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Responses of generalized diffusion-elasticity problems with variable material properties

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ABSTRACT

The main goal of the manuscript is to capture the transient responses of non-Fick diffusion-elasticity problems based on concentration-dependent material properties by using finite element method. The principle of virtual work is performed to formulate the nonlinear finite element governing equations. The equations are solved in time domain directly. The problem of a thick circular plate with concentration-dependent material properties under chemical shock is studied. The results indicate that the wave feature of molar concentration is well depicted. The influences of concentration-dependent material properties on the transient responses are evaluated and discussed in detail.

1 INTRODUCTION

In practical engineering, the coupling between diffusion and mechanics is of great significance in domains of artificial skins of robots, actuators of adaptive structures and artificial muscles and so on. The problems of mechanical deformation of solids in non-uniform concentration field have aroused great interests due to their extensive engineering applications in micro-electromechanical (MEMS) and nano-electromechanical (NEMS) systems, such as micro-beam resonator (Khanchehgardan 2014) and porous micro-electrodes (Le 2017). It is known that the diffusion of atoms can produce the chemical stresses (diffusion-induced stresses). With the rapid development of multifunctional materials, the effect of chemical stress on their mechanical behavior becomes increasingly important in material systems of nano-sized circular elastic matrix, Cu-Cr nano-layered films, lithium-ion batteries (LIBs) and so on. To better understand interaction mechanism between strain and concentration fields, much investigation efforts have been focused on the theoretical modeling of coupled diffusion-mechanics (Prussin, 1961, Yang, 2005).
However, when the concerned time period is as short as femtosecond/ picosecond, the aforementioned models may be challenged. For example, the extremely fast mass transfer usually occurs at ultra-short time period during the rapid solidification of

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micro/nano-sized binary mixtures. At the moving solid-liquid interfaces, the produced high concentration gradient accompanying the phase change processes are under far from equilibrium condition. It implies that the non-equilibrium approach needs to be used in such situation. Instead of the classical local equilibrium diffusion equation (i.e. Fick law), the local non-equilibrium diffusion equation of hyperbolic type (i.e. non-Fick law) is more reasonable to characterize the transport feature of mass diffusion in medium at extreme short time. This model is expected to capture the relaxation effect of mass diffusion, namely, the abrupt change of concentration at one point could not be felt at distant points immediately. This suggests that the mass diffuses at a finite velocity. A through and comprehensive understanding on the characteristics of mass diffusion can refer to Sobolev (2014). Nowadays, the non-Fick diffusion model is widely used in rapid solidification of metal alloys (Sobolev 2012a) and colloidal crystallization (Sobolev 2012b) and so on. Enlightened by this, the coupled non-Fick diffusion-elasticity theories have been put forward with the consideration of non-Fick effect of mass diffusion. Due to the consideration of non-Fick effect, the paradox of infinite speed of mass diffusion in both the uncoupled and coupled theories of classical diffusion-elasticity is eliminated and the wave feature can be depicted by the coupled non-Fick diffusion-elasticity theories. Based on this theory, much efforts have been devoted on the transient responses of coupled non-Fick diffusion-elasticity problems by using Laplace transformation (LT) technique, meshless local Petrov-Galerkin (MLPG) method (Hosseini 2013) and mesh free generalized finite difference (MGFD) method (Hosseini 2015). Discrete and truncation errors are introduced in inverse Laplace transformation when using LT. In particular, when the concerned problems involve nonlinear terms (higher-order and coupled terms), the nonlinear solutions in Laplace domain are even hardly obtained. To compensate for the defects of the abovementioned methods, time-domain finite element method (Tian 2006) may be a better choice. It solves the governing equations (linear and nonlinear) in time domain directly.

Until now, the investigations of transient shock behavior of coupled non-Fick diffusion-elasticity problems are mostly focused on the structure composed of concentration independent material properties. However, numerous theoretical and experimental studies indicate that the pronounced concentration-dependent effect on material performance of metal nanocrystals (Ramezani 2015), microgel (Yang 2017) and so on. It has been reported that both the elastic modulus and diffusivity share the concentration-dependent feature. For example, the intrinsic mechanical property of electrodes changes greatly due to the changed elastic modulus in charging process (Qi 2014).

