

## A Modeling Framework for Coupling Plasticity with Species Diffusion

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**Abstract.** This paper presents a modeling framework—mathematical model and computational framework—to study the response of a plastic material due to the presence and transport of a chemical species in the host material. Such a modeling framework is important to a wide variety of problems ranging from Li-ion batteries, moisture diffusion in cementitious materials, hydrogen diffusion in metals, to consolidation of soils under severe loading-unloading regimes. The mathematical model incorporates experimental observations reported in the literature on how (elastic and plastic) material properties change because of the presence and transport of a chemical species. Also, the model accounts for one-way (transport affects the deformation but not *vice versa*) and two-way couplings between deformation and transport subproblems. The resulting coupled equations are not amenable to analytical solutions; so, we present a robust computational framework for obtaining numerical solutions. Given that popular numerical formulations do not produce nonnegative solutions, the computational framework uses an optimized-based nonnegative formulation that respects physical constraints (e.g., nonnegative concentrations). For completeness, we also show the effect and propagation of the negative concentrations, often produced by contemporary transport solvers, into the overall predictions of deformation and concentration fields. Notably, anisotropy of the diffusion process exacerbates these unphysical violations. Using representative numerical examples, we discuss how the concentration field affects plastic deformations of a degrading solid. Based on these numerical examples, we also discuss how plastic zones spread because of material degradation. To illustrate how the proposed computational framework performs, we report various performance metrics such as optimization iterations and time-to-solution.

**AMS subject classifications:** 74C05, 74F25, 74S05

**Key words:** Species diffusion, plasticity, non-negative solutions, damage mechanics, degradation/healing, coupled problem.

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# 1 Introduction and motivation

## 1.1 Motivation

Degradation of materials has a substantial economic cost tag; for example, corrosion—a prominent degradation mechanism—itself costs several trillion dollars worldwide [1, 2]. External stimuli are often the primary causes of material degradation. These stimuli could be in the form of mechanical loading, high/low temperatures, transport of chemical species, chemical reactions, radiation, to name a few. The damage incurred from such stimuli could diminish the serviceability or even make the material unusable altogether because of complete rupture. Knott [3] lists the various ways of mechanical failure as elastic instability (buckling), large elastic deformations, tensile instability (necking), plastic deformation (yielding), and cracking (fracture and fatigue). Given the subject's breadth, a comprehensive study of degradation of materials, addressing all the causes and ways of failure mentioned above, will be out of reach of any single research article. Duly, we restrict our study to the harmful effects of a chemical species' presence and transport on mechanical material properties and refer to such a phenomenon as degradation from here-on.

Prior experiments have shown that the presence and diffusion of a chemical species affect the plastic material properties; for example, the elastic yield function could depend on the species' concentration [4]. Such dependence on material properties affects the plastic deformation of the material. Diffusion-induced degradation of a solid undergoing plastic deformation poses several challenges in a wide variety of industrial applications. We now briefly outline four such challenges.

*First*, metal structures exposed to hydrogen gas (such as storage tanks) often suffer from hydrogen embrittlement. In these structures, hydrogen atoms infiltrate into the metal's crystalline structure, interacts with defects such as dislocations, grain boundaries, and voids, compromising material properties and strength [5]. *Second*, in material systems operating under severe loading and environmental conditions, the diffusion of matter under mechanical stresses can degrade the microstructure, triggering nucleation of local damage in the form of vacancy clusters or micro-voids. Some specific examples include vacancy diffusion-driven cavitation in nuclear reactor components and thin films' damage in semiconductor devices [6,7]. *Third*, diffusion of Li ions induces swelling during charge-discharge cycles in Li-ion batteries [8]. This swelling compromises the efficiency of Li-ion batteries. *Fourth*, a well-known degradation in concrete occurs because of alkali-silica reaction (ASR)—often referred to as concrete cancer [9]. This reaction leads to swelling at the aggregate level, altering elastoplastic material properties, and creating cracks. An aggressive ASR adversely affects the capacity and durability of a concrete structure [10].