$D_i(T) = D_{i,ref} \exp \left[-\frac{E_{a,D}}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right] \quad (26)$$

where ($D_i(T)$) is the diffusion coefficient at temperature (T), ($D_{i,ref}$) is its reference value, ($E_{a,D}$) is the activation energy for diffusion, and (R) is the universal gas constant. Separate modeling will be performed for reactions controlled processes with temperature dependent electrochemical kinetics parameters. The importance of combining temperature effects with electrochemical corrosion mechanisms has been clearly demonstrated by previous studies [13,14].

Mathematically, the occurrence of small defects and high temperatures can cause very steep gradients in concentration and potential, which makes the localized spatial refinement even more important. The proposed physics-weighted adaptive finite element method will focus on the electrochemically active regions with high computational resolution, using residual-based error indicators and electrochemical gradients. Its performance will be assessed through mesh convergence, conservation analysis and comparisons with uniformly refined reference solutions.

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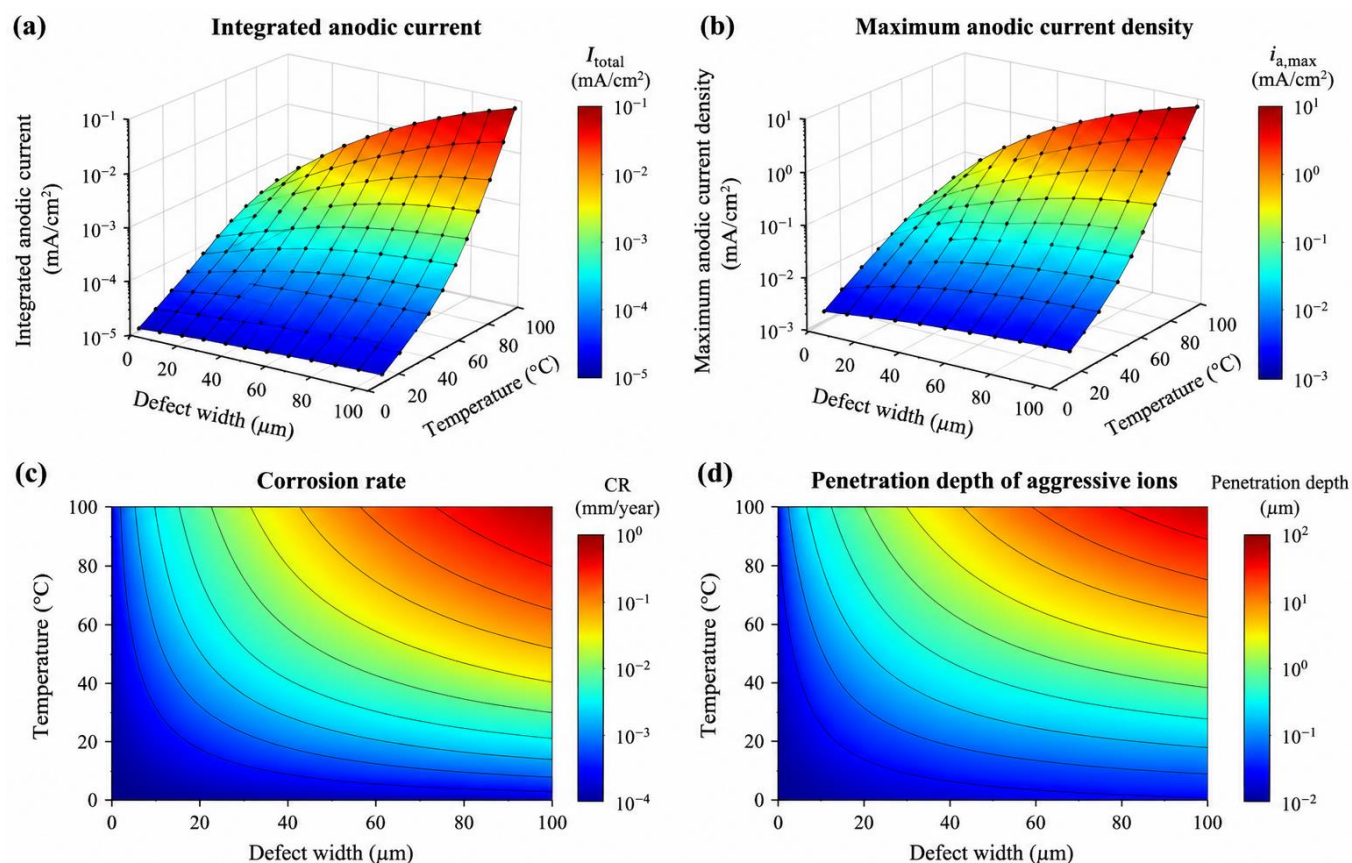


Fig. 6. Conceptual influence of coating defect width and temperature on corrosion-related parameters: (a) three-dimensional variation of integrated anodic current, (b) maximum anodic current density, (c) contour distribution of corrosion rate, and (d) penetration depth of aggressive ionic species. The illustrations represent anticipated qualitative trends associated with increasing defect dimensions and temperature rather than validated numerical simulation results.

NUMERICAL OPTIMIZATION OF COATING PARAMETERS

Once the numerical model is validated, an optimization analysis will be performed to find the best coating configurations that reduce the amount of simulated anodic dissolution and increase the protection. The main design parameters will be the thickness of the coating, the connected porosity and the shape of the defects. All these factors influence the movement of ions, the availability of electrolytes and the electrochemical activity. Fig. 7(a–d) shows the proposed strategy to improve the things; it shows response surfaces, transport resistance, Pareto-optimal solutions and the best coating configurations.

The main objective, illustrated in Fig. 7(a), is to minimize the total anodic dissolution activity on the metal surface by achieving the minimum possible integrated anodic current. The conceptual response surface indicates that the coating could be thickened to reduce the anodic current by increasing the length of the ion pathways. Also, it could be made porous to allow more electrolytes to pass through and enhance the electrochemical activity. But at a certain point adding more coating thickness may not protect as well, this is called diminishing returns. This behavior demonstrates the importance of finding the right coating dimensions to protect against corrosion without using too much material.

The second response shown in Fig. 7(b) illustrates the expected behavior of the predicted relationship between coating thickness, porosity and transport resistance. Coatings of higher thickness and lower interconnected porosity are generally believed to be more resistant to ion transport. But, if we only focus on the improvement of anodic current and transport resistance, we may get the same coating configuration, rather than different ones. So the optimization will look at things like how much coating material is being used, the cost of production or design limits regarding thickness to make engineering trade-offs that are

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meaningful. Figure 7(c) shows the concept of multi-objective optimization as a non-dominated Pareto front, which displays coating configurations that are not dominated. Each Pareto-optimal solution has a design that improves one of the competing goals and worsens another. For example, a reduction of the anodic current density can lead to thicker coatings and a reduction of the material consumption can lead to thinner coatings. Thus, the Pareto front provides a means to choose coating configurations that satisfy the corrosion protection requirements and remain within the bounds of practical engineering.

The corresponding coating design space is shown in Figure 7(d). The contour distribution and proposed Pareto-optimal pathway guide the search for promising thickness and porosity combinations. The design priorities for the representative configurations A, B, C are varied, e.g. maximum protection, balanced optimization and minimum coating material. These settings are just recommendations until the optimization process is run with validated numbers. The proposed study will also examine nonlinear interactions between coating thickness, porosity, and defect geometry. Response-surface methods and sensitivity analysis will be used to identify which factors have the greatest influence on the total anodic current, the highest local current density and the transport resistance. Coating defects will be particularly addressed as the amount of current in some areas can still be high even if the global ionic permeability decreases.

The physics-weighted adaptive finite element framework will make optimization easier by allowing for easy discovery of numbers in electrochemically active areas. Convergence tests and comparison with improved reference solutions will give an accurate assessment of the objective function. Surrogate models can also be used to reduce cost of computation when optimization calculations are repeated again and again.

