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Application of meshless local integral equations to two dimensional analysis of coupled non-Fick diffusion–elasticity

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ABSTRACT

This work presents the application of meshless local Petrov–Galerkin (MLPG) method to two dimensional coupled non-Fick diffusion–elasticity analysis. A unit step function is used as the test functions in the local weak-form. It leads to local integral equations (LIEs). The analyzed domain is divided into small subdomains with a circular shape. The radial basis functions are used for approximation of the spatial variation of field variables. For treatment of time variations, the Laplace-transform technique is utilized. Several numerical examples are given to verify the accuracy and the efficiency of the proposed method. The molar concentration diffuses through 2D domain with a finite speed similar to elastic wave. The propagation of mass diffusion and elastic waves are obtained and discussed at various time instants. The MLPG method has a high capability to track the diffusion and elastic wave fronts at arbitrary time instants in 2D domain. The profiles of molar concentration and displacements in two orthogonal directions are illustrated at various time instants.

1. Introduction

From engineering perspective, one of the most important problems in mass transfer problems is diffusion of mass in solids such as diffusion of a gas in the metal. To have a realistic simulation for diffusion of gas in solids, the interaction between diffusion and elasticity should be considered in models used for calculations. Some models including diffusion, elasticity and temperature effects have been published in literature. The non-Fick effects on steady-state and transient mass diffusion were studied by Jiang and Liu [1] for various boundary and initial conditions. Ellery and Simpson [2] presented an analytical approach to study nonlinear reactive transport models. An exact analytical solution was presented by Magyari [3,4] for analysis of linear or nonlinear reaction–diffusion in porous catalysts. Sun et al. [5] studied on diffusion and reaction in porous catalysts by the decomposition method and nonlinear model as an approximate solution. In another work, Abbasbandy [6] presented other approximate solution for the nonlinear model diffusion and reaction in porous catalysts by means of the homotopy analysis method. By introducing coupling between diffusion and elasticity, Gorsky [7] analyzed the interaction of diffusion and stresses. Peter and Smith [8] discussed the influence of advective transport on coupled chemical and mechanical consolidation of clays. Based on some of experimental works in micro- and nano-scales [9], it can be concluded that the diffusion of mass appears with a finite speed. Consequently, the non-Fick effects should be considered in calculations using coupled diffusion–elasticity based on non-Fick theories [10,11]. Recently, Suo and Shen [12] derived the exact variational principles for dynamical theoretical model and variational principles for coupled temperature–diffusion–mechanics with some numerical examples in which the molar concentration propagates with a finite speed.

Although the analytical methods are very valuable even for coupled problems in engineering (for example coupled thermo-elasticity problem [13]), some numerical methods such as finite element (FE) and boundary element (BE) methods have been successfully developed in this area of engineering because of mathematical limitations of analytical methods. In spite of the great success of the finite element and boundary element methods as the most efficient numerical tools for the solution of coupled problems [14] in complex domains, there has been a growing interest in the so-called meshless of mesh-free methods over the past decade. One of the most efficient meshless techniques is the meshless local Petrov–Galerkin (MLPG) method [16–19]. Recently, the authors employed this method successfully for coupled thermoelasticity analysis [20] and nonlinear diffusion equations [21]. Considering uncertainty in mechanical properties, the stochastic MLPG method was developed for coupled thermo-elasticity analysis by Hosseini et al. [22].

In the present paper, the authors have extended a meshless method based on the local Petrov–Galerkin weak form to coupled

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non-Fick diffusion–elasticity problem. In our meshless method, nodal points are regularly and/or randomly distributed over the 2D domain. Each node is the center of a circle surrounding this node. The Laplace-transform technique is applied to the set of coupled governing equations for the 2D non-Fick diffusion–elasticity in order to eliminate the time variable temporarily. Then, the unknown Laplace-transforms of the relevant physical quantities are constrained by the prescribed boundary conditions and the local integral equations developed as the weak form of the governing equations on local subdomains. Two kinds of shock loading are considered to illustrate the applicability of the proposed method. The profiles of 2D propagation of molar concentration and displacements waves are obtained at various time instants.

2. Mathematical formulations

The governing equations of coupled non-Fick diffusion–elasticity are given as [11,12]

$$\sigma_{ij,j}+f_i=\rho\ddot{u}_i \tag{1}$$

$$\dot{\mu}+\dot{\mu}^{(a)}=\frac{I}{c_0}-\frac{\beta' J_{i,i}}{c_0} \tag{2}$$

where f_i, ρ, u_i, $\mu^{(a)}$, I and c_0 are the body force, mass density, displacement, inertia chemical potential, diffusion source term and reference concentration, respectively. The constitutive equations can be found as

$$\sigma_{ij}=C_{ijkl}\varepsilon_{kl}-\alpha_{ij}c \tag{3}$$

$$\mu=\alpha_{ij}\varepsilon_{ij}+\beta c \tag{4}$$

where σ_{ij}, ε_{ij}, c and μ are the stress, strain, molar concentration (mol/m^3) and chemical potential (J/mol), respectively. The term J_i is the diffusion flux ($\mathrm{mol}/(m^2 s)$), which is given by the following equation (Fick's law) for isotropic and homogenous material

$$J_i=-D_{ij}c_{,j}=-D_0\delta_{ij}c_{,j}=-D_0c_{,i} \tag{5}$$

with D_0 being the diffusion coefficient. Furthermore, $\mu^{(a)}$ is assumed to be proportional to the rate of the concentration that is

$$\mu^{(a)}=\gamma\dot{c} \tag{6}$$

where γ is a proportionality coefficient. The term β' is equal to RT, with R being the universal gas constant and T is the absolute temperature. The relationship between β' and β is

$$\beta=\frac{\beta'}{c_0} \tag{7}$$

In this work, the body force and diffusion source terms are neglected, thus, we have

$$\sigma_{ij,j}=\rho\ddot{u}_i \tag{8}$$

or

$$\sigma_{ij,j}(X,t)=\rho\ddot{u}_i(X,t) \tag{9}$$

$$\dot{\mu}(X,t)+\dot{\mu}^{(a)}(X,t)=-\frac{\beta' J_{i,i}}{c_0}=-\beta J_{i,i}(X,t) \tag{10}$$