One can conclude that the concentration-dependent elasticity and diffusivity play important roles in engineering. Thus, it is strongly necessary to evaluate their effects on the transient shock responses of coupled non-Fick diffusion elasticity problems. In engineering problems, the investigations of transient shock responses of multifunctional structures have significant meanings in the exploitation and fabrication of MEMS/NEMS devices. Most investigations available on non-Fick diffusion-elasticity problems are limited to the constant diffusivity and elastic modulus. The concentration-dependence effect on them should be seriously considered. Present work aims to study the transient shock responses of non-Fick diffusion-elasticity problems with concentration-dependent material properties. By using the principle of virtual work, the finite element governing

equations are formulated and solved in time domain directly. As numerical example, the problem of a thick circular plate composed of material with concentration-dependent material properties under chemical shock is investigated. The nonlinear transient solutions are obtained and illustrated graphically. Parametric studies are conducted to evaluate the effects of concentration-dependent material properties on the transient responses.

2 CONCENTRATION-DEPENDENT MATERIAL PROPERTIES

In the present study, the concentration-dependent material properties involve two parts: concentration-dependent elastic modulus and diffusivity.

2.1 Concentration-dependent elastic modulus

In terms of energy conservation law and Clausius inequality (i.e. the first and second principles of thermodynamics), the internal energy $\mathrm{d}U_{ie}$, heat energy storage $\mathrm{d}Q_{he}$ and strain energy $\mathrm{d}U_{se}$ per unit volume satisfy the following relation:

$$\mathrm{d}U_{ie} = \mathrm{d}Q_{he} + \mathrm{d}U_{se} = T\mathrm{d}S + \sigma_{ij}\mathrm{d}\varepsilon_{ij} \tag{1}$$

where σ_{ij} are the components of stress tensor, ε_{ij} are the components of strain tensor, S is the entropy per unit volume and T is the absolute temperature. The Helmholtz free energy function is introduced as:

$$\psi = U_{ie} - TS \tag{2}$$

Substitution of Eq. (2) into Eq. (1) yields:

$$\mathrm{d}\psi = -S\mathrm{d}T + \sigma_{ij}\mathrm{d}\varepsilon_{ij} \tag{3}$$

which implies that

$$\sigma_{ij} = \frac{\partial \psi}{\partial \varepsilon_{ij}} \tag{4}$$

Using Eq. (4), the elastic modulus tensor C_{ijkl} is calculated as:

$$C_{ijkl} = \frac{\partial \sigma}{\partial \varepsilon_{ij}} = \frac{\partial^2 \psi}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}} \tag{5}$$

For an elastic solid, the Helmholtz free energy can be expanded in a Taylor series as:

$$\psi\left(\varepsilon_{ij}, c\right) = \psi\left(\varepsilon_{ij}, 0\right) + \frac{\partial \psi\left(\varepsilon_{ij}, 0\right)}{\partial c}c + \frac{1}{2}\frac{\partial^2 \psi\left(\varepsilon_{ij}, 0\right)}{\partial c^2}c^2 + \cdots \tag{6}$$

where c is molar concentration ($\mathrm{J/mol}$). Substitution of Eq. (6) in Eq. (5) results in:

$$\begin{aligned} C_{ijkl}\left(c\right) &= C^0_{ijkl} + \frac{\partial^3 \psi\left(\varepsilon_{ij}, 0\right)}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}\partial c}c + \frac{1}{2}\frac{\partial^4 \psi\left(\varepsilon_{ij}, 0\right)}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}\partial c^2}c^2 + \cdots \\ &= C^0_{ijkl} + \left(\Delta C_{ijkl}\right)c + \cdots = C^0_{ijkl} + \zeta c + \cdots = C^0_{ijkl}\left(1 + \chi_C c\right) \end{aligned} \tag{7}$$

where C^0_{ijkl} is the elastic modulus without concentration-dependent effect and ΔC_{ijkl} is the change of elastic modulus per unit concentration. The first order of approximation in Eq.(7) indicates that the elastic modulus has a linear dependence relation with molar

concentration. The parameter χ_C in this linear formulation can be used to measure the influences of the molar concentration on the elastic modulus. For isotropic materials, it has been found that the Young's modulus presents a linear dependence relation with molar concentration:

$$E = E_0 + \xi c \tag{8}$$

where E_0 and ξ are Young's modulus without concentration-dependent effect and the change of Young's modulus per unit concentration, respectively. The effect of concentration-dependent elastic modulus on the transient shock behavior of coupled non-Fick diffusion-elasticity problems are rarely reported.

