Variational Multiscale Enrichment for Modeling Coupled Mechano-Diffusion Problems

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Abstract

In this manuscript, a new multiscale-multiphysics computational methodology is devised for analysis of coupled diffusion-deformation problems. The proposed methodology is based on the variational multiscale principles. The basic premise of the approach is accurate fine-scale representation at a small subdomain where it is known a-priori that important physical phenomena are likely to occur. The response within the remainder of the problem domain is idealized based on coarse-scale representation. We apply this idea to evaluate a coupled mechano-diffusion problem that idealizes the response of titanium structures subjected to thermo-chemo-mechanical environment. The proposed methodology is employed to devise a multiscale model, in which the transport of oxygen into titanium is modeled as a diffusion process, whereas the mechanical response is idealized using concentration dependent elasticity equations. A coupled solution strategy based on operator split is formulated to evaluate the coupled multiphysics and multiscale problem. Numerical experiments are conducted to assess the accuracy and computational performance of the proposed methodology. Numerical simulations indicate that the variational multiscale enrichment has reasonable accuracy and computationally efficient in modeling the coupled mechano-diffusion response.

Keywords: Variational multiscale enrichment; Multiphysics; Coupled problems; Titanium, Oxygen ingress

1 Introduction

Time-dependent deterioration of structural materials subjected to aggressive environments poses significant challenges for many engineering systems. Examples that have received increased attention recently include embrittlement-induced fracture in hydrogen containment structures [1], oxide formation in metallic and ceramic matrix composite aerospace structures operating at high temperatures [2, 3], concrete deterioration due to ingress of sulfate, chloride and other aggressive agents [4], among others.

In the aerospace arena, there is an increased interest in modeling and prediction of the oxygen ingress induced deterioration of titanium structures employed in hypersonic air vehicles operating

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Figure 1: (a) Multiple physical processes affecting the response prediction of oxygen-rich titanium; (b) Multiple scales affecting the response prediction of oxygen-rich titanium.

under extreme thermo-mechanical environment. In the presence of high temperatures, atmospheric oxygen tends to diffuse into titanium along the surface of the structure. Time-dependent deterioration phenomena in titanium is marked by a strong coupling between the transport of oxygen through the structural material and the deformation process as illustrated in Fig. 1a. The transport of oxygen typically leads to increase in hardness, loss of ductility, loss of fatigue life and strength [5, 6] as a result of occupation of interstitials by oxygen atoms, phase transformations, and oxide formation based on the available amount of oxygen within the material. The diffusion of oxygen is also affected by the mechanical processes since the microcrack formation within the brittle oxygen-rich layer accelerates diffusion of oxygen. The response of titanium structures operating in extreme environments is affected by phenomena occurring at multiple spatial scales in addition to multiple physical processes as illustrated in Fig. 1b. Oxygen ingress and ingress induced changes in deformation response is limited to a boundary region with a thickness in the order of tens of microns. In contrast, the overall thickness of the titanium structure is in the order of millimeters. The heterogeneity of the material microstructure also significantly affects the response at the boundary region since the size of the statistically representative volume is often in the order or greater than the boundary region thickness.

Modeling and prediction of the response of titanium structures operating in extreme environments requires: (a) constitutive models capable of accurately capturing the coupling between transport phenomena and the deformation response at the microstructural as well as the phenomenological levels, and; (b) a multiscale-multiphysics computational framework capable of evaluating the coupled response. The current manuscript is concerned with the development of such a multiscale-multiphysics computational approach for analysis of mechano-diffusion problems.

In view of recent developments in computational multiscale modeling, a number of new investigations focused on devising multiscale computational methodologies for coupled diffusion-deformation problems. For instance, Terada *et al.* [7] formulated a coupled mechano-diffusion model based on the computational homogenization method [8–12]. Lee and Sundararaghavan [13] employed a similar homogenization based approach for the analysis of oxidation in ceramic matrix composites. Multiscale models based on computational homogenization theory for the analysis of other coupled parabolicelliptic systems such as thermo-mechanical response were proposed recently (e.g., Yu and Fish [14], Ozdemir *et al.* [15]).

The current manuscript provides a novel computational framework for the analysis of coupled

mechano-diffusion problems based on the multiscale variational enrichment idea originally proposed by Hughes and coworkers [16, 17], and further developed for solid and fluid systems (see e.g., Refs. [18-20] among others). 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- and fine-scale components without the assumption of scale separation (i.e., $\zeta \equiv l_m/l_M \rightarrow 0$, where $l_{\rm m}$ and $l_{\rm M}$ denote the characteristic lengths at the micro- and macro-scales). With the exception of recent efforts on extending the capabilities of computational homogenization (e.g., [21]), the majority of the computational homogenization-based methods operate under the scale separation limit. The proposed framework is therefore advantageous in 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. 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 based on phenomenological models. The scale decomposition is achieved by employing residual free bubble functions [22–24]. This manuscript details the formulation and implementation of a system of parabolic diffusion and elliptic elasticity equations to model the coupled transport and deformation processes. A novel operator split methodology is devised and implemented to efficiently evaluate the coupled multiscale-multiphysics problem. The proposed coupled solution algorithm is parallelizable and provides the possibility of efficient evaluation of largescale structural systems.

The remainder of this manuscript is organized as follows: Section 2 provides the problem statement, and the governing equations of the boundary value problem describing mechano-diffusion. Section 3 describes the variational multiscale enrichment methodology and the discretization of the resulting multiscale-multiphysics governing equations. Section 4 details the computational strategy employed in the numerical evaluation of the discrete system of equations. In Section 5, the diffusion and mechanical material models that couple the diffusion and deformation processes are provided. Two numerical examples are included to verify the proposed multiscale-multiphysics approach, and assess the performance and capabilities. Section 6 presents conclusions and the future research directions.

2 Problem Statement

We start by setting the governing equations of the coupled problem, which defines the transport of an aggressive agent into a solid material and the deformation response under mechanical loading. The following restrictions are considered for the transport and deformation processes: (1) The transport phenomena is taken to be a purely diffusion process: no chemical reactions causing formation of reaction products or phase transformations take place at the concentration levels of interest; and, (2) Deformations remain elastic.

Let $\Omega \subset \mathbb{R}^{n_{sd}}$ be the domain of the structure as illustrated in Fig 2a. n_{sd} is the number of spatial dimensions. The diffusion process is provided by the following governing partial differential equation:

$$\dot{c}(\mathbf{x},t) = \nabla \cdot [D(\mathbf{x},t) \nabla c(\mathbf{x},t)]; \quad \mathbf{x} \in \Omega$$
(1)

in which, *c* denotes the concentration field; *D* the apparent diffusivity; **x** position coordinate vector; $t \in \mathcal{T} \subset \mathbb{R}^+$ the time coordinate; and, superposed dot the time derivative of the corresponding field. The boundary and initial conditions are given as:

- Dirichlet B.C.: $c(\mathbf{x},t) = \tilde{c}(\mathbf{x},t); \quad \mathbf{x} \in \Gamma$ (2)
- Initial condition: $c(\mathbf{x}, t = 0) = c_0(\mathbf{x}); \quad \mathbf{x} \in \Omega$ (3)



Figure 2: (a) The problem domain; (b) The boundary region, and; (c) The heterogeneous microstructure associated with an enrichment domain.

where, \tilde{c} the prescribed Dirichlet boundary condition along the domain boundary, $\Gamma \equiv \partial \Omega$; and, c_0 the prescribed initial concentration distribution. The apparent diffusivity within the domain is affected by the stress state, $\boldsymbol{\sigma}$, stress history, and temperature, *T*. In the general form:

$$D(\mathbf{x},t) = \bar{D}(\mathbf{x},t;\boldsymbol{\omega},\boldsymbol{\sigma},T) > 0 \tag{4}$$

in which, $\boldsymbol{\omega}$ denotes the internal state variables for the effect of stress history on diffusivity. Overbar distinguishes the value and the form of the function. The specific choice of form for diffusivity does not affect the subsequent formulation, and the form employed in the numerical verification studies is provided in Section 5.1.