For isotropic and homogenous materials, the elasticity tensor and material coefficients α_{ij} become

$$C_{ijkl}=\frac{2\nu G}{1-2\nu}\delta_{ij}\delta_{kl}+G\delta_{ik}\delta_{jl}+G\delta_{il}\delta_{jk}, \quad \alpha_{ij}=\alpha_o\delta_{ij} \tag{11}$$

Applying the Laplace transformation to the constitutive and governing equations, we obtain

$$\overline{\sigma}_{ij}(X,S)=\frac{2\nu G}{1-2\nu}\delta_{ij}\overline{u}_{k,k}(X,S)+G\overline{u}_{i,j}(X,S)+G\overline{u}_{j,i}(X,S)-\alpha_0\delta_{ij}\overline{c}(X,S) \tag{12}$$

and

$$\overline{\sigma}_{ij,j}(X,S)=\rho S^2\overline{u}_i(X,S)-\rho S u_i(X,0)-\rho\dot{u}_i(X,0)=\rho S^2\overline{u}_i(X,S)-k_i(X,S) \tag{13}$$

where

$$k_i(X,S)=\rho S u_i(X,0)+\rho\dot{u}_i(X,0) \tag{14}$$

Following the derivation of the local integral equation for the first governing equation on local sub-domain Ω_s, we can write

$$\int_{\Omega_s}\{\overline{\sigma}_{ij,j}(X,S)-\rho S^2\overline{u}_i(X,S)+k_i(X,S)\}F^*_{ik}(X)d\Omega=0 \tag{15}$$

where $F^*_{ik}(X)$ are test functions.

Hence, in view of the Gauss divergence theorem, we obtain

$$\int_{\partial\Omega_s}n_j(X)\overline{\sigma}_{ij}(X,S)F^*_{ik}(X)d\Gamma-\int_{\Omega_s}\overline{\sigma}_{ij}(X,S)F^*_{ik,j}(X)d\Omega \\ -\int_{\Omega_s}\{\rho S^2\overline{u}_i(X,S)-k_i(X,S)\}F^*_{ik}(X)d\Omega=0 \tag{16}$$

Having chosen the test functions as the Heaviside unit step function with support on the local sub-domain, i.e.

$$F^*_{ik}(X)=\begin{cases}\delta_{ik}, & X\in\Omega_s\\ 0, & X\notin(\Omega_s\cup\Gamma_s)\end{cases}$$

one obtains the LIE

$$\int_{\partial\Omega_s}n_j(X)\overline{\sigma}_{ij}(X,S)d\Gamma-\int_{\Omega_s}\{\rho S^2\overline{u}_i(X,S)-k_i(X,S)\}d\Omega=0 \tag{17}$$

which is the expression for the momentum balance. Recall that $\overline{\sigma}_{ij}$ is expressed in terms of the displacement gradients and the concentration according to Eq. (12).

In view of Eqs. (4)–(6) and (10), we may write

$$\alpha_0\dot{u}_{i,i}(X,t)+\beta\dot{c}(X,t)+\gamma\ddot{c}(X,t)=\beta D_0 c_{,i\,i}(X,t) \tag{18}$$

Hence, by applying the Laplace transformation technique, one can obtain

$$\begin{gathered}\alpha_0 S\overline{u}_{i,i}(X,S)-\alpha_0 u_{i,i}(X,0)+\beta S\overline{c}(X,S)-\beta c(X,0)\\ +\gamma S^2\overline{c}(X,S)-\gamma S c(X,0)-\gamma\dot{c}(X,0)=\beta D_0\overline{c}_{,ii}\\ \text{or}\\ \alpha_0 S\overline{u}_{i,i}(X,S)+\beta S\overline{c}(X,S)+\gamma S^2\overline{c}(X,S)-\beta D_0\overline{c}_{,ii}(X,S)=L_i(X,S)\end{gathered} \tag{19}$$

where

$$L_i(X,S)=\alpha_0 u_{i,i}(X,0)+\beta c(X,0)+\gamma S c(X,0)+\gamma\dot{c}(X,0) \tag{20}$$

The weak form of the governing Eq. (19) on local sub-domain Ω_s is given as

$$\int_{\Omega_s}[\alpha_0 S\overline{u}_{i,i}(X,S)+\beta S\overline{c}(X,S)+\gamma S^2\overline{c}(X,S)-\beta D_0\overline{c}_{,i\,i}(X,S)]G^*(X)d\Omega \\ =\int_{\Omega_s}L_i(X,S)G^*(X)d\Omega \tag{21}$$

where $G^*(X)$ is a test function.

Having used the Gauss divergence theorem, one obtains from (21)

$$\int_{\partial\Omega_s}[\alpha_0 S\overline{u}_i(X,S)-\beta D_0\overline{c}_{,i}(X,S)]n_i(X)G^*(X)d\Gamma \\ -\int_{\Omega_s}[\alpha_0 S\overline{u}_i(X,S)-\beta D_0\overline{c}_{,i}(X,S)]G^*_{,i}(X)d\Gamma \\ +\int_{\Omega_s}[\beta S\overline{c}(X,S)+\gamma S^2\overline{c}(X,S)]G^*(X)d\Omega=\int_{\Omega_s}L_i(X,S)G^*(X)d\Omega \tag{22}$$