2.2 Concentration-dependent diffusivity

In most of isotropic solids/fluids systems, it has been found that the diffusion coefficient has a close relation with the distribution of molar concentration (Siebel 2015). For a homogeneous medium without diffusion sources, Fick's mass diffusion law with concentration-dependent diffusivity can be written as:

$$J_i = -D(c)c_{,i} \tag{9}$$

where J_i are the components of diffusion flux. The concentration-dependent diffusivity $D(c)$ is taken as a function of the concentration with linear relation as follows (Roussel 2001):

$$D(c) = D_m\left(1+\chi_D c\right) \tag{10}$$

where D_m is constant diffusion coefficient, χ_D is the parameter to measure the influence of concentration on diffusivity. The mass diffusion equation with concentration-dependent diffusivity is used to the transient shock analysis of coupled non-Fick diffusion-elasticity problems in this paper.

3 GOVERNING EQUATIONS

When the concentration-dependent elastic modulus and diffusivity are taken into account in the coupled non-Fick diffusion-elasticity problems (Suo 2012, 2013), the governing equations can be written as follows:

The motion equation and non-Fick diffusion equation (in the absence of body force and diffusion source):

$$\sigma_{ij,j} = \rho\ddot{u}_i \tag{11}$$

$$\dot{\mu} + \dot{\mu}^{(a)} = -\beta J_{i,i} \tag{12}$$

where

$$\beta = \frac{\beta'}{c_0}, \quad \beta'=RT, \quad \dot{\mu}^{(a)} = \gamma\dot{c}$$

where u_i, μ, $\mu^{(a)}$, c_0, γ, R and T are respectively the components of displacement vector, chemical potential, inertial chemical potential, reference concentration, proportionality coefficient, the universe gas constant and absolute temperature.

The constitutive relation:

$$\sigma_{ij} = C_{ijkl}(c)\varepsilon_{kl} - \alpha_{ij}c \tag{13}$$

$$\mu = \alpha_{ij}\varepsilon_{ij} + \beta c \tag{14}$$

where α_{ij} and β are the mechanical diffusion coefficients and the chemical potential constant, respectively.

The relation between the strain and displacement is given as:

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \tag{15}$$

The Fick's law for isotropic and homogeneous material with concentration-dependent diffusivity is shown in Eq.(9).

Then, the governing equations of displacement field and concentration field can be obtained:

$$C_{ijkl}(c)u_{k,lj} + \left[C_{ijkl}(c)\right]_{,j} u_{k,l} - \alpha_{ij}c_{,j} = \rho\ddot{u}_i \tag{16}$$

$$\left[D(c)\right]_{,i} c_{,i} + D(c)c_{,ii} = \frac{\alpha_{ij}}{\beta}\dot{\varepsilon}_{ij} + \dot{c} + \tau\ddot{c} \tag{17}$$

where $\tau = \gamma/\beta$ is the diffusion relaxation time. Note that if the coupled term in Eq. (17) is ignored, the non-Fick diffusion equation with concentration- dependent diffusivity reads as:

$$\dot{c} + \tau\ddot{c} = \left[D(c)\right]_{,i} c_{,i} + D(c)c_{,ii} \tag{18}$$

which can degenerate into following limiting cases:

1) The non-Fick mass diffusion model is obtained when the diffusivity is assumed to be constant.

2) The classical Fick's mass diffusion model with concentration- dependent diffusivity is derived when the diffusion relaxation time is ignored.

Eq. (18) implies that the molar concentration diffuses at a finite speed of $v = \sqrt{D(c)/\tau}$.

Thus far, the governing equations of the coupled non-Fick diffusion-elasticity problems based on concentration-dependent elastic modulus and diffusivity are formulated.

4 FINITE ELEMENT FORMULATIONS

Due to the presence of nonlinear terms in the governing equations, the mostly used numerical methods, such as LT, may be not applicable. To address the nonlinear problem formulated in Section 3, finite element method is applied to solve the nonlinear coupled non-Fick diffusion-elasticity based on concentration-dependent elastic modulus and diffusivity in time domain directly. This method avoids the tedious processes and precision losses in the applications of numerical methods of LT.

