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High-Order Unconditionally Energy-Stable Decoupled Method for Phase Field Modeling of Pitting Corrosion with Adaptive Implementation

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Abstract. Pitting corrosion, recognized as one of the most catastrophic forms of localized corrosion, frequently leads to premature structural failures. A major computational challenge is the development of accurate and efficient numerical methods that can capture both the initiation and the nonlinear evolution of corrosion pits. In this work, we propose a third-order, decoupled, unconditionally energy-stable implicit-explicit (IMEX) Runge-Kutta scheme for a phase-field model of pitting corrosion, which is formulated as a gradient flow of a coupled free energy functional involving a phase field variable and a normalized ion concentration. The proposed scheme is rigorously proven to satisfy a discrete energy dissipation law, regardless of time step size. To further enhance computational performance, we integrate an adaptive mesh refinement and dynamic time-stepping strategy, enabling efficient resolution of interface dynamics. Comprehensive numerical experiments validate the high accuracy, unconditional energy stability, and effectiveness of adaptive implementation in simulating the complex spatio-temporal evolution of pitting corrosion.

AMS subject classifications: 35K55, 65M60, 65M12

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Key words: Pitting corrosion, phase field model, high-order IMEX Runge-Kutta methods, unconditional energy stability, adaptive finite element method.

1 Introduction

Most materials are inherently heterogeneous due to the presence and interaction of microstructures within, which consist of grains or domains with different structures, orientations, and chemical compositions. Understanding the formation and evolution of these microstructures is critical to predicting material performance under service conditions. Among the multitude of degradation mechanisms in structural materials, corrosion stands out as a particularly insidious threat, manifesting itself as a complex electrochemical interplay between metallic surfaces and aggressive environmental agents, posing significant risks to long-term integrity, reliability, and service life. A passive film is typically coated on the surface of high-strength alloys such as stainless steel and aluminum alloys to restrain corrosion. However, pitting corrosion is a highly localized form of material degradation triggered by the partial rupture of the passive film on the metal surface. Once initiated, these localized corrosion sites can propagate rapidly due to the formation of pits and crevices, which generate stress concentrations and significantly increase the likelihood of fatigue crack initiation. To mitigate the risks of premature failure and extend service life, designing computationally efficient and physically accurate algorithms to simulate corrosion damage from pitting has become a fundamental challenge in both materials science and structural engineering.

Several numerical models are derived to simulate the evolving morphology of the pit during the corrosion process, including the sharp interface model [50,76,80], the level set model [26], and the phase field model [4,32,33,56]. Based on numerical techniques such as the finite element method [80], the level set method [26], the arbitrary Lagrangian-Eulerian [73], meshfree methods [62], and the finite volume method [64], the velocity of the moving interface in the sharp interface model is incorporated in the boundary conditions assigned along the pitting interface, which increases the complexity of implementation and computational cost. This approach has also been applied to model fatigue corrosion cracking and stress corrosion cracking phenomena [42,72]. The diffusive interface phase field method has been extensively employed to address challenges involving dynamic phase interface geometries and evolving topological configurations [9,17,22,75,79], such as solidification of materials [10], dislocation interactions [81], superconductivity phenomena [8], dendritic growth [16, 78, 86], contact line dynamics [39, 65, 83], two-phase fluid flows [71], biological and medical processes [25, 38], liquid crystal modeling [18,77,87], and topology optimization [34,53]. Kim and co-authors [47] proposed the phase field model for solidification in binary alloys, commonly referred to as the Kim-Kim-Suzuki (KKS) model. Through rigorous asymptotic analysis under the thin-interface approximation, a relationship between the phase field mobility and the interfacial kinetic