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ANALYTICAL SOLUTIONS FOR A ONE-DIMENSIONAL CHEMO-MECHANICAL COUPLING PROBLEM**

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ABSTRACT Chemo-mechanical coupling exists in a lot of intelligent materials including hydrogels, biological tissues and other soft materials. These materials are able to respond to external stimulus, such as temperature, chemical concentration, and pH value. In this paper, a one-dimensional theoretical model for chemo-mechanical coupling is proposed for analyzing the uniaxial stress/strain state of coupling materials. Based on the chemo-mechanical coupled governing equation, the displacement function and concentration function are derived and the stress and chemical potential are obtained. It is shown that the present chemo-mechanical theory can characterize the chemo-mechanical coupling behavior of intelligent materials.

KEY WORDS intelligent materials, chemo-mechanical coupling, analytical solution, theoretical model, constitutive equations, hydrogel

I. INTRODUCTION

In modern industry and engineering practice, many materials employed have multi-field coupling behavior and are often known as smart material. Commonly used smart materials include shape memory alloys (SMA), mass-energy optical fibers, piezoelectric materials, pH-response hydrogels and their composites. Applications of these smart materials are widely found in the automotive industry, telephony, architecture, food and so on. Intelligent hydrogel is such a class of material that its properties can vary significantly with the changes of external environmental conditions, including physical and chemical stimuli. Physical stimuli are defined as physical environmental factors, including light, temperature, sound, electric and magnetic field, whereas chemical stimuli include pH value of the solution and ionic concentration.

It is noted that smart gels are generally swelling or shrinking in response to external chemical stimuli[1]. Such chemo-mechanical coupling phenomena also exist in other types of materials including clay[2–4], cement paste[5,6], geomaterials[7] and biological soft tissues[8–10] and hard tissues[11–13]. Therefore, it is important from the viewpoint of engineering application to evaluate the chemo-mechanical coupling behavior of these multifield materials. During the past few decades, researchers have developed some experimental methods, numerical simulations and theoretical models for analyzing chemo-mechanical coupling of these widely used materials. For example, Ballhause et al.[14] investigated the mechanical

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mechanism of the chemical stimulation, and he indicated that the osmotic pressure of polymer and solution would undergo a change in response to the variation of the external chemical condition. The concentration, the chemical potential, and the displacement can be analyzed by the coupled chemo-electro-mechanical model. Vallenton et al.[15] involved the material expansion caused by enzyme reaction in consideration of the coupled effects of fluid flow, diffusion and chemical reaction. Doi et al.[16] studied the colloid dynamic behavior under a static electric field. Thomas et al.[17] observed that the mechanical properties of the gel were affected by electric charge in the electrophoresis solution. The anion and cationic concentration and potential between the interior and exterior of the colloid can be calculated according to the ionic concentration in the surrounding solvent, when chemical and electric simulation sparks occurred at the same time. It is shown that, with the large expansion of colloid fibers, the ion concentration variation along the positive direction of the anion colloid leads to relatively large results. Recently, Lu et al.[18] designed a uniaxial tensile experiment to explore the critical strain of polymer-supported metal. Yashin et al.[19] found that self-consistent vibration of the hydrogel depends on its model size and external force. Loeffel et al.[20] dealt with the polymer surface properties of the TBC material, including the diffusion of oxygen of surface materials and redox characteristics.

For studies on numerical simulation in chemo-mechanical coupling problems, Li et al.[21] developed a Hermite-Cloud method to model chemo-mechanical deformation and ionic concentration of hygrogels subjected to chemical and electrical stimulation, and numerical results are in good agreement with experimental data. Kaasschieter et al.[22] applied the multiphasic theory and associated four-phase mixed finite element to model the mechanical behavior of cartilages. Hong et al.[23] presented a finite element method based on the Gibbs free energy and non-linear thermodynamics, and illustrated several examples including swelling-induced deformation, contact and bifurcation. Macrombe et al.[24] investigated the inhomogeneous swelling of pH-sensitive gels by implementing a finite element method. Furthermore, the theory has been embedded in the commercial software ABAQUS by writing a user-supplied subroutine. Yang et al.[25,26] formulated coupled constitutive equations for analyzing general thermo-electro-chemo-mechanical coupling behavior of hydrogels by introducing the thermo-electro-chemo-mechanical effects into the Gibbs free energy. Based on the Gibbs free energy functional, a coupled finite element procedure is developed to model the swelling, shrinking and redistribution of ions with the smart hydrogels in some chemo-mechanical environments.

For analytical solutions to chemo-mechanical problems, De et al.[27] derived steady- and transient-state chemo-mechanical coupled equations where the ion transportation is described by the Nernst-Planck flux equations, and the osmotic pressure of mechanical field was introduced by the extended Darcy's law. Li et al.[28,29] and Lai et al.[30] presented a MEC model for the glucose-stimulus hydrogel and pH-sensitive hydrogel considering the effects of enzyme catalysis. Giovanni et al.[31] derived a one-dimensional distributed model based on the Euler-Bernoulli beam theory and a parallel-plate approximation, and validated his theoretical findings through a series of experiments. Unlike the theoretical solutions mentioned above, this paper is focused on the theoretical stress/strain analysis of intelligent materials with the objective of deriving a series of closed-form solutions. The solution can then be used to obtain results of displacement, stress, concentration and chemical potential of smart gels. In particular, we proposed a uniaxial stress/strain theoretical model by considering mechanical equilibrium and mass conservation. Two numerical examples are considered to assess the effectiveness of the model and applicability of the corresponding solution.

II. GOVERNING EQUATIONS OF CHEMO-MECHANICAL COUPLING

Consider a chemo-mechanical body of volume Ω bounded by surface S. The governing equations are the equilibrium equations of stresses and diffusion equations of ions. The equilibrium equations are

$$\sigma_{ij,j} + f_i = \rho \ddot{u}_i \qquad (\text{in} \quad \Omega) \tag{1}$$

and boundary conditions

$$u_i = \bar{u}_i \quad (\text{on} \quad S_u), \qquad \sigma_{ij} n_j = \bar{t}_i \quad (\text{on} \quad S_t) \tag{2}$$

where σ_{ij} is stress tensor, f_i is the body force, u_i is displacement, $\bar{u}_i$ and $\bar{t}_i$ are the prescribed surface displacements and tractions on the surface S, n_j is the unit outward normal vector to the surface S, $S = S_u + S_t$.