This section is mainly devoted to establish the finite element formulations of the coupled non-Fick diffusion-elasticity problems with concentration- dependent modulus and diffusivity. The constitutive equations (13) and (14) can be written as the following matrix forms:

$$\{\sigma\} = \left[C(c)\right]\{\varepsilon\} - \{\alpha\}\{c\} \tag{19}$$

$$\{\mu\} = \{\alpha\}^{\mathrm{T}}\{\varepsilon\} + [\beta]\{c\} \tag{20}$$

The matrix form of Fick law of mass diffusion equation is given as:

$$\{J\} = -\left[D(c)\right]\{c'\} \tag{21}$$

where $c' = c_{,i}$. For a given element, the displacement $\{u\}$ and concentration $\{c\}$ can be expressed with shape functions $\left[N_1^e\right]$ and $\left[N_2^e\right]$:

$$\{u\} = \left[N_1^e\right]\{u^e\}, \quad \{c\} = \left\{N_2^e\right\}^{\mathrm{T}}\{c^e\} \tag{22}$$

In terms of the nodal values of displacement $\{u^e\}$ and molar concentration $\{c^e\}$, the elastic strain $\{\varepsilon\}$ and concentration gradient $\{c'\}$ can be expressed as:

$$\{\varepsilon\} = [B_1]\{u^e\}, \quad \{c'\} = [B_2]\{c^e\} \tag{23}$$

where $[B_1]$ and $[B_2]$ are the strain matrix and concentration gradient matrix. The variational form of Eq. (23) can be written as:

$$\delta\{\varepsilon\} = [B_1]\delta\{u^e\}, \quad \delta\{c'\} = [B_2]\delta\{c^e\} \tag{24}$$

The principle of virtual work for the coupled non-Fick diffusion-elasticity problems with concentration-dependent elastic modulus and diffusivity has the following form:

$$\begin{aligned}&\int_V \left[\delta\{\varepsilon\}^{\mathrm{T}}\{\sigma\} + \left(\{\dot{\mu}\} + \{\dot{\mu}\}^{(a)}\right)\delta\{c\} + \delta\{c'\}^{\mathrm{T}}\{J\}\right]\mathrm{d}V \\ &= -\int_V \delta\{u\}^{\mathrm{T}}\rho\{\ddot{u}\}\,\mathrm{d}V + \int_{A_\sigma}\delta\{u\}^{\mathrm{T}}\{\bar{f}\}\,\mathrm{d}A + \int_{A_c}\delta\{c\}^{\mathrm{T}}\{\bar{J}\}\,\mathrm{d}A\end{aligned} \tag{25}$$

where $\{\bar{f}\}$ is the traction vector on surface A_σ and $\{\bar{J}\}$ is the mass flux vector on surface A_c. Substitution of Eqs. (19)-(21) into Eq. (25) yields:

$$\sum_{i=1}^{ne}\left(\mathbf{M}\ddot{\mathbf{X}} + \mathbf{C}\dot{\mathbf{X}} + \mathbf{K}\mathbf{X} = \mathbf{F}_{\mathrm{ex}}\right) \tag{26}$$

where ne is the total number of elements. $\mathbf{M}$, $\mathbf{C}$, $\mathbf{K}$, $\mathbf{X}$ and $\mathbf{F}_{\mathrm{ex}}$ are mass matrices, damping matrices, stiffness matrices, vector of unknown constitutive variables and external force vector, respectively, which can be represented as:

$$\mathbf{M} = \begin{bmatrix} M_{mm}^e & 0 \\ 0 & M_{cc}^e \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} 0 & 0 \\ C_{cm}^e & C_{cc}^e \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} K_{mm}^e(c) & -K_{mc}^e \\ 0 & K_{cc}^e(c) \end{bmatrix}, \quad \mathbf{X} = \begin{Bmatrix} u^e \\ c^e \end{Bmatrix}, \quad \mathbf{F}_{ex} = \begin{Bmatrix} f_m^e \\ c_c^e \end{Bmatrix}$$

where

$$\left[M_{mm}^e\right] = \int_V \left[N_1^e\right]^{\mathrm{T}}\rho\left[N_1^e\right]\mathrm{d}V, \quad \left[M_{cc}^e\right] = \int_V \tau\left[N_2^e\right][\beta]\left[N_2^e\right]^{\mathrm{T}}\mathrm{d}V$$

$$\left[C_{cm}^e\right] = \int_V \left\{N_2^e\right\}\{\alpha\}^{\mathrm{T}}[B_1]\,\mathrm{d}V, \quad \left[C_{cc}^e\right] = \int_V \left\{N_2^e\right\}[\beta]\left\{N_2^e\right\}^{\mathrm{T}}\mathrm{d}V$$