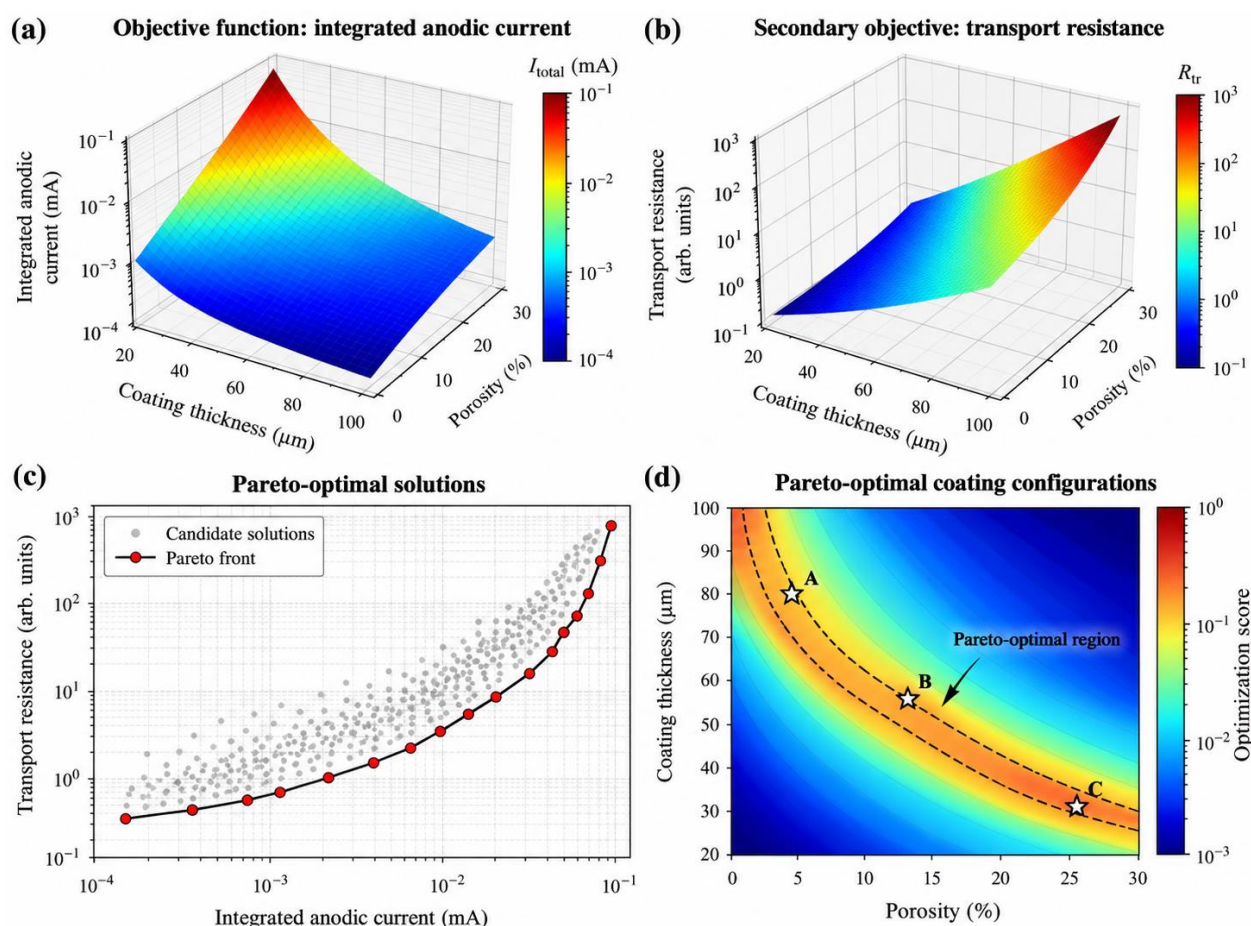


Fig. 7. Conceptual response surfaces and Pareto-optimal coating configurations obtained from the proposed numerical optimization framework: (a) response surface of the primary objective function represented by integrated anodic current, (b) response surface of the secondary objective related to transport resistance, (c) Pareto front showing non-dominated candidate solutions, and (d) contour map illustrating the Pareto-optimal coating-parameter region in terms of thickness and porosity.

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COMPARISON WITH PUBLISHED NUMERICAL STUDIES

We will compare the proposed physics-weighted adaptive finite element framework to other well-known numerical methods for modeling electrochemical corrosion, such as uniform finite element methods (FEM), residual-based adaptive FEM, and phase-field formulations. We will compare them in terms of their accuracy, behavior in convergence, computation speed, representation of the real world, and their ability to resolve localized electrochemical phenomena near coating defects. The pros and cons of each numerical method are summarized in Table 4, taking into account the computational requirements, model complexity and capability to resolve localized corrosion processes.

Standard finite element methods [20], [33] and [35] are used for studying electrochemical potential distribution, galvanic corrosion and corrosion defect evolution in metal systems. These approaches provide a flexible approach to using computers for solving coupled transport and electrochemical equations with complex boundary and geometrical conditions. However, uniform mesh refinement may necessitate a large number of finite elements to accurately resolve the steep gradients in concentration and current density near coating discontinuities. This limitation can lead to increased computation time and memory usage when considering nonlinear electrochemical reactions and transient transport processes.

Some of these problems can be solved using residual-based adaptive finite element methods that refine the computational mesh in regions where large discretization errors are present. The mathematics of a posteriori error estimation and adaptive refinement has been studied already by researchers and they proved how important are for controlling computational resources and improving the accuracy of the numbers [7–9], [23–24], [30–31]. However, standard residual estimators focus mainly on the discretization error of the governing equations and corrosion-related quantities like maximum anodic current density or integrated anodic current are not necessarily the first choice. Thus, more work is needed to assess whether incorporating physically meaningful electrochemical indicators can enhance predictions of localized corrosion behavior.

Phase-field numerical methods provide an alternative to demonstrate the evolution of corrosion morphologies with time and the interplay of electrochemical reactions, ionic transport and mechanical degradation. The use of these has already been demonstrated by researchers for pitting corrosion, galvanic corrosion, crevice corrosion and mechanically assisted degradation [4, 5, 10, 14]. Unlike the fixed-boundary FEM formulations, the phase-field models can deal with moving interfaces without the need to track the corrosion front explicitly. In contrast, adding more field variables and nonlinear couplings usually makes computations harder. In addition, phase-field formulations introduce additional numerical parameters, e.g., interface regularization length scales, that have to be carefully chosen and verified. Other computer studies have been carried out on reaction-diffusion equations, damage due to corrosion, and methods to find solutions that make efficient use of computers [25–27], [29–32], [34]. These studies emphasize the importance of ensuring stability and convergence of the numerical schemes, of correctly estimating the errors and of the physical consistency of the models when developing computer models for coupled degradation processes. However, the literature contains a vast range of different numerical objectives and physical assumptions. This complicates a direct comparison of performance unless the same benchmark problems and accuracy criteria are employed.

To overcome these issues, the proposed physics-weighted adaptive FEM framework integrates the classical residual-based error estimation with supplementary refinement indicators based on variations of electrochemical current density and ionic concentration gradients. The aim of this strategy is to focus computational effort on coating defects and electrochemically active interfaces, while maintaining a relatively coarse discretization in areas with predominantly smooth solution fields. Unlike the traditional residual-only approach, the proposed method includes physical information about corrosion into the mesh-marking process. Systematic comparisons with uniform FEM, residual-adaptive FEM and highly refined numerical reference solutions will demonstrate its performance.

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The comparison will involve the relative numerical error, total degrees of freedom, computational time, convergence behavior and conservation residuals. Much care will be taken to see if the suggested method gives an improvement in accuracy for quantities related to localized corrosion while having the same cost of computations. This comparison will also show the difference between electrochemical models with fixed geometry and phase field formulations that explicitly simulate the evolution of the corrosion front. In this way, one will not draw wrong conclusions from models that can not do the same things physically.

Table 4. Comparison of existing numerical approaches and the proposed physics-weighted adaptive finite element framework for corrosion modeling.