The mechanical response of the structure is modeled using the elasticity equations:

$$\nabla \cdot (\mathbf{L}(\mathbf{x},t) : \nabla^{s} \mathbf{u}(\mathbf{x},t)) = \mathbf{0}; \quad \mathbf{x} \in \Omega$$
(5)

in which, **u** denotes the displacement vector; **L** the tensor of elastic moduli; and, ∇^s the symmetric gradient operator. The boundary conditions for the mechanical problem are:

Displacement B.C.:
$$\mathbf{u}(\mathbf{x},t) = \tilde{\mathbf{u}}(\mathbf{x},t); \quad \mathbf{x} \in \Gamma_u$$
 (6)

Traction B.C.:
$$\mathbf{\sigma}(\mathbf{x},t) \cdot \mathbf{n} = \tilde{\mathbf{t}}(\mathbf{x},t); \quad \mathbf{x} \in \Gamma_t$$
 (7)

where, $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{t}}$ displacements and tractions prescribed along boundaries Γ_u and Γ_t , respectively, such that $\Gamma = \Gamma_u \cup \Gamma_t$; $\Gamma_u \cap \Gamma_t \equiv \emptyset$; and, \mathbf{n} the unit vector normal to the domain boundary. The concentration field affects the deformation response through the tensor of elastic moduli. In the general form:

$$\mathbf{L}(\mathbf{x},t) = \bar{\mathbf{L}}(\mathbf{x},t;c) \tag{8}$$

The tensor of elastic moduli is assumed to satisfy the conditions of major and minor symmetries and positivity (i.e., $\exists C_0 > 0$ such that $\boldsymbol{\xi} : \mathbf{L} : \boldsymbol{\xi} \ge C_0 \boldsymbol{\xi} : \boldsymbol{\xi} \forall$ symmetric $\boldsymbol{\xi}$) for all concentration values ($0 \le c \le 1$).

Equations 1-8 provides the governing equations for the coupled mechano-diffusion process. The weak form of the coupled boundary value problem is given as follows:

Find $c \in W$ and $\mathbf{u} \in \mathcal{V}$ for each $t \in \mathcal{T}$ such that:

$$\int_{\Omega} v \dot{c} d\Omega + \int_{\Omega} \nabla v D \nabla c d\Omega = 0$$
⁽⁹⁾

$$\int_{\Gamma_t} \mathbf{w} \cdot \tilde{\mathbf{t}} \, d\Gamma - \int_{\Omega} \nabla \mathbf{w} : \mathbf{L} : \nabla \mathbf{u} \, d\Omega = 0 \tag{10}$$

are satisfied for all $v \in H_0^1(\Omega)$ and $\mathbf{w} \in [H_0^1(\Omega)]^{n_{sd}}$. The trial spaces for the concentration and displacement fields are:

$$\mathcal{W} \equiv \left\{ \hat{c} \in H^1(\Omega) \, \middle| \, \hat{c} = \tilde{c} \text{ on } \mathbf{x} \in \Gamma \right\}$$
(11)

$$\mathcal{V} \equiv \left\{ \hat{\mathbf{u}} \in \left[H^1(\Omega) \right]^{n_{sd}} \middle| \hat{\mathbf{u}} = \tilde{\mathbf{u}} \text{ on } \mathbf{x} \in \Gamma_u \right\}$$
(12)

where, $H^1(\Omega)$ is the Sobolev space of functions with square integrable values and derivatives defined in the domain, Ω , and $H_0^1(\Omega)$ is the subspace of functions in $H^1(\Omega)$ that are homogeneous along the domain boundary, Γ .

3 Variational Multiscale Enrichment

Let the problem domain, Ω , consists of two non-overlapping subdomains Ω^b and Ω^s such that $\Omega \equiv \Omega^b \cup \Omega^s$ as illustrated in Fig. 2. The problem domain is split such that significant rise in concentration levels and associated deformation phenomena during the observation window, \mathcal{T} , remains within the boundary region, Ω^b . Within the boundary region, the coupled mechano-diffusion response is accurately characterized by modeling and resolving at the scale of the microstructural heterogeneities. The extent of the boundary region within the observation period is assumed to remain small compared to the overall size of the structure. Within the substrate domain, Ω^s , the concentration levels remain insignificant and the mechanical response is not affected by the diffusion process. Coarse scale (i.e., phenomenological) modeling is considered to be capable of accurately capturing the response within Ω^s . It is implicitly assumed that the overall structure is large enough to computationally prohibit the full resolution of the microscale heterogeneities throughout the structure.

The boundary region, Ω^b , is partitioned into simple enrichment (microstructural) domains in such a way that each enrichment domain can be represented by a standard finite element as illustrated in Fig. 2b:

$$\Omega^{b} = \bigcup_{\alpha=1}^{n_{en}} \Omega^{b}_{\alpha}; \text{ such that } \Omega^{b}_{\alpha} \cap \Omega^{b}_{\beta} \equiv \emptyset \text{ when } \alpha \neq \beta$$
(13)

in which, n_{en} is the total number of enrichment domains. Each enrichment domain coincides with a macroscopic finite element for the coarse scale solution of the problem described below. Within each enrichment domain, the microscale heterogeneity is discretized and numerically evaluated for the local fine scale solution (Fig. 2c). To this extent, the response fields are expressed in terms of micro- and macroscale counterparts using the following decompositions:

$$c(\mathbf{x},t) = c^{M}(\mathbf{x},t) + \sum_{\alpha=1}^{n_{en}} \mathcal{H}(\Omega^{b}_{\alpha}) c^{m}_{\alpha}(\mathbf{x},t)$$
(14)

$$\mathbf{u}(\mathbf{x},t) = \mathbf{u}^{M}(\mathbf{x},t) + \sum_{\alpha=1}^{n_{en}} \mathcal{H}(\Omega_{\alpha}^{b}) \mathbf{u}_{\alpha}^{m}(\mathbf{x},t)$$
(15)

where, superscripts M and m denote the macroscale and microscale response fields, respectively; and:

$$\mathcal{H}(\Omega^b_{\alpha}) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega^b_{\alpha} \\ 0 & \text{elsewhere} \end{cases}$$
(16)

The decompositions provided in Eqs. 14-15 are inadmissible since the response functions may lie outside the trial function spaces due to discontinuities across the enrichment domain boundaries. Proper boundary conditions for the microscale response fields must therefore ensure inter-enrichment domain continuity. We adopt the concept of residual free bubbles developed in Refs. [22–24] to ensure admissible decomposition of the response fields. The microscale response fields are considered to have homogeneous boundary conditions at the enrichment domain boundaries:

$$c^m_{\alpha}(\mathbf{x},t) = 0 \text{ and } \mathbf{u}^m_{\alpha}(\mathbf{x},t) = \mathbf{0} \text{ on } \mathbf{x} \in \Gamma_{\alpha} \equiv \partial \Omega^b_{\alpha}; \ \alpha = 1, 2, \dots, n_{en}$$
 (17)

In addition to ensuring that the response fields, c and \mathbf{u} , lie within the trial spaces \mathcal{W} and \mathcal{V} , respectively, the choice of homogeneous microscale boundary conditions ensures that the nodal values of the macroscale response fields c^M and \mathbf{u}^M coincide with the nodal values of the corresponding total response fields upon discretization, similar to the finite element method with standard Lagrangian shape functions.