$$\left[K_{mm}^e(c)\right] = \int_V [B_1]^{\mathrm{T}}\left[C(c)\right][B_1]\mathrm{d}V, \quad \left[K_{mc}^e\right] = \int_V [B_1]^{\mathrm{T}}\{\alpha\}\left\{N_2^e\right\}^{\mathrm{T}}\mathrm{d}V$$

$$\left[K_{cc}^e(c)\right] = \int_V [B_2]^{\mathrm{T}}\left[D(c)\right][B_2]\mathrm{d}V, \quad \left\{f_m^e\right\} = \int_{A_\sigma}\left[N_1^e\right]^{\mathrm{T}}\left\{\bar{f}\right\}\mathrm{d}A$$

$$\left\{c_c^e\right\} = \int_{A_\eta}\left\{N_2^e\right\}\left\{\bar{J}\right\}\mathrm{d}A$$

For convenience, the following dimensionless quantities are introduced:

$$\left(x_i^*,\, u_i^*\right)=\sqrt{\frac{\lambda+2\mu}{\rho}}\,\frac{1}{D_m}\left(x_i,\, u_i\right),\quad \left(t^*,\, \tau^*\right)=\frac{\lambda+2\mu}{\rho}\,\frac{1}{D_m}\left(t,\, \tau\right),$$
$$\sigma_{ij}^*=\frac{\sigma_{ij}}{\mu},\quad c^*=\frac{c}{c_0},\quad \chi_C^*=c_0\chi_C,\quad \chi_D^*=c_0\chi_D \tag{27}$$

The nonlinear finite element governing equation (26) can be solved directly in time domain by associating with appropriate initial and boundary conditions. Note that the present formulations can degenerate into the case of the coupled non-Fick diffusion-elasticity problems when the concerned elastic modulus and diffusivity are assumed to be constants.

5 NUMERICAL EXAMPLE: RESULTS AND DISCUSSIONS

In this section, transient responses of non-Fick diffusion-elasticity problems based on concentration-dependent elastic modulus and diffusivity for an isotropic homogeneous elastic solid is studied. The elastic modulus and material coefficient α_{ij} have the following forms:

$$C_{ijkl}=\lambda(c)\delta_{ij}\delta_{kl}+\mu(c)\delta_{ik}\delta_{jl}+\mu(c)\delta_{il}\delta_{jk},\quad \alpha_{ij}=\alpha\delta_{ij} \tag{28}$$

Then, the governing equations can be written as:

$$\sigma_{ij,\,j}=\rho\ddot{u}_i,\quad \dot{\mu}+\dot{\mu}^{(a)}=-\beta J_{i,i} \tag{29}$$

$$\sigma_{ij}=\lambda(c)\varepsilon_{kk}\delta_{ij}+2\mu(c)\varepsilon_{ij}-\alpha c\delta_{ij},\quad \mu=\alpha\varepsilon_{kk}+\beta c \tag{30}$$

$$\varepsilon_{ij}=\frac{1}{2}\left(u_{i,\,j}+u_{j,i}\right),\qquad J_i=-D(c)c_{,i} \tag{31}$$

Substitution of Eqs. (30) into Eqs. (29) leads to:

$$\mu(c)u_{i,jj}+\left[\lambda(c)+\mu(c)\right]u_{j,ij}-\alpha c_{,i}+\left[\lambda(c)\right]_{,i}u_{j,\,j}+2\left[\mu(c)\right]_{,\,j}u_{i,\,j}=\rho\ddot{u}_i \tag{32}$$

$$\left[D(c)\right]_{,i}c_{,i}+D(c)c_{,ii}=\frac{\alpha_{ij}}{\beta}\varepsilon_{ij}+\dot{c}+\tau\ddot{c} \tag{33}$$

In the governing equations of motion and molar concentration (i.e. Eqs. (32) and (33)), it needs to be pointed out that the concentration-dependent elastic modulus (i.e. $\lambda(c)$ and $\mu(c)$) and diffusivity (i.e. $D(c)$) have the following forms:

$$\lambda(c)=\lambda(1+\chi_C c),\quad \mu(c)=\mu(1+\chi_C c),\quad D(c)=D_m(1+\chi_D c) \tag{34}$$

For numerical evaluations, the material parameters are shown in Table 1.

Table 1 Material constant in numerical simulation.