Numerical approach	Main advantages	Limitations and challenges	Relevant references
Uniform FEM	Straightforward implementation; flexible treatment of complex geometries and coupled electrochemical equations	High computational cost for resolving localized gradients; inefficient element distribution in regions with smooth fields	[20], [33], [35]
Residual-adaptive FEM	Established error-based refinement; improved allocation of computational resources; suitable for adaptive error control	Refinement may not specifically target corrosion-related quantities of interest; requires reliable error estimators	[7]–[9], [23], [24], [30], [31]
Phase-field FEM	Represents evolving corrosion morphology; accommodates interface evolution and coupled electrochemical–mechanical degradation	Additional nonlinear equations; higher computational requirements; sensitivity to interface regularization parameters	[4], [5], [10]–[14]
Stabilized and advanced numerical schemes	Improved treatment of transport-dominated equations; potential improvements in stability and numerical convergence	Stabilization parameters and discretization choices require careful verification; may introduce numerical diffusion	[22], [29], [32]
Proposed physics-weighted adaptive FEM	Combines residual-based error estimation with electrochemical gradient indicators; targets localized corrosion-sensitive regions; potentially improves computational efficiency	Requires calibration of refinement weights; verification of convergence and conservation; validation against benchmark and experimental data	Present study

From Table 4 it can be seen that the novelty of the proposed framework lies in the combination of numerical error information with electrochemical field characteristics in the adaptive refinement process. This method should be especially useful for nanocomposite-coated metals with localized defects because concentration and potential gradients can be very large near visible metal–electrolyte interfaces. Adding more physical indicators, however, does not necessarily lead to better numerical performance. The proposed method is expected to achieve quantitative improvements over current refinement strategies with reproducible numbers.

NUMERICAL BENCHMARK AND MODEL VERIFICATION

To obtain a qualitative picture of transport in a porous coating we solved a one-dimensional steady-state reaction-diffusion model. The governing equation is:

$$D_{eff} \frac{d^2c}{dx^2} - kc = 0 \tag{27}$$

subject to:

$$c(0) = c_b, c(L) = 0 \tag{28}$$

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where D_{eff} is the effective diffusion coefficient, k represents a first-order reaction or removal coefficient, L is coating thickness, and c_b is the imposed concentration at the electrolyte-facing boundary.

The corresponding analytical solution is:

$$c(x) = c_b \frac{\sinh[\alpha(L-x)]}{\sinh(\alpha L)} \quad (29)$$

with:

$$\alpha = \sqrt{\frac{k}{D_{\text{eff}}}} \quad (30)$$

The calculated flux at the metal-facing boundary is:

$$J_m = \frac{D_{\text{eff}} c_b \alpha}{\sinh(\alpha L)} \quad (31)$$

The benchmark was calculated using $D_o=10^{-9}$ m²/s, $k=0.02$ s⁻¹, $c_b=600$ mol/m³, a 50 μm coating, and 5% porosity.

These assumptions are illustrated by using the exact reference flux $J_m = 8.7694e^{-5}$ mol.m⁻².s⁻¹. It is not a corrosion current density, it is a reactant transport flux. To convert it to corrosion current we need to know the stoichiometry of the electrochemical reaction and to show that the reactant flux limits the reaction rate.

MESH CONVERGENCE ANALYSIS

The proposed reaction–diffusion benchmark was numerically tested with mesh convergence analysis for accuracy, computational consistency and discretization sensitivity. We solved the one-dimensional steady-state reaction–diffusion equation using a second-order finite-difference approximation with two different ways of dividing the space into discrete elements: uniform and geometrically graded meshes. To systematically investigate the effect of the spatial refinement on the calculated metal-interface reactant flux, five spatial resolutions were examined: 12, 24, 48, 96, and 192 elements. The numerical predictions were compared to the accompanying analytical solution to provide a means of assessing discretization errors and convergence characteristics. The resulting numbers are presented in Fig. 8(a–c), and the calculated relative flux errors are listed in Table 5.

Table 5. Relative error in the calculated metal-interface reactant flux for uniform and geometrically graded finite-difference meshes.

Number of elements (N)	Uniform mesh flux error (%)	Graded mesh flux error (%)
12	0.7829	5.8919
24	0.1943	1.5681
48	0.0485	0.4060
96	0.0121	0.1034
192	0.0030	0.0261

Fig. 8(a) shows that the relative flux error decreases with increasing mesh resolution for both numerical discretization strategies. The relative error of the uniform mesh is reduced from 0.7829 % with 12 elements to 0.0030 % with 192 elements, a total reduction of about 99.62%. Similarly, the geometrically graded mesh exhibits an error reduction from 5.8919% to 0.0261%, which is a 99.56% error reduction. It is clear from these results that the predicted metal-interface reactant flux is much more accurate when more computational elements are included. However, for the same number of elements, the geometrically graded mesh exhibits always larger errors than the uniform mesh, which shows the important role of spatial distribution of the mesh elements on the efficiency of the mesh.

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For the coarsest discretization (12 elements) the relative error of the graded mesh is about 7.53% larger than the uniform mesh. This difference is still visible at higher resolutions where the graded mesh has an error of 0.0261% and the uniform mesh only 0.0030% at 192 elements. The graded configuration is less accurate, which shows that increasing the computing nodes in some area does not always make it easier to predict a given physical quantity. Uniform discretization for this benchmark implies a better distribution of elements to compute the metal-interface flux while prescribed geometrical grading results in larger discretization errors. Therefore, if mesh refinement is to be carried out, it should be based on the numerical features of the governing equations and the sensitivity of the output quantity, rather than geometrical considerations alone.

Fig. 8(b) shows the corresponding convergence of the calculated metal-interface reactant flux. Both discretization strategies converge toward the analytical reference value of around $8.7694 \times 10^5 \text{ mol.m}^{-2}.\text{s}^{-1}$ with increasing number of elements. The geometrically graded mesh gives more accurate flux values at relatively low mesh resolutions, while the uniform mesh gives more accurate values that are closer to the analytical reference. The more detail we add, the smaller the difference between the two numerical solutions, until they are almost the same. The numerical flux is stable for higher element counts; the influence of spatial discretization becomes negligible, and this supports the consistency of the numerical approximations for the benchmark studied.

The agreement between the two discretization methods at higher mesh resolutions is very important because it indicates that they are converging to the same reference solution, despite starting with different numbers of computational elements distributed in space. The rate of approach to the analytical flux is different for each method, however. The uniform mesh has a smaller relative error for the same number of elements, which indicates that it is more numerically efficient in the sense of degrees of freedom for the given one-dimensional problem. However, to properly assess computational efficiency one would also need to measure solution time, memory consumption and performance of numerical solvers, which are not taken into account in this benchmark.

To know more about working of features of convergence, relative flux errors are plotted against number of elements in logarithmic scale as shown in Fig. 8(c). Thus, the error decreases almost linearly with increasing mesh resolution, indicating that both discretization strategies are of about second order. This is expected for the second order finite-difference approximation, and the relative error is reduced by about four times when the number of elements in a uniform mesh is doubled. For the geometrically graded mesh there is a similar fall-off but absolute errors are higher over the range studied.

The observed convergence order can be evaluated using the relationship:

$$E_N \propto N^{-p} \quad (32)$$

where (E_N) is the numerical error, (N) represents the number of mesh elements, and (p) denotes the observed convergence order. For two successive mesh resolutions, the order can be estimated from:

$$p = \frac{\ln\left(\frac{E_{N_1}}{E_{N_2}}\right)}{\ln\left(\frac{N_2}{N_1}\right)} \quad (33)$$

where E_{N_1} and E_{N_2} are the numerical errors associated with mesh resolutions N_1 and N_2 , respectively, with $N_2 > N_1$.

The overall convergence order is expected to be approximately 2.01 for the uniform mesh and 1.96 for the geometrically graded mesh, as indicated by the relative flux errors in Table 6. These numbers indicate that both discretization strategies converge toward second-order accuracy in the range of refinements studied. In Fig. 8(c) the convergence trends are almost the same, although the absolute error amounts are different, indicating similar asymptotic behavior.