Considering additive two-scale decompositions for the test functions, v and \mathbf{w} , analogous to Eqs. 14-15, the weak form of the original problem given in Eqs. 9-10 is decomposed into a macroscale diffusion and deformation problems defined over the problem domain, Ω , and a series of local microscale diffusion and deformation problems defined over the enrichment domains. The weak form of the resulting multiscale problem is given as follows:

Find the macroscale concentration field, $c^M \in \mathcal{W}$, macroscale displacement field, $\mathbf{u}^M \in \mathcal{V}$, the microscale concentration fields, $c^m_{\alpha} \in \mathcal{W}_{\alpha}$, and the microscale displacement fields, $\mathbf{u}^m_{\alpha} \in \mathcal{V}_{\alpha}$, for each $t \in \mathcal{T}$ such that:

Macroscale diffusion problem:

$$a\left(v^{M},c^{M}\right)_{\Omega}^{c}+\left(v^{M},\dot{c}^{M}\right)_{\Omega}^{c}=-\sum_{\alpha=1}^{n_{en}}\left[a\left(v^{M},c_{\alpha}^{m}\right)_{\Omega_{\alpha}^{b}}^{c}+\left(v^{M},\dot{c}_{\alpha}^{m}\right)_{\Omega_{\alpha}^{b}}^{c}-\left(v^{M},q_{\alpha}^{m}\right)_{\Gamma_{\alpha}}^{c}\right]$$

$$\tag{18}$$

Microscale diffusion problems: $(\alpha = 1, 2, ..., n_{en})$

$$a\left(v_{\alpha}^{m},c_{\alpha}^{m}\right)_{\Omega_{\alpha}^{b}}^{c}+\left(v_{\alpha}^{m},\dot{c}_{\alpha}^{m}\right)_{\Omega_{\alpha}^{b}}^{c}=-a\left(v_{\alpha}^{m},c^{M}\right)_{\Omega_{\alpha}^{b}}^{c}-\left(v_{\alpha}^{m},\dot{c}^{M}\right)_{\Omega_{\alpha}^{b}}^{c}\tag{19}$$

Macroscale mechanical problem:

$$a\left(\mathbf{w}^{M},\mathbf{u}^{M}\right)_{\Omega}^{u}-\left(\mathbf{w}^{M},\tilde{\mathbf{t}}\right)_{\Gamma_{t}}^{u}=-\sum_{\alpha=1}^{n_{en}}\left[a\left(\mathbf{w}^{M},\mathbf{u}_{\alpha}^{m}\right)_{\Omega_{\alpha}^{b}}^{u}-\left(\mathbf{w}^{M},\mathbf{t}_{\alpha}^{m}\right)_{\Gamma_{\alpha}}^{u}\right]$$
(20)

Microscale mechanical problems: $(\alpha = 1, 2, ..., n_{en})$

$$a\left(\mathbf{w}_{\alpha}^{m},\mathbf{u}_{\alpha}^{m}\right)_{\Omega_{\alpha}^{b}}^{u}=-a\left(\mathbf{w}_{\alpha}^{m},\mathbf{u}^{M}\right)_{\Omega_{\alpha}^{b}}^{u}$$
(21)

(10)

(01)

are satisfied for all $v^{M} \in H_{0}^{1}(\Omega)$, $\mathbf{w}^{M} \in [H_{0}^{1}(\Omega)]^{n_{sd}}$, $v_{\alpha}^{m} \in H_{0}^{1}(\Omega_{\alpha}^{b})$, and $\mathbf{w}_{\alpha}^{m} \in [H_{0}^{1}(\Omega_{\alpha}^{b})]^{n_{sd}}$. $q_{\alpha}^{m} = D\nabla c_{\alpha}^{m} \cdot \mathbf{n}$ and $\mathbf{t}_{\alpha}^{m} = (\mathbf{L} : \nabla \mathbf{u}_{\alpha}^{m}) \cdot \mathbf{n}$ denote the microscale boundary flux and tractions, respectively. The trial spaces for the microscale concentration and displacement fields are given as: $\mathcal{W}_{\alpha} \equiv H_{0}^{1}(\Omega_{\alpha}^{b})$ and $\mathcal{V}_{\alpha} \equiv [H_{0}^{1}(\Omega_{\alpha}^{b})]^{n_{sd}}$, respectively; $(u, w)_{[\cdot]}^{c} := \int_{[\cdot]} u w d[\cdot]$ and $(\mathbf{u}, \mathbf{w})_{[\cdot]}^{u} = \int_{[\cdot]} \mathbf{u} \cdot \mathbf{w} d[\cdot]$ denote L_{2} inner products defined over the domain $[\cdot]$, and; $a(u, w)_{[\cdot]}^{c} := \int_{[\cdot]} \nabla u D\nabla w d[\cdot]$ and $a(\mathbf{u}, \mathbf{w})_{[\cdot]}^{u} := \int_{[\cdot]} \nabla \mathbf{u} \cdot \mathbf{L} : \nabla \mathbf{w} d[\cdot]$ are bilinear forms for the diffusion and deformation problems, respectively.

The couplings between the micro- and macroscopic scales are due to the right hand size terms in Eqs. 18-21, whereas the coupling between the diffusion and deformation processes is due to the concentration and deformation dependent material behavior. The macroscale mechano-diffusion problem defined over the macrostructure, Ω , is discretized using a coarse finite element grid, which coincides with the enrichment domains within the boundary region. Within each enrichment domain, a fine

discretization resolving the microstructural heterogeneity is considered. The macroscale and the microscale response fields are approximated using the standard Galerkin discretization. The concentration fields and the corresponding test functions are expressed as:

$$c^{M}(\mathbf{x},t) = \sum_{A=1}^{M} N_{A}(\mathbf{x}) \hat{C}_{A}(t); \qquad v^{M}(\mathbf{x},t) = \sum_{A=1}^{M} N_{A}(\mathbf{x}) \hat{V}_{A}(t)$$
(22)

$$c_{\alpha}^{m}(\mathbf{x},t) = \sum_{a=1}^{m^{\alpha}} n_{a}^{\alpha}(\mathbf{x}) \hat{c}_{a}^{\alpha}(t); \qquad v_{\alpha}^{m}(\mathbf{x},t) = \sum_{a=1}^{m^{\alpha}} n_{a}^{\alpha}(\mathbf{x}) \hat{v}_{a}^{\alpha}(t)$$
(23)

in which, M and m^{α} denote the number of nodes in the macroscale mesh, and the microscale mesh associated with the enrichment domain, Ω^b_{α} , respectively; N_A and n^{α}_a are the macro and microscale shape functions, respectively. Overhat denotes the nodal coordinates of the corresponding response field. The deformation fields and the corresponding test functions are expressed as:

$$\mathbf{u}^{M}(\mathbf{x},t) = \sum_{A=1}^{M} N_{A}(\mathbf{x}) \hat{\mathbf{U}}_{A}(t); \qquad \mathbf{w}^{M}(\mathbf{x},t) = \sum_{A=1}^{M} N_{A}(\mathbf{x}) \hat{\mathbf{W}}_{A}(t)$$
(24)

$$\mathbf{u}_{\alpha}^{m}(\mathbf{x},t) = \sum_{a=1}^{m^{\alpha}} n_{a}^{\alpha}(\mathbf{x})\hat{\mathbf{u}}_{a}^{\alpha}(t); \qquad \mathbf{w}_{\alpha}^{m}(\mathbf{x},t) = \sum_{a=1}^{m^{\alpha}} n_{a}^{\alpha}(\mathbf{x})\hat{\mathbf{w}}_{a}^{\alpha}(t)$$
(25)

The superscript, α in the microscale discretizations (Eqs. 23 and 25) indicates that the present formulation permits using different microstructural representations at each enrichment domain throughout the boundary region.

