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A coupled theory for chemically active and deformable solids with mass diffusion and heat conduction

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ABSTRACT

To analyse the frequently encountered thermo-chemo-mechanical problems in chemically active material applications, we develop a thermodynamically-consistent continuum theory of coupled deformation, mass diffusion, heat conduction and chemical reaction. Basic balance equations of force, mass and energy are presented at first, and then fully coupled constitutive laws interpreting multi-field interactions and evolving equations governing irreversible fluxes are constructed according to the energy dissipation inequality and the chemical kinetics. To consider the essential distinction between mass diffusion and chemical reactions in affecting free energy and dissipations of a highly coupled system, we regard both the concentrations of diffusive species and the extent of reaction as independent state variables. This new formulation then distinguishes between the energy contribution from the diffusive species entering the solid and that from the subsequent chemical reactions occurring among these species and the host solid, which not only interact with stresses or strains in different manners and on different time scales, but also induce different variations of solid microstructures and material properties. Taking advantage of this new description, we further establish a specialized isothermal model to predict precisely the transient chemo-mechanical response of a swelling solid with a proposed volumetric constraint that accounts for material incompressibility. Coupled kinetics is incorporated to capture the volumetric swelling of the solid caused by imbibition of external species and the simultaneous dilation arised from chemical reactions between the diffusing species and the solid. The model is then exemplified with two numerical examples of transient swelling accompanied by chemical reaction. Various ratios of characteristic times of diffusion and chemical reaction are taken into account to shed light on the dependency on kinetic time scales of evolution patterns for a diffusion-reaction controlled deformable solid.

1. Introduction

The multi-field coupling problems concerning mass transport, heat exchange, composition change and mechanical deformation of a chemically active medium is of significance in modern advanced technology and engineering applications such as self-healing materials (Aliko-Benítez et al., 2015; Bekas et al., 2016; Blaiszik et al., 2010), environmental-sensitive materials (Chester and Anand, 2011; Hong et al., 2008; Wallmersperger et al., 2008, 2004), natural fiber reinforced composites (Pan and Zhong, 2014a, b, 2015), mechanochemically responsive materials (Black et al., 2011; Caruso et al., 2009),

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energy storage and conversion devices (Bove, 2008; Brassart and Suo, 2012; Cui et al., 2012; Haftbaradaran and Qu, 2015; Haftbaradaran et al., 2011; Schalkwijk and Scosati, 2002), biological tissues (Frijns et al., 2003; Peradzyński, 2010) and porous mixtures of geomaterials (Coussy, 2004, 2010; Gawin et al., 2006; Lecampion, 2013). Thermo-chemo-mechanically coupled dynamic processes are the common features of these problems and hence constitute the major concerns of relevant investigations, either in the development of advanced functionalities of new materials or in the evaluation of potential adverse impacts on long-term performances of engineering structures or machine parts.

Considerable efforts have been devoted to various theories in the past decades on coupling problems. For most cases, the coupling problems can be abstracted as a host deformable solid surrounding with liquid chemical species, gaseous mixtures and solute atoms or ions, which can migrate into or out of the solid and induce expansion or shrinkage. Because the imposed mechanical constraints in the interior or on the boundary of an expanding or shrinking solid will lead to internal stresses that can reversely affect the transport of chemical species (Chester and Anand, 2010), the coupling of mechanical stress and mass transport in solids becomes the research focus in extensive literature, from the early studies of Gibbs (1878) on fluid diffusion in solids and Biot (1941) on saturated soils to recent attempts on the macroscopic field theory (Chester, 2012; Chester and Anand, 2010; Hong et al., 2008; Yang et al., 2010) and the mixture theory (Coussy, 2004; Huyghe and Janssen, 1999). The scope of application has also been greatly enlarged, especially to biological tissues (Ateshian, 2007; Frijns et al., 2003; Peradzyński, 2010), responsive materials like gels and polyelectrolyte (Wallmersperger et al., 2008), where the migration of ions and the electrochemical effect are incorporated with hyperelastic responses of solids. Meanwhile, with the development of batteries and fuel cells, the problem of solid state diffusion driven by chemo-mechanical forces has been extensively studied (Haftbaradaran and Qu, 2014, 2015; Swaminathan and Qu, 2007; Swaminathan et al., 2007). In these works, the chemo-mechanical coupling is formulated by the governing equations of stress-dependent mass transport considering the volumetric constraints such as the intrinsic incompressibility of each constituent.