The total interpretation of Fig. 8(a–c) provides a complete picture of numerical convergence. The relative error decreases with the refinement of the mesh (Fig. 8(a)), the computed metal-interface reactant flux

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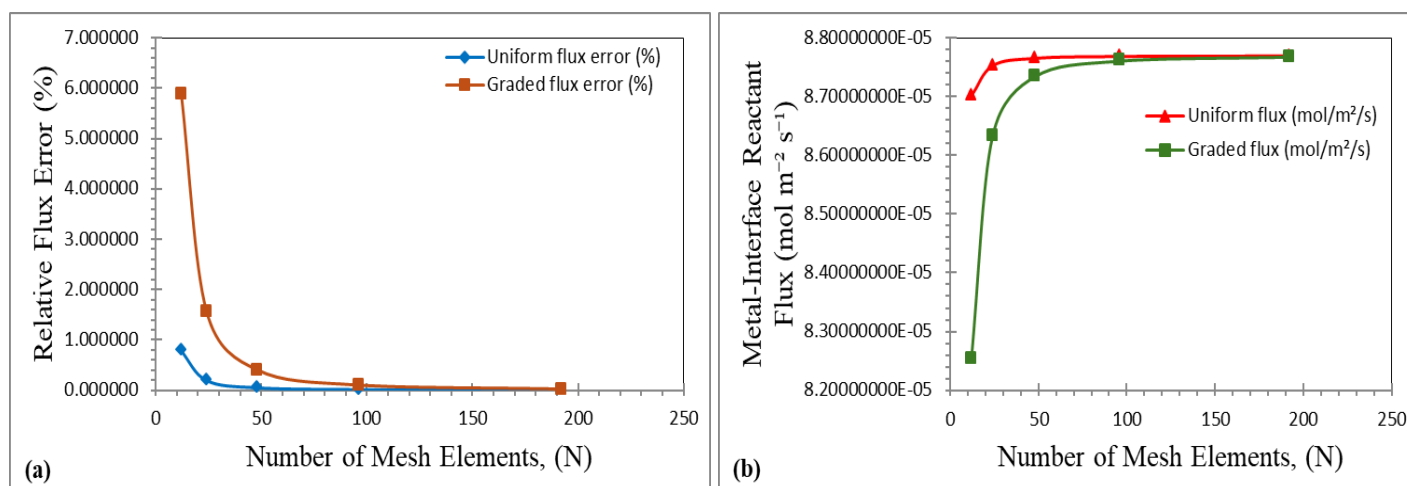
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approaches the analytical reference solution (Fig. 8(b)), and the convergence order is demonstrated by the logarithmic analysis (Fig. 8(c)). The results show the consistency of both discretization methods in relation to the mesh refinement, while the uniform mesh is more accurate for the chosen benchmark, when the number of elements is kept fixed.

The differences observed between uniform and geometrically graded meshes are a good starting point for making a better refinement strategy from the point of view of adaptive numerical analysis. Results show that the non-uniform density of the mesh alone is not sufficient to ensure improved numerical accuracy. Rather, an adaptive method should locate the areas that cause a lot of discretization error and refine them using mathematically sound criteria. In the proposed physics-weighted adaptive finite element framework, residual-based error indicators will be coupled with physically meaningful quantities, such as variations in electrochemical current density and ionic concentration gradients, to help refine the mesh around coating defects and electrochemically active interfaces.

The aim of this approach is to optimize the use of the computer resources by using a finer spatial resolution in areas where there are steep gradients, while keeping relatively coarse elements in areas where the numerical solution is smoother. However, the physics-weighted refinement indicator proposed here needs to be tested on its own with numerical benchmarks and compared with traditional adaptive methods to see the performance. In particular, future simulations should verify if the additional electrochemical indicators improve the accuracy of the localized corrosion-related quantities without complicating the mesh or being computationally expensive.

The convergence study is based on a simplified one-dimensional reaction-diffusion problem solved by finite differences. It is important to point out that this is different from the full two-dimensional adaptive finite element formulation proposed for electrochemical corrosion modeling. Therefore the results show that the preliminary benchmark is numerically consistent, but do not show directly that the proposed adaptive FEM method is more accurate or better. More numerical studies will include coupled Nernst–Planck transport, electrolyte potential distribution, nonlinear electrochemical reaction kinetics and localized coating defects to test the performance of the whole computational framework.



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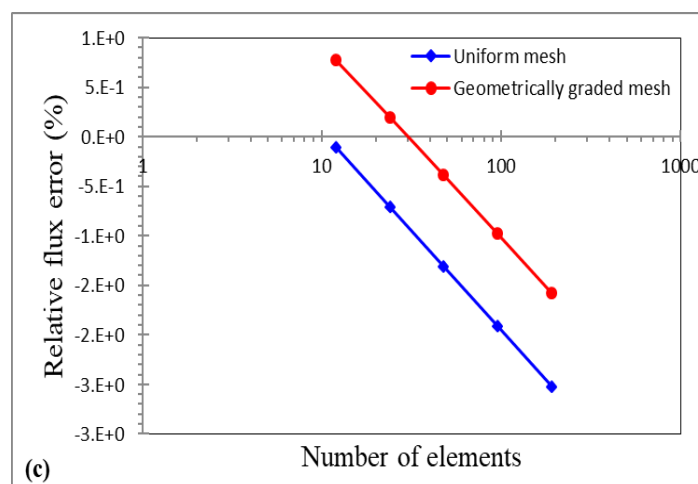


Fig. 8. Mesh convergence analysis of the metal-interface reactant flux using uniform and geometrically graded finite-difference meshes: (a) relative flux error as a function of mesh elements on a linear scale, (b) convergence of the calculated reactant flux toward the analytical reference solution, and (c) log–log representation of relative flux error demonstrating approximately second-order numerical convergence.

NUMERICAL CONCENTRATION DISTRIBUTION

A simplified one-dimensional reaction–diffusion model was used to investigate the steady-state reactant concentration distribution and the effect of the porosity of the coating on the distribution. In the numerical analysis, a nanocomposite coating with a thickness of 50 μm and four different levels of porosity, i.e. 1%, 3%, 5% and 10% was considered. The concentration and the rate of the bulk reactant were kept on the same level, so as to isolate the effect of porosity on the transport behavior. The concentration profiles which were made are shown in Fig. 9. This shows how the concentration of the reactant changes when you move through the protective coating. The equation describing steady-state diffusion with a first-order reaction is Eq. (27):

To get an estimate of the effective diffusion coefficient, which takes into account the effects of connected porosity and tortuosity, use Equation 2: The computational benchmark (Eq. 28) was limited by the following constraints: The zero-concentration boundary at the metal-facing interface is not a general electrochemical boundary condition, but a perfect-sink condition in theory. 29 and 30 give the analytical solution of Equation 27, provided that the boundary conditions are satisfied. As shown in Figure 9, the concentration decreases gradually from the electrolyte-facing boundary to the metal-facing boundary for all porosity levels studied. The effective medium model has a lot of attenuation at the first part of the coating at 1% porosity as the concentration falls faster. This is due to the relatively low value of the effective diffusion coefficient, which makes it difficult for the reactants to travel through the connected pore network. So the concentration profile is strongly curved, which means that the reactant is consumed faster inside the coating.

When the coating porosity increases to 3%, the corresponding curve of the concentration drop in Fig. 9 shows that the effect is less obvious. The effective diffusion coefficient increases as more connected pores are available for reactants to move through the coating. So the calculated concentration is larger than the one obtained for the 1% porosity configuration at a certain distance from the outside. This behavior indicates that for the same reaction and boundary conditions, transport resistance decreases with increasing porosity. As seen in Fig. 9, for the 5% porosity configuration, the concentration of the reactant increases even more inside the coating. The concentration profile is less curved, indicating that diffusion has more effect than the first order reaction. This is in agreement with the idea that the characteristic parameter α is mathematically related to the effective diffusion coefficient. As D_{eff} increases, α decreases and the attenuation of concentration across the coating is less severe.