Substituting Eqs. 22-25 into the weak forms of the micro and macroscale problems, discretizing the time coordinate, and employing the backward difference approximation to discretize the time derivatives, the following nonlinear coupled system of equations are obtained (in vector notation):

Macroscale diffusion problem:
$$\Psi := (\mathbf{M}^{sc} + \Delta t \mathbf{K}^{sc}(\mathbf{u})) \hat{\mathbf{C}} - \mathbf{M}^{sc}{}_{t}\hat{\mathbf{C}} - \mathbf{f}^{sc}(\mathbf{u}) = \mathbf{0}$$
 (26)

Microscale diffusion problems:
$$\boldsymbol{\Psi}^{\alpha} := \left(\mathbf{M}^{bc}_{\alpha} + \Delta t \mathbf{K}^{bc}_{\alpha}(\mathbf{u}) \right) \hat{\mathbf{c}}^{\alpha} - \mathbf{M}^{bc}_{\alpha t} \hat{\mathbf{c}}^{\alpha} - \mathbf{f}^{bc}_{\alpha}(\mathbf{u}) = \mathbf{0}$$
 (27)

Macroscale mechanical problem: $\mathbf{\Phi} := \mathbf{K}^{su}(c) \hat{\mathbf{U}} - \mathbf{f}^{su}(c) = \mathbf{0}$ (28)

Microscale mechanical problem:
$$\mathbf{\phi}^{\alpha} := \mathbf{K}^{bu}_{\alpha}(c) \,\hat{\mathbf{u}}^{\alpha} - \mathbf{f}^{bu}_{\alpha}(c) = \mathbf{0}$$
 (29)

in which, $\hat{\mathbf{C}} = {\{\hat{C}_1, \hat{C}_2, \dots, \hat{C}_M\}}^T$ and $\hat{\mathbf{U}} = {\{\hat{\mathbf{U}}_1^T, \hat{\mathbf{U}}_2^T, \dots, \hat{\mathbf{U}}_M^T\}}^T$ denote the macroscale nodal concentration and displacement coefficients in vector form, respectively; *T* the transpose operator; $\hat{\mathbf{c}}^{\alpha} = {\{\hat{c}_1^{\alpha}, \hat{c}_2^{\alpha}, \dots, \hat{c}_{m^{\alpha}}^{\alpha}\}}^T$ and $\hat{\mathbf{u}}^{\alpha} = {\{(\hat{\mathbf{u}}_1^{\alpha})^T, (\hat{\mathbf{u}}_2^{\alpha})^T, \dots, (\hat{\mathbf{u}}_{m^{\alpha}}^{\alpha})^T\}}^T$ the microscale nodal concentration and displacement fields within enrichment domain α , respectively; and, left subscript *t* denotes the value at the previous time step. The finite element matrices for the diffusion problems are:

$$\mathbf{M}^{sc} = \mathop{\mathbf{A}}_{A,B} (N_A, N_B)^c_{\Omega}; \quad \mathbf{K}^{sc} = \mathop{\mathbf{A}}_{A,B} a (N_A, N_B)^c_{\Omega}$$
(30)

$$\mathbf{M}_{\alpha}^{bc} = \mathbf{A}_{a,b} \left(n_{a}^{\alpha}, n_{b}^{\alpha} \right)_{\Omega_{\alpha}^{b}}^{c}; \quad \mathbf{K}_{\alpha}^{bc} = \mathbf{A}_{a,b} a \left(n_{a}^{\alpha}, n_{b}^{\alpha} \right)_{\Omega_{\alpha}^{b}}^{c}$$
(31)

$$\mathbf{f}^{sc} = \mathbf{A}_{A} \sum_{\alpha=1}^{n_{en}} \sum_{a=1}^{n_{m}^{\alpha}} \left[-\Delta t \hat{c}_{a}^{\alpha} a \left(N_{A}, n_{a}^{\alpha} \right)_{\Omega_{\alpha}^{b}}^{c} - \Delta \hat{c}_{a}^{\alpha} \left(N_{A}, n_{a}^{\alpha} \right)_{\Omega_{\alpha}^{b}}^{c} + \left(N_{A}, q_{\alpha}^{m} \right)_{\Gamma_{\alpha}}^{c} \right]$$
(32)

$$\mathbf{f}_{\alpha}^{bc} = \mathbf{A}_{a} \sum_{A=1}^{M} \left[-\Delta t \hat{C}_{A} a \left(n_{a}^{\alpha}, N_{A} \right)_{\Omega_{\alpha}^{b}}^{c} - \Delta \hat{C}_{A} \left(n_{a}^{\alpha}, N_{A} \right)_{\Omega_{\alpha}^{b}}^{c} \right]$$
(33)



Figure 3: Implementation strategy for the evaluation of coupled deformation and diffusion response of microscale and macroscale problems.

in which, **A** denotes standard finite element assembly operation, and $\Delta(\cdot) = (\cdot) - (\cdot)$. The finite element matrices for the mechanical problems are given as:

$$\mathbf{K}^{su} = \mathop{\mathbf{A}}_{A,B} a \left(N_A, N_B \right)^u_{\Omega}; \quad \mathbf{K}^{bu}_{\alpha} = \mathop{\mathbf{A}}_{a,b} a \left(n^{\alpha}_a, n^{\alpha}_b \right)^u_{\Omega^b_{\alpha}}$$
(34)

$$\mathbf{f}^{su} = \mathbf{A}_{A} \left\{ \left(N_{A}, \tilde{\mathbf{t}} \right)_{\Gamma_{t}}^{u} - \sum_{\alpha=1}^{n_{en}} \sum_{a=1}^{n_{m}^{m}} \hat{\mathbf{u}}_{a}^{\alpha} a \left(N_{A}, n_{a}^{\alpha} \right)_{\Omega_{\alpha}^{b}}^{u} + \sum_{\alpha=1}^{n_{en}} \left(N_{A}, \mathbf{t}_{\alpha}^{m} \right)_{\Gamma_{\alpha}}^{u} \right\}$$
(35)

$$\mathbf{f}_{\alpha}^{bu} = \mathbf{A}_{a} \left\{ -\sum_{A=1}^{M} \hat{\mathbf{U}}_{A} a \left(n_{a}^{\alpha}, N_{A} \right)_{\Omega_{\alpha}^{b}}^{u} \right\}$$
(36)

From the physical perspective, the solutions of the macroscale problems provide the homogenized response of the system, whereas the microscale problems provide the enrichment of the boundary region due to the resolution of the heterogeneities. The momentum and mass balance across the enriched and substrate elements at the macroscale, as well as in the microscale problems are satisfied separately in the weak sense as in standard finite element approaches. It is noted that a direct reconstruction of the original response fields would violate the mass and momentum balance across the enrichment domain - substrate interface due to different resolutions of the micro- and macroscale representations.

