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Modeling High Performing Structures at Extreme Environments: Effects of Environmental Degradation

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Modeling and prediction of the deterioration of material and structural performance under severe environmental conditions has been a tremendous challenge to computational and modeling communities. Examples of such problems that display environmental-deformation response coupling are ubiquitous across the engineering landscape. Problems that attracted recent attention include oxidation of metallic structural components of hypersonic air vehicles that operate under high temperature and high amplitude loads; hydrogen embrittlement in renewable energy infrastructure; among many others.

We are concerned with developing a modeling framework that can accurately describe coupled aggressive agent transport- mechanical deformation and failure processes. The proposed framework has two components: (1) Formulation and implementation of the coupling mechanisms between transport and mechanical processes, and (2) Development of a multiscale modeling approach that can accurately describe the degradation phenomenon emanating from structural boundaries and propagating towards the interior of the material or the structure. We will present a three-field finite element formulation for the evaluation of coupled transport-deformation problems. A stabilized advection-diffusion-reaction model is employed to idealize the mass transport of an aggressive environmental agent within a solid medium, whereas the deformation response of the medium is formulated using the mixed finite element approach with pressure and displacement as unknown variables. The proposed model accurately captures the pressure and pressure gradient fields that characterize the reaction and advection terms of the mass transport model. The proposed transport-deformation model is calibrated and applied to evaluate the response of titanium structures operating in high temperature environments. We also propose a new multiscale approach for the analysis of coupled mechano-diffusion problems on the basis of the multiscale variational enrichment idea. In this approach, the response (i.e., concentration and deformation) fields and the associated partial differential equations describing the physical phenomenon are decomposed into coarse-scale and fine-scale components without the assumption of scale separation. The proposed framework is advantageous in the analysis of problems, where the ingress of the aggressive agent (e.g., oxygen) is limited to a surface layer with a thickness in the order of the statistically representative volume of microstructural heterogeneity or less. The coupled mechano-diffusion response is fully resolved at the scale of the material heterogeneity, whereas the substrate material that is unaffected by the transport process is idealized on the basis of the phenomenological modeling.

Caglar Oskay is an Associate Professor of Civil and Environmental Engineering at Vanderbilt University, where he has been a faculty member since 2006. He received his PhD from the Civil Engineering department at Rensselaer Polytechnic University in 2003. He worked as a Research Associate at the Scientific Computation Research Center and the Civil Engineering department at RPI before joining Vanderbilt. Prof. Oskay's primary research focus is on multiscale computational modeling and simulation of material and structure systems subjected to extreme environments and loading conditions.