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It can be seen from Fig. 9 that for the case of the highest porosity (10%), the interior region of the coating has the highest concentration of reactants at any given time. This behavior is due to the interconnected pore network which allows the ions to reach different parts of the material. This improves transport and reduces the concentration gradient to deliver reactants to these areas. With increasing importance of the diffusion relative to the desired first-order reaction, the concentration profile becomes more linear in nature. The comparison of the four concentration profiles shows the significant effect of the coating porosity on the spatial distribution of the reactant concentration under the assumed transport conditions. When the concentration is calculated at a fixed position in the coating, it generally proceeds in the following order:

$$c_{10\%} > c_{5\%} > c_{3\%} > c_{1\%} \quad (34)$$

for the positions between 0 and L. The concentrations at the edges are equal since the same boundary conditions are imposed for all porosities. Fick's first law gives us the diffusion flux that accompanies it:

$$J(x) = -D_{eff} \frac{dc}{dx} \quad (35)$$

where $J(x)$ represents the local reactant flux ($\text{mol.m}^{-2}.\text{s}^{-1}$). Substitution of Eq. 29 into Eq. 35 gives:

$$J(x) = D_{eff} c_b \alpha \frac{\cosh[\alpha(L-x)]}{\sinh(\alpha L)} \quad (36)$$

What is the flux at the interface of metal and reactant? Equation 31 also gives a numerical value for the amount of reactant that migrates to the metal-facing side. The connected porosity, when increased, leads to a higher effective diffusion coefficient, allowing more reactants to reach the interface, according to the reaction-diffusion assumptions made. However, the transport flux cannot be used as a direct measure of anodic corrosion current unless the electrochemical kinetic and stoichiometric relationships are known. From the numerical analysis point of view, the concentration profiles in Fig. 9 show the importance of correctly resolving spatial gradients within coatings with different effective transport properties. Coatings with higher porosity can exhibit smoother concentration distributions, while coatings with low porosity can exhibit steeper local gradients, especially close to the boundary facing the electrolyte. Such variations are important for adaptive numerical discretization, as regions with strong gradients may require higher spatial resolution to maintain the accuracy of the numerical solution. Therefore the analytical concentration distributions are a good reference for testing the accuracy of the proposed adaptive finite element framework. In future simulations ionic transport coupling, electrolyte potential distribution and electrochemical reaction kinetics will be incorporated to explore more real world like nanocomposite coated metallic systems. The number of predictions will be verified by mesh convergence analysis, estimation of the concentration field error and mass conservation.

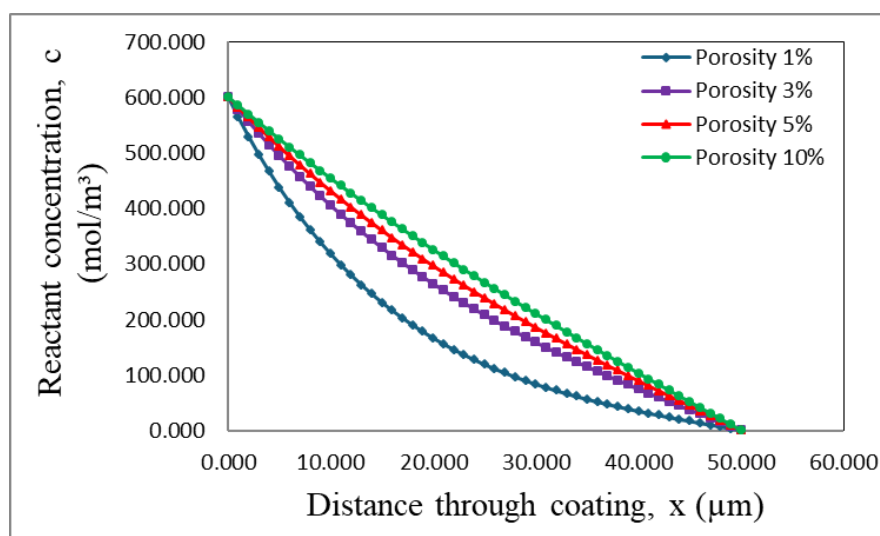


Fig. 9. Calculated steady-state reactant concentration profiles across a 50 μm nanocomposite coating for connected porosities of 1%, 3%, 5%, and 10%.

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EFFECT OF COATING THICKNESS AND POROSITY

The metal-interface reactant flux was calculated, and the effects of coating thickness and porosity on the transport behavior of nanocomposite coatings were quantitatively examined. The transport of reactive species to the underlying metal substrate was studied under the influence of four coating thicknesses (25, 50, 75 and 100 μm) and four connected porosity levels (1%, 3%, 5% and 10%). The calculations were performed by the simplified steady-state reaction–diffusion model with first-order reaction kinetics and effective diffusion properties. The calculated flux values are summarized in Table 5 and their dependence on the thickness and porosity of the coating is shown in Fig. 10 and Table 6.

Table 6. Calculated metal-interface reactant flux as a function of coating thickness and porosity ($\mu\text{mol.m}^{-2}.\text{s}^{-1}$).

Coating thickness (μm)	Porosity 1%	Porosity 3%	Porosity 5%	Porosity 10%
25	29.371	142.248	266.784	601.221
50	3.129	36.826	87.694	242.369
75	0.337	10.219	32.317	116.665
100	0.036	2.850	12.087	58.354

Figure 10 shows that the metal-interface reactant flux decreases monotonically with increasing coating thickness for all levels of porosity studied. This behavior can be explained by the longer diffusion path and the effects of diffusion resistance and first-order reactant consumption in the coating. At smaller thicknesses, the shorter transport paths of the reactive species to the metal-facing interface result in larger calculated flux values. Increasing the coating thickness increases the transport distance and slows down the reactant more before it reaches the substrate below. The calculated reactant flux decreases from $29.371 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ to $3.129 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ at 25 to 50 μm for the coating with 1% porosity. Increasing the thickness to 75 and 100 μm decreases the flux to 0.337 and $0.036 \mu\text{mol.m}^{-2}.\text{s}^{-1}$, respectively. The results show that the transport of the reactant is considerably hindered in low-porosity cases that reduces the total flux by about 99.88% for the coating thickness between 25 and 100 μm . The large drop is consistent with the relatively low effective diffusion coefficient for less connected porosity, meaning that reactant consumption is a larger factor in transport.

The trend is analogous for the 3% porosity configuration, see Fig. 10. The calculated flux is reduced from $142.248 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ for 25 μm to $36.826 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ for 50 μm . Then it reduces further to a value of $10.219 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ for 75 μm and $2.850 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ for 100 μm . This means that the total amount has been reduced by about 98%. While the flux is reduced considerably with increasing thickness, the fluxes are still higher than for the coating with 1% porosity at the same thicknesses. This difference indicates that the mobility of reactants is increased by more connected pores through an increase of the effective diffusion coefficient.

For the coating with 5% porosity, the reactant flux falls from $266.784 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ at 25 μm to $87.694 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ at 50 μm . The decreases are 32.317 and $12.087 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ at the thickness of 75 and 100 μm , respectively. The general reduction of $\sim 95.47\%$ demonstrates that the coating thickness remains a significant factor despite the increasing of the connected porosity. However, the increased flux values in comparison to the coatings with fewer pores indicate that the protective effect of the longer transport path is only partially compensated by the better effective diffusion.

As seen in Fig. 10, the coating with 10% porosity has the highest reactant flux values. The calculated flux is $601.221 \mu\text{mol.m}^{-2}.\text{s}^{-1}$ at a thickness of 25 μm which is much higher than the values for the 1%, 3% and 5% porosity configurations. With increase in thickness to 50, 75 and 100 μm flux decreases to 242.369, 116.665 and $58.354 \mu\text{mol.m}^{-2}.\text{s}^{-1}$. Although the overall reduction is about 90.29%, the flux that remains at 100 μm is much higher than expected for coatings with less connected porosity. This behavior shows the importance of controlling the connectivity of pores and the effective permeability along with the thickening of the coating.

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The analysis of both Table 5 and Fig. 10 shows that the motion of the reactive species is influenced in a complex manner by the thickness and porosity of the coating. The metal-interface flux is always increased with the increase in porosity at a constant coating thickness. For example, at 50 μm , the flux increases from 3.129 $\mu\text{mol.m}^{-2}.\text{s}^{-1}$ at 1% porosity to 242.369 $\mu\text{mol.m}^{-2}.\text{s}^{-1}$ at 10% porosity, a 77.5 times increase. At 100 μm , the flux goes from 0.036 to 58.354 $\mu\text{mol.m}^{-2}.\text{s}^{-2}$ when the porosity goes from 1% to 10%. Thus, these results demonstrate that the porosity plays a larger role when the effective diffusion coefficient controls the amount of reactant attenuation within the coating.