4 Multiscale-Multiphysics Coupled Solution Algorithm

In this section, we describe the solution methodology to evaluate the discrete system (Eqs. 26-29) describing the coupled mechano-diffusion problem. The proposed approach is based on operator split methodology, in which Eqs. 26-29 are sequentially evaluated at each time step. The coupling relationships and the basic approach are illustrated in Fig. 3. The microscale mechano-diffusion problem (Eqs. 27 and 29) defined within each enrichment domain is strongly coupled to the macroscale mechano-diffusion problem (Eqs. 26 and 28) through the coupling terms in Eqs. 32-36. In contrast, no coupling term exists between microscale mechano-diffusion problems defined over different enrichment domains. This is due to the particular choice of homogeneous boundary conditions for the microscale concentration and response fields. The field continuity is ensured by imposing continuity of the macroscale response fields. The present form based on uncoupled microscale systems of equations is attractive because our formulation facilitates a simple and parallelizable solution strategy illustrated in Fig. 3. The proposed solution algorithm is implemented in the commercial software package DiffPack, which is an object oriented development framework for the numerical solution of partial differential equations [25]. DiffPack provides a library of C++ classes to facilitate development of solution algorithms for complex PDEs. The staggered solution strategy adopted in this study consists of the following steps:

Given: Material parameters $D(\mathbf{u})$ and $\mathbf{L}(c)$ in functional form, boundary data for concentration field, \tilde{c} , and the deformation response, $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{t}}$, as well as the initial concentration field, c_0 :

1. Let k denote the time step counter (k = 0). Initialize diffusion and deformation problems by computing the initial state of the macroscale and the microscale fields based on the given initial data (i.e., c_0) at t = 0.

Set:
$$_{0}\hat{\mathbf{C}}; \ _{0}\hat{\mathbf{C}} = 0; \ _{0}\hat{\mathbf{U}} = \mathbf{0}; \ _{0}\hat{\mathbf{U}} = \mathbf{0}$$
(37)

Set:
$$_{0}\hat{\mathbf{c}}^{\alpha}$$
, $_{0}\hat{\mathbf{u}}^{\alpha} = \mathbf{0}$, $\alpha = 1, 2, \dots, n_{en}$ (38)

in which, left subscript denotes time step. The nodal coordinates of the macroscale concentration field coincide with the values of the total concentration field evaluated at the nodes due to the homogeneity of the microscale boundary conditions and since the macroscale field discretization is taken to coincide with the boundaries of the enrichment domains. The initial state of the microscale concentration field is computed as the difference between the initial condition data and the macroscale concentration field approximation based on Eq. 22a.

- 2. Increase time step: $k \leftarrow k + 1$ (until the end of observation period):
 - (a) Initialize convergence iterations: i = 0.
 - (b) Set: ${}^{i}_{k}\hat{\mathbf{c}}^{\alpha} = {}_{k-1}\hat{\mathbf{c}}^{\alpha}$ and ${}^{i}_{k}\hat{\mathbf{u}}^{\alpha} = {}_{k-1}\hat{\mathbf{u}}^{\alpha}$; $\alpha = 1, 2, \ldots, n_{en}$.
 - (c) Compute the macroscale field predictors:

$$\hat{\mathbf{C}}_{k} = k^{-1} \hat{\mathbf{C}} + \Delta t_{k-1} \dot{\hat{\mathbf{C}}}$$
(39)

$${}^{l}_{k}\hat{\mathbf{U}} = {}_{k-1}\hat{\mathbf{U}} + \Delta t_{k-1}\hat{\mathbf{U}}$$

$$\tag{40}$$

Let $0 < tol^c \ll 1$ and $0 < tol^u \ll 1$ be the convergence tolerance parameters defined for the diffusion and mechanical response equations, respectively; and $e^c \ge 0$ and $e^u \ge 0$ denote the error measures for the concentration and the displacement fields, respectively.

- (d) While $e^c tol^c > 0$ and $e^u tol^u > 0$:
 - i. $i \leftarrow i+1$
 - ii. Compute the microscale concentration field coefficients, ${}^{i}_{k}\hat{\mathbf{c}}^{\alpha}$, by solving $\tilde{\mathbf{\Psi}}^{\alpha} = \mathbf{0}$ over each enrichment domain $(1 \le \alpha \le n_{en})$:

$$\tilde{\boldsymbol{\Psi}}^{\alpha} := \left(\mathbf{M}^{bc}_{\alpha} + \Delta t \mathbf{K}^{bc}_{\alpha}(\tilde{\mathbf{u}}) \right)^{i}_{k} \hat{\mathbf{c}}^{\alpha} - \mathbf{M}^{bc}_{\alpha \ k-1} \hat{\mathbf{c}}^{\alpha} - \mathbf{f}^{bc}_{\alpha}(\tilde{\mathbf{u}})$$
(41)

$$\tilde{\mathbf{u}} := {}^{i-1}_{\ k} \mathbf{u}^M + \sum_{\alpha=1}^{n_{en}} \mathcal{H}(\Omega^b_\alpha) {}^{i-1}_{\ k} \mathbf{u}^m_\alpha(\mathbf{x}, t)$$
(42)

iii. Compute the microscale deformation field coefficients, ${}^{i}_{k}\hat{\mathbf{u}}^{\alpha}$, by solving $\tilde{\boldsymbol{\phi}}^{\alpha} = 0$ over each enrichment domain $(1 \le \alpha \le n_{en})$:

$$\tilde{\boldsymbol{\phi}}^{\alpha} := \mathbf{K}^{bu}_{\alpha}(\tilde{c})^{i}_{k} \hat{\mathbf{u}}^{\alpha} - \mathbf{f}^{bu}_{\alpha}(\tilde{c})$$
(43)

$$\tilde{c}(\mathbf{x},t) = {}^{i-1}_{\ k} c^{M}(\mathbf{x},t) + \sum_{\alpha=1}^{n_{en}} \mathcal{H}(\Omega^{b}_{\alpha}) {}^{i}_{\ k} c^{m}_{\alpha}(\mathbf{x},t)$$
(44)

iv. Compute the macroscale concentration field coefficients, ${}^{i}_{k}\hat{\mathbf{C}}$, by solving $\tilde{\mathbf{\Psi}} = 0$:

$$\tilde{\boldsymbol{\Psi}} := \left(\mathbf{M}^{sc} + \Delta t \mathbf{K}^{sc} \begin{pmatrix} i \\ k \mathbf{u} \end{pmatrix} \right)_{k}^{i} \hat{\mathbf{C}} - \mathbf{M}^{sc}_{k-1} \hat{\mathbf{C}} - \mathbf{f}^{sc} \begin{pmatrix} i \\ k \mathbf{u} \end{pmatrix}$$
(45)

v. Compute the macroscale deformation field coefficients, ${}^{i}_{k}\hat{\mathbf{C}}$, by solving $\tilde{\mathbf{\Phi}} = 0$:

$$\tilde{\mathbf{\Phi}} := \mathbf{K}^{su} \begin{pmatrix} i \\ k \end{pmatrix} \begin{pmatrix} i \\ k \end{pmatrix} \hat{\mathbf{U}} - \mathbf{f}^{su} \begin{pmatrix} i \\ k \end{pmatrix}$$
(46)

vi. Compute the error measures for the concentration and the displacement fields, e^c and e^u , respectively:

$$e^{c} = \frac{\begin{vmatrix} i & \hat{\mathbf{C}} - i & \hat{\mathbf{C}} \end{vmatrix}}{\begin{vmatrix} i & \hat{\mathbf{C}} \end{vmatrix}}; \quad e^{u} = \frac{\begin{vmatrix} i & \hat{\mathbf{U}} - i & \hat{\mathbf{U}} \end{vmatrix}}{\begin{vmatrix} i & \hat{\mathbf{U}} \end{vmatrix}}$$
(47)