On the other hand, the diffusive species may react with the host solid or between themselves, which frequently encounters in reaction-based self-healing polymers (Blaiszik et al., 2010), redox of metals (Dong et al., 2012), hydration and dissolution of geomaterials (Gawin et al., 2006; Lecampion, 2013), degradation of macromolecules (Rajagopal et al., 2007). Reaction-diffusion kinetics is crucial in studying these coupling processes (Aliko-Benítez et al., 2015; Drozdov, 2014), which are accompanied by the chemical dilation or shrinkage, the variation of mass and density, the change of mechanical properties and the stress redistribution. For example, the reaction–diffusion process of oxygen accompanied by irreversible shrinkage strains is the main concern in thermo-oxidation of polymers (Gigliotti and Grandidier, 2010). In the study of degradation of material properties, internal variables were introduced to quantify the damage processes (Pan and Zhong, 2014b; Rajagopal et al., 2007), yet there is still a shortage of theoretical models based on full coupling analysis of reaction, diffusion and deformation. In addition, despite the stress could influence the chemical process intrinsically through activation energy (Black et al., 2011; Caruso et al., 2009) or extrinsically by reactant supply, the corresponding theoretical description remains open in most existing theories.

Though different in mechanism, both the stress-assisted mass transport and the stress-related reaction process in solids are referred to as chemo-mechanical coupling. However, a fully coupling theory has not yet been well formulated, which should embody not only the mass balance that controls reaction-diffusion but also the individual evolution relations linking deformation with diffusion and reaction. Furthermore, the temperature effect is necessary to be considered, since the temperature also directly influences the reaction rate, and the reaction, in turn, brings about temperature perturbation, other than the thermoelastic effect.

A few coupling models have been established based on irreversible thermodynamics and linear phenomenological laws. Loeffel and Anand (2011) presented a thermodynamically consistent large-deformation theory for the durability problem of thermal barrier coatings with coupled temperature variation, elastic-viscoplastic deformation, oxygen diffusion and oxidation. Rambert et al. (2007) obtained a complete set of constitutive equations for heat conduction, mass diffusion, chemical process and gradient-type elastic strain for geomaterials. Gigliotti and Grandidier (2010) investigated the reaction–diffusion–mechanical couplings in polymers exposed to thermo-oxidative environments. Rambert et al. (2006) proposed a thermo-chemo-mechanical model for water and gas transport in polymers. Hu and Shen (2013) developed a theoretical framework and variational principles for thermal–mechanical–chemical coupling media. These important contributions specialize in different aspects, yet the treatment of reactions is restricted to linear evolution laws which take effect only in diffusion-controlled near-equilibrium systems (Gurtin et al., 2013).

On these grounds, it is necessary to formulate a fully coupled thermo-chemo-mechanical theory to meet the demand for both a general framework with broader applications and the complete kinetics regarding each evolution process. Thereupon, the present work aims to develop a macroscopic field theory of coupled deformation, diffusion, chemical reaction and heat conduction for a chemically active solid based on non-equilibrium thermodynamics of continua. This theory is expected to describe efficiently both the transient evolution and the quasi-static response of a coupling system, where the specific kinetics for diffusion and reaction are included to cover problems with various time scales. A generalized chemo-elastic theory is also established to address the combined effects of volumetric swelling and reaction dilation/shrinkage of a reactive elastic solid subjected to surrounding chemical species.

The present paper is organized as follows. We first consider in Section 2 the basic conservation equations and the entropy inequality for the continuum body of solid-diffusing species mixtures. We next derive in Section 3 the state equations, constitutive relations and overall heat conduction equation that directly couple the state variables. Three special cases will also be briefly discussed to cover most practical applications. Section 4 is devoted to discuss the complementary