From Fig. 10, the logarithmic graph also shows that the reactant flux does not depend linearly on coating thickness. The curves become flatter with increasing thickness, which is the mathematical behavior of the steady-state reaction-diffusion solution. Eq. 31 shows the flux at the metal interface with the boundary conditions given. This relation shows that the flux computed is a function of the coating thickness and the effective diffusivity. The relative importance of these parameters is decided by the competition between reaction and diffusion. You can get an idea of how much effect adding more coating has by calculating the percent drop in reactant flux using:

$$R_J = \frac{J_{25} - J_{100}}{J_{25}} \times 100 \quad (37)$$

where J_{25} and J_{100} are the calculated metal-interface fluxes for coating thicknesses of 25 and 100 μm , respectively.

Table 6 shows that the reductions are approximately 99.88% for coatings with 1% porosity, 98.00% for coatings with 3% porosity, 95.47% for coatings with 5% porosity, and 90.29% for coatings with 10% porosity. The percentage benefit decreases with increasing levels of porosity. This shows that a larger effective diffusion can compensate for the effect of coating thickness on the attenuation of the reactants. So just making the coating thicker may not be enough to get good transport resistance if it has a lot of large pores that are all connected to each other. The results indicate that the most effective method to prevent the movement of reactive electrolyte species in the design of protective coatings is to minimize the number of connected pores. In most cases the calculated flux decreases with increasing coating thickness. But, if you control both thickness and porosity at the same time, you have other options for improving transport resistance. For example, a low thickness coating with few interconnected pores may have less flux of reactants than a much thicker coating with more pores. This point makes it clear that, in judging the barrier performance, the geometric thickness as well as the coating microstructure should be considered.

Numerical trends also provide us with good information for the next step of optimization, as demonstrated in Fig. 10. The proposed computational framework enables one to use the coating thickness and the corresponding porosity as design variables and find the combinations of parameters that minimize the reactant transport while satisfying practical constraints related to the coating preparation, materials usage and the feasibility of the coating fabrication. However, these calculations are based on a simple one-dimensional reaction-diffusion benchmark which do not consider the electrochemical potential distributions, interfacial reaction kinetics or coating defects that occur in only a few places. The calculated reactant flux should not be considered as a direct measure of corrosion current density or corrosion resistance proved by experiments.

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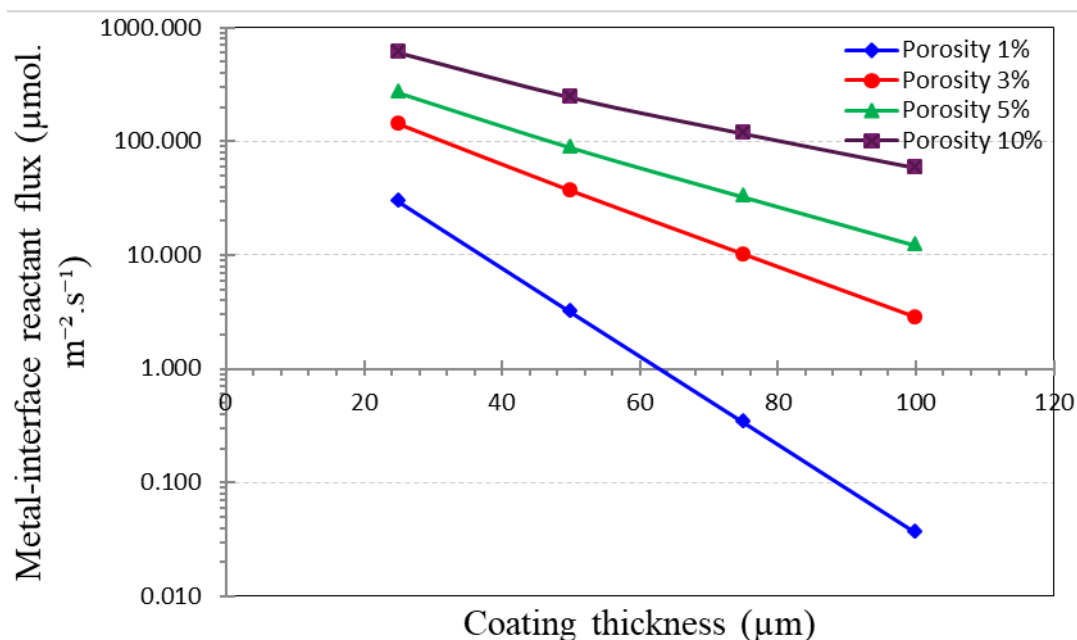


Fig. 10. Calculated dependence of metal-interface reactant flux on coating thickness (25–100 μm) for nanocomposite coatings with connected porosities of 1%, 3%, 5%, and 10%.

COMPARISON BETWEEN ANALYTICAL AND NUMERICAL SOLUTIONS

Numerical discretization accuracy and reliability were checked by comparing the steady-state reactant concentration distributions with the analytical solution of the one-dimensional reaction–diffusion equation. The two numerical discretization strategies considered were uniform and geometrically graded finite-difference meshes, and were examined with 24 elements for the same material properties, reaction parameters and boundary conditions. This comparison was performed to investigate the effect of the mesh distribution on the accuracy of the numbers and the ability of each discretization strategy to reproduce the concentration profile obtained from the analysis. Figure 11 shows the computed concentration distributions and a larger inset showing the difference between the numerical and analytical solutions.

Figure 11 shows that the concentration of the reactant decreases slowly from 600 mol.m⁻³ at the boundary facing the electrolyte to nearly zero at the boundary facing the metal, which corresponds to a coating thickness of 50 μm. This behavior is understandable when considering the boundary conditions and the interaction between diffusion and consumption of the reactant of first order inside the coating. The concentration distribution decreases nonlinearly with distance indicating that diffusive transport and removal of reactive species compete with each other. The characteristic reaction-diffusion length, which governs the global form of the concentration profile, is derived from the comparison of the reaction-rate coefficient and the effective diffusion coefficient.

The analytical distribution of concentration is used as a reference to check the accuracy of the numerical estimates. (29) (30) where the analytical solution for the steady-state reaction-diffusion model being studied. The blue line in Fig. 11 shows the concentration profile with the uniform mesh. The numerical distribution is very close to the analytical profile for most of the coating thickness. This shows that there are only small deviations for the chosen benchmark conditions. As the computational nodes are equally spaced, the governing concentration gradient may be represented consistently in space. This means that the numerical approximation can represent the decay of the overall concentration. The analytical and uniform-mesh curves are very close to each other, which means that 24 uniformly spaced elements are a good way of approximating the concentration field in the simplified problem.

The geometrically graded mesh shown by the red curve in Fig. 11 shows a similar overall concentration trend but a larger difference from the analytical reference solution. This difference is especially pronounced in the middle of the coating, where the concentration of the graded mesh is less than the analytical and

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uniform mesh. Such a behavior reveals that the planned irregular distribution of computational nodes does not give a totally correct picture of the concentration field in the computational domain. The use of graded meshes may increase numerical resolution in some regions, but the effectiveness of such meshes depends on the relation between local element size, concentration gradients and the quantity to be evaluated.