(e) Update microscale and macroscale converged concentration and displacement fields:

$$_{k}\hat{\mathbf{c}}^{\alpha} = {}^{i}_{k}\hat{\mathbf{c}}^{\alpha}; \quad _{k}\hat{\mathbf{u}}^{\alpha} = {}^{i}_{k}\hat{\mathbf{u}}^{\alpha}; \quad _{k}\hat{\mathbf{C}} = {}^{i}_{k}\hat{\mathbf{C}}; \quad _{k}\hat{\mathbf{U}} = {}^{i}_{k}\hat{\mathbf{U}}$$
(48)

3. Go to Step 2 until end of observation period.

The proposed staggered solution algorithm employs macroscale error measures to ensure convergence as described by Eq. 47. The computational algorithm also incorporates an adaptive time stepping methodology, in which, the time step cut-backs are introduced in case of failure of convergence in the proposed staggered evaluation procedure, whereas the time step size is adaptively increased in case of smooth response based on total number of iterations to convergence. The advantages of employing the proposed staggered algorithm over strong coupling methodologies, in which the diffusion and deformation problems are simultaneously evaluated are: (1) The system size to be evaluated increases for both macroscale and microscale diffusion-deformation problems when strong coupling methodologies are employed. (2) The staggered approach provides the capability to use separate time step sizes for diffusion and deformation problems, where the temporal variation of the deformation and diffusion processes are of the same scale, yet disparate. The time step size employed to evaluate the microscale and macroscale boundary value problems are taken to be identical in the proposed algorithm. It is straightforward to extend the algorithm to include separate time step sizes for the macroscale and the microscale problems to improve the efficiency, accuracy and convergence characteristics. The convergence, accuracy and efficiency characteristics of the proposed algorithm is provided in Section 5.2.

5 Numerical Testing

The implementation of the proposed multiscale-multiphysics computational method is verified based on numerical simulations. In this section, we describe the particular constitutive relationships employed to describe the diffusivity of the aggressive agent as a function of deformation, and the tensor of elastic moduli as a function of concentration; and, verify the proposed methodology using two examples. The first example is concerned with single-physics multiscale problems evaluated to assess the accuracy and performance characteristics of the proposed approach (Section 5.2). In the second example, a fully coupled mechano-diffusion problem defined on a panel subjected to non-uniform thermo-mechanical environment is evaluated (Section 5.3).

5.1 Diffusion-deformation coupling

Diffusivity within the microconstituents as well as the homogenized substrate region is modeled as a function of temperature and the mechanical stress state of the structure:

$$D(\omega,T) = D_0 [1 + D_i(\omega) + D_p(\omega)] \exp\left(-\frac{Q}{RT}\right)$$
(49)

in which, D_0 is the pre-exponential constant; Q the activation energy; and, R the universal gas constant. ω is a scalar indicating the state of mechanical damage at the material point, providing the coupling between the deformation processes and diffusivity. In this approach, the apparent diffusivity of the solid medium is affected by microcrack density, which is quantified by the damage variable, ω . The relationship between the apparent diffusivity and ω is modeled based on the theory of percolation [26]. This idea was employed to idealize the effect of mechanical damage state on the sulfate ingress into cementitious materials by Krajcinovic *et al.* [27], and more recently, on the oxygen ingress into titanium and titanium alloys by Oskay and Haney [28]. The physical justification of the coupling relationship between mechanical deformation and the diffusivity as well as the model employed in this study is described in detail in Ref. [28]. Only a brief review of the model is provided herein. The effect of mechanical damage on diffusivity is expressed in terms of initiation, D_i , and percolation, D_p , components:

$$D_i = a\omega \tag{50}$$

$$D_{p} = \begin{cases} 0 & \omega < \omega_{c} \\ \frac{(\omega - \omega_{c})^{2}}{(\omega - \omega_{ec})} & \omega_{c} \le \omega < \omega_{ec} \\ \infty & \omega \ge \omega_{ec} \end{cases}$$
(51)

At relatively low levels of microcrack density $\omega < \omega_c$, the diffusivity of the aggressive agent is a linear function of the mechanical damage state [29]. ω_c is the conduction percolation threshold. When damage exceeds elastic percolation threshold, ω_{ec} , a continuous path across the material point develops, causing free flow of the aggressive agent. In the intermediate values of mechanical damage, the value of diffusivity increases with increasing mechanical damage. In this study, a simple damage law provides the relationship between damage formation and the stress state:

$$\boldsymbol{\omega}(\mathbf{x},t) = \frac{\boldsymbol{\kappa}(\mathbf{x},t)}{p_{cr}}; \quad \boldsymbol{\kappa}(\mathbf{x},t) = \max_{\tau} \left\{ \left\langle \frac{1}{3} \operatorname{tr}(\boldsymbol{\sigma})(\mathbf{x},\tau) \right\rangle \middle| \tau \le t \right\}$$
(52)

where, σ denotes stress tensor, and p_{cr} is the critical expansive stress, which causes cracking within the material; and, $\langle \cdot \rangle := ((\cdot) + |\cdot|)/2$ are MacCauley brackets indicating that an increase in compressive stress does not lead to an increase in the damage state. In the present model, the mechanical response is not affected by the damage state and remains elastic.

The material stiffness is taken to increase as a function of concentration. For simplicity, the material constituents at the microscale, as well as the homogenized response within the substrate are taken to be isotropic. The tensor of elastic moduli, **L**, is therefore expressed in terms of two independent constants:



Figure 4: Variation of the material stiffness as a function of concentration.

Young's modulus, E, and Poisson's ratio, v. The Poisson's ratio is taken to be invariant under changes in the concentration level. E varies as a function of concentration, c, based on the following relationship:

$$E = E_0 \left[\frac{r-1}{\pi} \operatorname{atan} \left(\frac{\pi E'_{cr}}{E_0(r-1)} (c - c_{crit}) \right) + \frac{r+1}{2} \right]$$
(53)

in which, E_0 , $r = E_{\text{max}}/E_0$, E'_{cr} and c_{crit} are material parameters describing the evolution of the mechanical stiffness as a function of concentration as illustrated in Fig. 4.