The larger inset in Fig. 11 shows the distribution of the concentrations in a layer of the coating of thickness between 20 and 30 μm better. The agreement between the analytical and uniform-mesh profiles is quite good, and the inset shows that the downward deviation is larger for the geometrically graded mesh. These differences clearly show the dependence of numerical concentration predictions on the placement of computational nodes in space. However, the visual separation of the curves provides only a coarse impression of the accuracy of the numbers; for a more thorough evaluation the numerical error must be directly calculated at similar spatial positions. The absolute concentration error can be used to measure the agreement between the analytical and numerical concentration distributions:

$$E_c(x) = |c_{\text{num}}(x) - c_{\text{analytical}}(x)| \quad (38)$$

where $(c_{\text{num}}(x))$ and $(c_{\text{analytical}}(x))$ represent the numerical and analytical concentrations, respectively. The relative concentration error may also be evaluated using an appropriate reference concentration:

$$E_{c,\text{rel}}(x) = \frac{|c_{\text{num}}(x) - c_{\text{analytical}}(x)|}{c_b} \times 100\% \quad (39)$$

This definition avoids the instability of the numbers when you divide by the local analytical concentration near the metal-facing boundary where the prescribed concentration approaches zero. The concentration field root-mean-square error (RMSE) can be obtained in a more complete way as follows:

$$\text{RMSE} = \sqrt{\frac{1}{M} \sum_{i=1}^M [c_{\text{num}}(x_i) - c_{\text{analytical}}(x_i)]^2} \quad (40)$$

where the number of comparison points is (M). These error measures provide a way to compare the accuracy of the two discretization strategies at numbers. When comparing geometrically graded meshes, the comparison should be made at the same physical locations or by consistent interpolation to avoid differences due to different nodal locations. From the comparison in Fig. 11 it seems that for the concentration profiles shown, the uniform mesh provides a better agreement with the analytical reference solution than the geometrically graded mesh. This is in line with the main result of the previous mesh-convergence study, which showed that for the selected one-dimensional transport benchmark, uniform discretization can perform better than prescribed geometric grading. However, the magnitude of the concentration-field error and the measured order of convergence should be determined using different numerical solutions and systematic mesh refinement.

From the perspective of adaptive numerical analysis, the comparison indicates a serious problem of using fixed mesh grading without taking into account the spatial distribution of numerical errors. A geometrically graded mesh could add more processing nodes to regions that do not contribute the most to the error of the chosen output quantity. Hence, increasing the density of the mesh near a certain boundary is not sufficient to guaranty better numerical accuracy. This discovery led to the development of the proposed physics-weighted adaptive finite element framework. The framework will utilize residual-based error indicators and physically meaningful electrochemical gradients to guide the mesh refinement. The proposed flexible framework will extend the initial one-dimensional benchmark to two-dimensional electrochemical transport problems involving coating defects, different material properties, electrolyte potential gradients and non-linear reaction kinetics at the interface. In these more complicated systems, differing local concentrations and current densities may call for varying levels of computational resolution. We will evaluate the performance of adaptive refinement by comparing it to analytical benchmarks, highly refined numerical results and, where appropriate, well-known residual based adaptive techniques.

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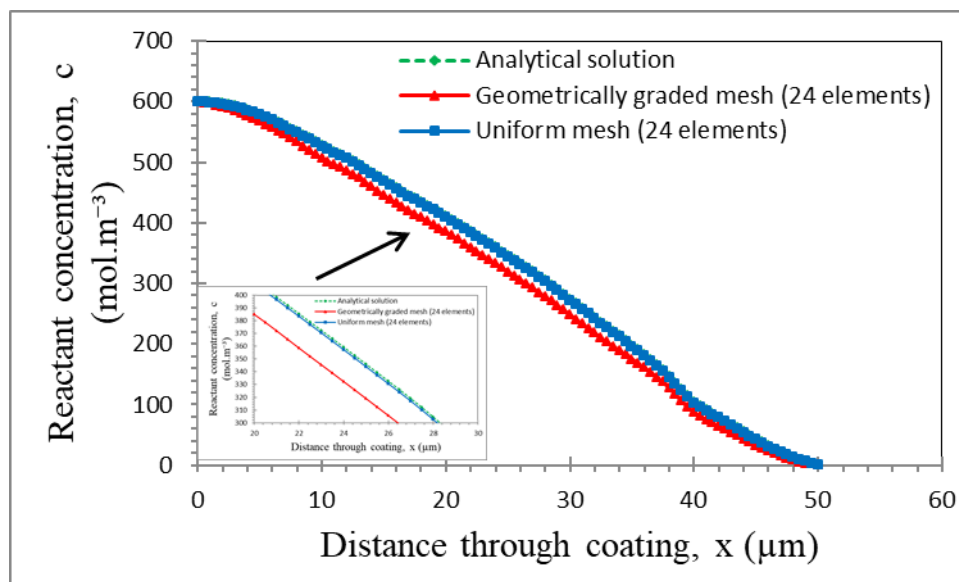


Fig. 11. Comparison of analytical and numerical steady-state reactant concentration profiles across a 50 μm nanocomposite coating using 24 uniform and geometrically graded finite-difference elements. The inset highlights differences between the analytical reference and the numerical concentration distributions within the intermediate coating region.

CONCLUSION

We demonstrate a way to use numbers to study localized corrosion in nanocomposite-coated metals, using coupled electrochemical modeling and adaptive numerical discretization. The proposed approach combines conservation of ionic species, Nernst-Planck transport, charge conservation and the kinetics of electrochemical reactions to examine the influence of coating properties and environmental conditions on corrosion related behavior. Preliminary computer studies with a one-dimensional reaction-diffusion benchmark suggested that a uniform and geometrically graded finite-difference mesh gave similar accuracy. The uniform discretization had smaller relative flux errors. The numbers also showed that the increase in the thickness of the coating and the decrease of the connected porosity greatly slowed the movement of reactants toward the metal interface. At 5% porosity, the calculated reactant flux dropped approximately 95.47% when the coating thickness increased from 25 to 100 μm , illustrating the significance of coating geometry and effective diffusivity. The comparison between analytical and numerical concentration profiles also demonstrated the importance of mesh distribution and systematic error evaluation. The suggested physics-weighted adaptive finite element method will combine residual-based error estimation and concentration-gradient and current-density indicators to achieve a better numerical resolution in the vicinity of more localized coating defects, based on these results. Future work will include coupled electrochemical transport, temperature dependent reaction kinetics, and numerical optimization to gain a better understanding of how corrosion behaves in real life. The expected contribution is a reusable computer method that can improve the accuracy of numbers and assist in the optimization of parameters for protective coatings. Ultimately, the framework could help make more accurate predictions about corrosion and help engineers make long-lasting nanocomposite coatings.

REFERENCES

- [1] L.-F. Huang, J. R. Scully, and J. M. Rondinelli, "Modeling Corrosion with First-Principles Electrochemical Phase Diagrams," *Annual Review of Materials Research*, vol. 49, pp. 53–77, 2019, doi: <https://doi.org/10.1146/annurev-matsci-070218-010105>.
- [2] E. Martínez-Pañeda, "Phase-field simulations opening new horizons in corrosion research," *MRS Bulletin*, vol. 49, pp. 603–612, 2024, doi: <https://doi.org/10.1557/s43577-024-00715-8>.

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- [3] C. Cui, R. Ma, and E. Martínez-Pañeda, “Electro-chemo-mechanical phase field modeling of localized corrosion: Theory and COMSOL implementation,” *Engineering with Computers*, vol. 39, pp. 3877–3894, 2023, doi: <https://doi.org/10.1007/s00366-023-01833-8>.
- [4] C. Lin, H. Ruan, and S.-Q. Shi, “Phase field study of mechanico-electrochemical corrosion,” *Electrochimica Acta*, vol. 310, pp. 240–255, 2019, doi: <https://doi.org/10.1016/j.electacta.2019.04.076>.
- [5] A. Imanian and M. Amiri, “Phase field modeling of corrosion damage,” *Corrosion Reviews*, vol. 40, no. 4, pp. 343–354, 2022, doi: <https://doi.org/10.1515/correv-2021-0063>.
- [6] J. Amador, J. M. Vega, E. García-Lecina, and F. Varas, “Quantitative phase-field model to simulate low carbon steel aqueous corrosion phenomena,” *Corrosion Science*, vol. 232, Art. no. 112045, 2024, doi: <https://doi.org/10.1016/j.corsci.2024.112045>.
- [7] I. Babuška and W. C. Rheinboldt, “Error estimates for adaptive finite element computations,” *SIAM Journal on Numerical Analysis*, vol. 15, no. 4, pp. 736–754, 1978, doi: <https://doi.org/10.1137/0715049>.
- [8] W. Dörfler, “A convergent adaptive algorithm for Poisson's equation,” *SIAM Journal on Numerical Analysis*, vol. 33, no. 3, pp. 1106–1124, 1996, doi: <https://doi.org/10.1137/0733054>.
- [9] O. C. Zienkiewicz and J. Z. Zhu, “The superconvergent patch recovery and a posteriori error estimates. Part 1: The recovery technique,” *International Journal for Numerical Methods in Engineering*, vol. 33, no. 7, pp. 1331–1364, 1992, doi: <https://doi.org/10.1002/nme.1620330702>.
- [10] W. Mai, S. Soghrati, and R. G. Buchheit, “A phase field model for simulating the pitting corrosion,” *Corrosion Science*, vol. 110, pp. 157–166, 2016, doi: <https://doi.org/10.1016/j.corsci.2016.04.001>.
- [11] W. Mai and S. Soghrati, “New phase field model for simulating galvanic and pitting corrosion processes,” *Electrochimica Acta*, vol. 260, pp. 290–304, 2018, doi: <https://doi.org/10.1016/j.electacta.2017.12.086>.
- [12] Z. H. Xiao, S. Y. Hu, J. L. Luo, S. Q. Shi, and C. H. Henager Jr., “A quantitative phase-field model for crevice corrosion,” *Computational Materials Science*, vol. 149, pp. 37–48, 2018, doi: <https://doi.org/10.1016/j.commatsci.2018.03.011>.
- [13] H. Zhi, P. Dong, K. Li, L. Gao, W. Zhou, and H. Zhang, “Phase field study of pitting corrosion: Electrochemical reactions and temperature dependence,” *Computational Materials Science*, vol. 244, Art. no. 113251, 2024, doi: <https://doi.org/10.1016/j.commatsci.2024.113251>.
- [14] S. Kovacevic, W. Ali, E. Martínez-Pañeda, and J. LLorca, “Phase-field modeling of pitting and mechanically-assisted corrosion of Mg alloys for biomedical applications,” *Acta Biomaterialia*, vol. 164, pp. 641–658, 2023, doi: <https://doi.org/10.1016/j.actbio.2023.04.011>.
- [15] A. A. Abubakar, S. S. Akhtar, and A. F. M. Arif, “Phase field modeling of V₂O₅ hot corrosion kinetics in thermal barrier coatings,” *Computational Materials Science*, vol. 99, pp. 105–116, 2015, doi: <https://doi.org/10.1016/j.commatsci.2014.12.004>.
- [16] J. Schneider, K. Kapfer, M. Mandel, A. Mittelbach, and L. Krüger, “Numerical simulation of corrosion in flanges under consideration of corrosion products and their porosity,” *Corrosion Science*, vol. 251, Art. no. 112898, 2025, doi: <https://doi.org/10.1016/j.corsci.2025.112898>.
- [17] J. Escobedo, F. A. Godínez, L. E. Muro, and R. Montoya, “Modeling pitting corrosion in stainless steels: A comprehensive review,” *Materials Today Communications*, vol. 51, Art. no. 114806, 2026, doi: <https://doi.org/10.1016/j.mtcomm.2026.114806>.
- [18] S. Amand, M. Musiani, M. E. Orazem, N. Pébère, B. Tribollet, and V. Vivier, “Constant-phase-element behavior caused by inhomogeneous water uptake in anti-corrosion coatings,” *Electrochimica Acta*, vol. 87, pp. 693–700, 2013, doi: <https://doi.org/10.1016/j.electacta.2012.09.061>.
- [19] F. Thébault, B. Vuillemin, R. Oltra, C. Allely, and K. Ogle, “Modeling bimetallic corrosion under thin electrolyte films,” *Corrosion Science*, vol. 53, no. 1, pp. 201–207, 2011, doi: <https://doi.org/10.1016/j.corsci.2010.09.010>.
- [20] S. R. Cross, S. Gollapudi, and C. A. Schuh, “Validated numerical modeling of galvanic corrosion of zinc and aluminum coatings,” *Corrosion Science*, vol. 88, pp. 226–233, 2014, doi: <https://doi.org/10.1016/j.corsci.2014.07.033>.
- [21] T. Schmid, O. B. Isgor, and U. Angst, “Pore-scale simulation of reactive transport processes at the steel–concrete interface,” *Cement and Concrete Research*, vol. 202, Art. no. 108132, 2026, doi: <https://doi.org/10.1016/j.cemconres.2026.108132>.

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- [22] A. N. Brooks and T. J. R. Hughes, "Streamline upwind/Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations," *Computer Methods in Applied Mechanics and Engineering*, vol. 32, nos. 1–3, pp. 199–259, 1982, doi: [https://doi.org/10.1016/0045-7825\(82\)90071-8](https://doi.org/10.1016/0045-7825(82)90071-8).
- [23] W. Bangerth and R. Rannacher, *Adaptive Finite Element Methods for Differential Equations*. Basel, Switzerland: Birkhäuser, 2003, doi: <https://doi.org/10.1007/978-3-0348-7605-6>.
- [24] R. Sandboge, "Adaptive finite element methods for systems of reaction-diffusion equations," *Computer Methods in Applied Mechanics and Engineering*, vol. 166, nos. 3–4, pp. 309–328, 1998, doi: [https://doi.org/10.1016/S0045-7825\(98\)00093-0](https://doi.org/10.1016/S0045-7825(98)00093-0).
- [25] F. Freddi and L. Mingazzi, "A predictive phase-field approach for cover cracking in corroded concrete elements," *Theoretical and Applied Fracture Mechanics*, vol. 122, Art. no. 103657, 2022, doi: <https://doi.org/10.1016/j.tafmec.2022.103657>.
- [26] X. Fang, Z. Pan, and A. Chen, "Phase field modeling of concrete cracking for non-uniform corrosion of rebar," *Theoretical and Applied Fracture Mechanics*, vol. 121, Art. no. 103517, 2022, doi: <https://doi.org/10.1016/j.tafmec.2022.103517>.
- [27] J. R. Galvele, "Transport processes and the mechanism of pitting of metals," *Journal of The Electrochemical Society*, vol. 123, no. 4, pp. 464–474, 1976, doi: <https://doi.org/10.1149/1.2132857>.
- [28] Y. Dong, Q. Zhou, et al., "Relationship between ion transport and the failure behavior of epoxy resin coatings," *Corrosion Science*, vol. 78, pp. 22–28, 2014, doi: <https://doi.org/10.1016/j.corsci.2013.08.017>.
- [29] H. Gao, L. Ju, et al., "An efficient second-order linear scheme for the phase field model of corrosive dissolution," *Journal of Computational and Applied Mathematics*, vol. 367, Art. no. 112472, 2020, doi: <https://doi.org/10.1016/j.cam.2019.112472>.
- [30] I. Babuška and W. C. Rheinboldt, "A-posteriori error estimates for the finite element method," *International Journal for Numerical Methods in Engineering*, vol. 12, no. 10, pp. 1597–1615, 1978, doi: <https://doi.org/10.1002/nme.1620121010>.
- [31] I. Babuška and W. C. Rheinboldt, "Adaptive approaches and reliability estimations in finite element analysis," *Computer Methods in Applied Mechanics and Engineering*, vols. 17–18, pp. 519–540, 1979, doi: [https://doi.org/10.1016/0045-7825\(79\)90042-2](https://doi.org/10.1016/0045-7825(79)90042-2).
- [32] J.-F. Remacle, P. Dular, A. Genon, et al., "A posteriori error estimation and adaptive meshing using error in constitutive relation," *IEEE Transactions on Magnetics*, vol. 32, no. 3, pp. 1369–1372, 1996, doi: <https://doi.org/10.1109/20.497501>.
- [33] L. Xu and Y. F. Cheng, "A finite element based model for prediction of corrosion defect growth on pipelines," *International Journal of Pressure Vessels and Piping*, vol. 153, pp. 70–79, 2017, doi: <https://doi.org/10.1016/j.ijpvp.2017.05.002>.
- [34] S. Kovacevic and E. Martínez-Pañeda, "A phase-field model for microbiologically influenced corrosion," *Corrosion Science*, vol. 270, Art. no. 114065, 2026, doi: <https://doi.org/10.1016/j.corsci.2026.114065>.
- [35] K. B. Deshpande, "Validated numerical modelling of galvanic corrosion for couples: Magnesium alloy (AE44)–mild steel and AE44–aluminium alloy (AA6063) in brine solution," *Corrosion Science*, vol. 52, no. 10, pp. 3514–3522, 2010, doi: <https://doi.org/10.1016/j.corsci.2010.06.031>.