5.2 Uniform loading

Diffusion and mechanical response characteristics of a 2.5 mm by 2.5 mm plane-strain specimen is considered to assess the performance and accuracy of the proposed computational methodology. The boundary region constitutes top 0.5 mm of the specimen including two phases illustrated as dark (phase a) and light (phase b) in Fig. 5. Young's modulus and pre-exponential constant ratios of the two phases are: $E^b/E^a = 1.5$ and $D_0^a/D_0^b = 4.5$, respectively, whereas the remainder of the material parameters are identical for both phases. Young's modulus, E^h , and pre-exponential diffusivity constant, D_0^h , within the substrate domain are equal to $0.76E^b$ and D_0^b , respectively. The performance of the proposed multiscale computational methodology is verified against direct numerical simulations based on the finite element method. In the direct numerical simulations, the heterogeneity within the boundary region is fully resolved. Four finite element meshes with element sizes of $h = 12.5 \,\mu\text{m}$, 25 μ m, 30 μ m, and 100 μ m are considered to discretize the boundary region. The substrate region is discretized using a coarse finite element mesh with element size of 0.5 mm. Penalty formulation is employed to ensure field continuity between the nonconforming boundary and substrate regions in the reference simulations as described in Ref. [28]. In the multiscale simulations, a coarse and regular macroscale grid with element size of 0.5 mm is considered. Four microscale discretizations of the enrichment domains are considered with average element size identical to boundary region element sizes in the direct numerical simulations. The macroscale discretization and the microscale enrichment domain discretization with $h = 25 \ \mu m$, along with the reference finite element mesh with $h = 25 \ \mu m$ is shown in Fig. 6.

The first series of simulations consider the diffusion phenomena within the specimen in the absence of mechanical loading or deformation. The concentration level at the top boundary is assumed to remain 10% throughout the simulations as shown in Fig 5a. The initial concentration within the material is 0.15%. The simulations are conducted for the duration of 1750 hours. Time step sizes for the multiscale and the reference simulations are chosen small enough such that further refinement of



Figure 5: The geometry of the specimen subjected to uniform loading conditions (a) configuration for the oxygen diffusion simulations, (b) configuration for the mechanical response simulations.

the time step size does not change the response significantly. Time step sizes employed to evaluate the multiscale and reference simulations are 5 hours and 0.5 hours, respectively. We first investigate the effect of convergence tolerance (tol^c) on the accuracy of the proposed multiscale method. Multiscale simulations with tolerances $tol^c = 1e^{-a}$ (a = 2, 3, ..., 8) are conducted on two meshes ($h = 25 \mu m$ and 50 μm). The results of the multiscale method are compared to reference simulations with same level of discretizations within the boundary region. Figure 7 illustrates the effect of the convergence tolerance parameter on the error associated with the multiscale model. The discrete L_2 error is computed as:

$$e_M = \frac{\|\hat{\mathbf{C}} - \hat{\mathbf{C}}_{ref}\|}{\|\hat{\mathbf{C}}_{ref}\|}$$
(54)

in which, $\hat{\mathbf{C}}_{ref}$, denotes concentration field coefficients at nodes that coincide with the macroscale mesh. Figure 7 shows that coupling tolerance does not have a significant effect on the accuracy of the multiscale simulations as the accuracy of the multiscale simulations remains nearly constant for all tolerance values considered. In contrast, total number of iterations per time step linearly increases as a function of the order of the tolerance parameter. $tol^c = 1e - 3$ is therefore employed as multiscale diffusion convergence tolerance in the subsequent simulations. Figure 8 illustrates the error of the proposed multiscale method as a function of discretization. The microscale error within an enrichment domain, α , is given as:

$$e_m = \frac{\left\| \hat{\mathbf{c}}^{\alpha} - \hat{\mathbf{c}}^{\alpha}_{ref} \right\|}{\left\| \hat{\mathbf{c}}^{\alpha}_{ref} \right\|}$$
(55)

where, $\hat{\mathbf{c}}_{ref}^{\alpha}$ denotes concentration field coefficients at nodes that coincide with the microscale mesh within the enrichment domain Ω_{α}^{b} . The microscale as well as the macroscale error remains less than 10% for all meshes considered. The discrepancy between the proposed approach and the reference finite element simulations is mainly due to employing the homogeneous boundary condition to describe the response at the microscale accuracy of the proposed approach is under investigation. Figure 9 compares the oxygen concentration field as a function of depth computed by the proposed multiscale method and reference finite element simulations for two time instances (t = 1000 hours and t = 1750



Figure 6: (a) Macroscale discretization of the specimen, (b) Microscale discretization of a single enrichment domain with $h = 25 \ \mu m$, (c) Discretization for the reference finite element simulations with $h = 25 \ \mu m$ within the boundary region.

hours) and two different meshes ($h = 25 \,\mu\text{m}$ and 50 μm). Figure 9 illustrates that the largest discrepancies between the multiscale and the reference simulations is concentrated within the top 1 mm depth. This is due to the fact that significant ingress of diffusant is limited to the top surface. Only a small increase in the diffusant concentration is observed beyond 1 mm depth within the observation period, justifying the use of coarse scale description at the substrate region. The proposed approach displays good overall accuracy compared to reference finite element method throughout the simulations.

The second series of simulations consider the deformation response of the specimen subjected to uniform uniaxial tension as illustrated in Fig 5b. The oxygen concentration is assumed to remain unchanged during loading. Figure 10 illustrates the equivalent stress profile within the specimen computed by the reference finite element method with average mesh size of $h = 12.5 \ \mu m$ within the boundary region. The figure illustrates a highly heterogeneous response due to the stiffness mismatch between the two phases within the boundary region. The displacement magnitude profiles computed using the multiscale model and the reference model are compared in Fig. 11. The non-uniform displacement fields display a reasonable match. The accuracy of the proposed method is further investigated as a function of discretization in Fig. 12. The microscale and macroscale errors remain within 8% for all four discretizations considered in the simulations. The macro- and microscale errors for the displacement field are computed analogous to the concentration field counterparts provided by Eqs. 54 and 55, respectively. The computational efficiency of the proposed multiscale method is shown in Fig. 13. The simulation performance of the multiscale model is significantly better compared to the reference simulations. Figure 13 illustrates that the simulation time for the proposed multiscale approach rises in the order of 1.5 as a function of the order of total number of degrees of freedom considered in the simulation. In contrast, the simulation time for the direct finite element method is in the order of 2.2. The multiscale model simulation for the densest mesh considered ($h = 12.5 \mu m$) is 22 times faster than the reference finite element method.



Figure 7: The effect of the convergence tolerance on multiscale simulation accuracy.



Figure 8: Microscale and macroscale discretization error in diffusion simulations.



Figure 9: Concentration as a function of depth.



Figure 10: Heterogeneous stress distribution within the boundary domain of the specimen when subjected to uniform tensile loading.



Figure 11: Comparison of the displacement profile computed by (a) Direct finite element method, and; (b) Multiscale model.



Figure 12: Microscale and macroscale discretization error in mechanical response simulations.



Figure 13: Computational cost comparison of the direct finite element and the multiscale simulations.

5.3 Mechano-diffusion in titanium panel

The capabilities of the proposed multiscale-multiphysics computational methodology are investigated by the analysis of the coupled mechano-diffusion response of a rectangular titanium alloy panel subjected to nonuniform thermo-mechanical loading and oxygen-rich environment. At elevated temperatures, oxygen tends to diffuse into titanium structures occupying the interstitials at low concentrations, forming alpha-case with significantly different structural properties such as embrittlement and increased hardness at moderate concentration levels, and causing oxidation at high concentration levels. The current investigation focuses on the response of titanium structures at low oxygen concentrations and oxygen and mechanical loading, in which, the effects of inelastic deformations, alpha-case formation and oxidation reactions are insignificant.

The geometry, loading and the boundary conditions of the panel are illustrated in Fig. 14. The length and thickness of the two-dimensional plane-strain panel are 25.5 mm and 2.45 mm, respectively. The panel is subjected to a nonuniform thermal flux along the top boundary. The amplitude of the flux spike is 3 W/mm² within the 3 mm wide central section of the boundary, whereas the remainder of the boundary is subjected to 1.25 W/mm^2 amplitude flux. The bottom of the panel is subjected to uniform temperature of 149 °C. The titanium alloy has an initial oxygen concentration of 0.15%. Along the top boundary, the panel is subjected to uniform oxygen concentration of 10% throughout the observation period of 100 hours. In addition to the thermal and chemical loading, the panel is also subjected to a uniform tensile loading of varying amplitude as illustrated in Fig. 14.

The characteristic time scale of the thermal process within the panel is orders of magnitude smaller than the characteristic time scale of the oxygen diffusion process. The thermal state reaches the steady state within first few seconds of the observation time. The steady state temperature profile of the panel is shown in Fig. 15. The steady state thermal profile is therefore employed as input to the chemo-



Figure 14: The geometry, boundary conditions and discretization of panel under coupled environment: (a) macroscale discretization; (b) boundary domain, and; (c) microscale discretization of an enrichment domain.

mechanical analysis of the titanium panel. The thermal profile includes a localized hot region with temperatures up to $630 \,^{o}$ C at the center of the top boundary due to the applied thermal flux spike. The elevated temperature at this region causes accelerated oxygen ingress.

The boundary region, Ω^b , is 4.8 mm wide and 50 μ m deep at center of the top boundary immediately below the applied thermal spike. The macroscale discretization of the problem domain is shown in Fig. 14a and a close-up of the macroscale discretization around the boundary region is shown in Fig. 14b. The macroscale discretization of the boundary region consists of 16 quadrilateral elements, each of which constitutes an enrichment domain. The enrichment domains consist of a two-phase microstructure, illustrated in Fig. 14c, with 70% vol. pct. alpha phase (light color) and 30% vol. pct. beta phase (dark color). The microstructural constitution is randomly generated based on the volume percentages of the two constituents. The microstructural element size is 5 μ m, which is the approximate grain size of the titanium alloy. The microstructural configurations for all enrichment domains are taken to be identical. The transport and mechanical properties of the microconstituents, as well as the homogenized substrate domain are shown in Table 1. The stiffness and pre-exponential constants of the two phases have the ratios: $E^{\beta}/E^{\alpha} = 1.5$ and $D_0^{\alpha}/D_0^{\beta} = 4.5$, respectively. The remaining material properties for the two phases within the microstructure, as well as the substrate domain are taken to be identical.

The panel with nonuniform thermal profile is subjected to uniaxial tensile loading of varying magnitudes and high oxygen concentration for 100 hours. Figure 16 illustrates the effect of the magnitude



Figure 15: The thermal profile under non-uniform boundary flux.

Table 1: Microconstituent and homogenized material parameters employed in the mechano-diffusion analysis of a titanium panel.

E^{α} [GPa]	E^{β} [GPa]	E ^h [GPa]	$D_0^{\alpha} [\mathrm{cm}^2/\mathrm{s}]$	$D_0^{\beta} [\mathrm{cm}^2/\mathrm{s}]$	D_0^h [cm ² /s]	Q [kJ/mole]
100.0	150.0	114.0	2.79	0.62	0.62	203.0
ν	E'_{max} [GPa]	E'_{cr} [GPa]	ω_c	ω _{ec}	a	$p_{cr}[MPa]$
0.32	200.0	1.0e3	0.1	0.5	3.56	700.0

of the applied mechanical stress on the diffusion characteristics of oxygen through the boundary region. An increase in the applied stress magnitude significantly increases the depth of the isocontours, which corresponds to the critical value of oxygen concentration ($c_{crit} = 0.045$) that causes significant embrittlement and hardening in the titanium alloy. The non-uniform transport of oxygen into the panel is evident in Fig 16. This nonuniform oxygen ingress is due to the heterogeneities within the microstructure. Figure 17 compares the evolution of oxygen concentration field as a function of depth and time computed by the proposed multiscale method and the reference finite element simulations, in which the microstructural heterogeneity within the boundary region is fully resolved. The figure illustrates the oxygen concentration profiles at the top - central section of the specimens subjected to 0, 100 and 200 MPa loading. Reasonable match between the oxygen concentration profiles are observed between the proposed and reference simulations, which verifies the accuracy characteristics of the proposed approach in the presence of combined mechanical and environmental loading conditions. The panel simulations show that the proposed multiscale model has the capability to effectively evaluate the coupled mechano-diffusion response.

6 Conclusions and Future Research

This manuscript presented a new multiscale-multiphysics computational methodology for modeling coupled mechano-diffusion problems. In the proposed approach a subdomain of interest within the structure is analyzed using fine scale approximation, whereas the remainder of the subdomain is idealized based on coarse scale (i.e., phenomenological) models. The present formulation circumvents the limiting condition of scale separation in multiscale computational models. A new coupled solution strategy based on operator split is devised for efficient evaluation in the presence of multiple spatial scales, and multiple and coupled physical processes. The proposed computational framework is implemented for two-dimensional problems and verified against direct finite element simulations. The multiscale-multiphysics approach has reasonable accuracy (within 10% of direct finite element simulations), and computational efficiency.



Figure 16: The effect of mechanical stress on the oxygen ingress into the panel.



Figure 17: Oxygen concentration within the enrichment domain as a function of depth based on the proposed multiscale approach and the direct finite element simulations when subjected to a tensile strength of: (a) 0 MPa; (b) 100 MPa; and, (c) 200MPa.

A number of computational issues remain outstanding and will be investigated in the near future. First, the transport processes into mechanical systems typically cause microcracking, as well as inelastic processes. The extension of the proposed methodology to incorporate the presence of inelastic processes as well as fracture within the boundary region is critical to realistic simulations of coupled mechano-diffusion problems, including the response of titanium structures subjected to extreme environments. Second, is devising efficient computational algorithms for the parallel implementation of the proposed computational methodology. While the present approach is computationally efficient compared to direct numerical simulations, analysis of large-scale three-dimensional structures will require implementation of parallel algorithms capable of efficiently evaluating the coupled multiscalemultiphysics response. The parallel implementation of the proposed methodology is promising because the enrichment domain (microscale) problems, associated with high computational costs, can be evaluated in parallel without the need of communication with the neighboring enrichment domains. This limits the interface communication overhead in domain decomposition based implementations. Third, employing homogeneous boundary conditions to describe the microscale response fields leads to significant errors. Increasing the fidelity of the proposed approach requires the development of new microscale boundary conditions that improve on the accuracy characteristics of the proposed approach, while keeping the scalability of the method for parallel implementation. Our near term efforts will include extending the proposed multiscale computational framework to parallel implementation for three-dimensional problems, and the development of novel boundary conditions for higher fidelity modeling of coupled transport-deformation processes.

7 Acknowledgements

The author gratefully acknowledges Air Force Summer Faculty Fellowship Program (AF SFFP), and the AFRL Structural Sciences Center (Contract No: GS04T09DBC0017 through High Performance Technologies, Inc.) for funding and support of this research.

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