α	φ	g	ν	E
1.870828693	0.0001978260870	0.58333	0.3	2.3×10^9 Pa

5.1 Verification

To check the validity of time-domain finite element method, the transient shock behavior of a plate with constant material properties is investigated. The medium is initially quiescent and the upper surface ($z=0$) is under the shock loading of molar

concentration in the form of a Heaviside unit step function of time. It is assumed that the dimension of *x*-axis and *y*-axis is much larger than the thickness (i.e. *z*-axis). During the analysis, time period is limited so that neither elastic wave nor diffusive wave reaches to the lower surface of the plate Hence, the problem considered can be treated as a one-dimensional case. Then, the dimensionless governing equations of motion and molar concentration can be written as (the asterisks of the dimensionless variables are omitted for brevity):

$$\varsigma^2 \frac{\partial^2 u}{\partial z^2} - \varphi \frac{\partial c}{\partial z} = \varsigma^2 \frac{\partial^2 w}{\partial t^2} \tag{35}$$

$$\frac{\partial^2 c}{\partial z^2} = g \frac{\partial^2 w}{\partial z \partial t} + \frac{\partial c}{\partial t} + \tau \frac{\partial^2 c}{\partial t^2} \tag{36}$$

where $\varsigma^2 = \frac{\lambda + 2\mu}{\mu}$, $\varphi = \frac{\alpha c_0}{\mu}$ and $g = \frac{\alpha}{\beta c_0}$. In terms of Eq. (36), the dimensionless velocity of mass diffusion can be calculated as $v'_{\mathrm{mc}} = \sqrt{1/\tau}$. When the dimensionless diffusion relaxation time is chosen as $\tau = 0.05$, the propagation velocity of the diffusive wave is 4.472 ($\sqrt{0.05}$) and the jump of molar concentration at diffusive wave front at different time should be at about $z|_{t=0.05} = 0.224$, $z|_{t=0.08} = 0.358$ and $z|_{t=0.10} = 0.447$. This suggests that the response of molar concentration vanishes identically when $z > 0.224$ at t=0.05. However, the value of molar concentration approaches to zero until when $z > 0.53$ in literature (Hosseini 2014). The finite propagation feature of molar concentration is not depicted exactly.

The dimensionless molar concentration are illustrated in Fig. 1. It is observed that the evaluated wave fronts from finite element analysis are almost the same as obtained from theoretical predictions. This implies that the finite element results are reliable.

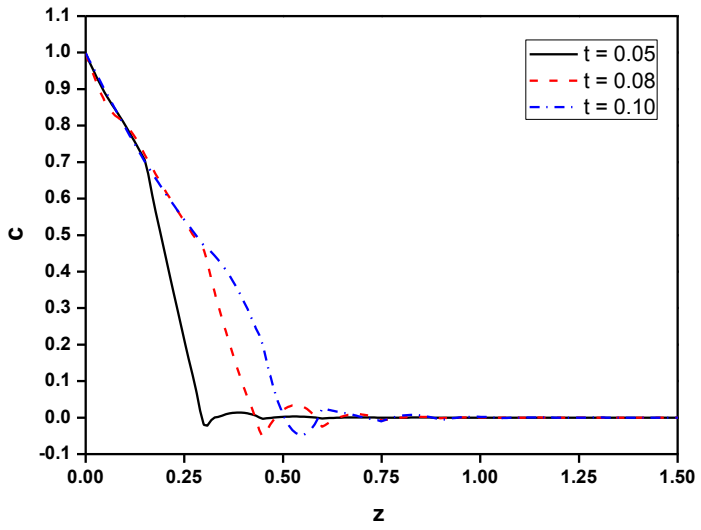


Fig. 1 The distribution of molar concentration at different time

5.2 Transient responses of a thick circular plate composed of a material with

concentration-dependent elastic modulus and diffusivity

To investigate the influences of concentration-dependent elastic modulus and diffusivity on the transient response of coupled non-Fick diffusion-elasticity problems, a circular plate of thickness of h composed of a material with concentration-dependent elastic modulus and diffusivity is taken as an example (see Fig. 2). The plate occupies the region $\Omega=\left\{(r,\theta,z)\,\middle|\, 0\le r<\infty, 0\le\theta\le 2\pi, 0\le z\le h\right\}$. The cylindrical system of coordinates (r,θ,z) with the *z*-axis coinciding with the axis of the cylinder is chosen. The initial state of the plate is assumed to be quiescent. The upper surface of the plate is taken to be traction free and its central parts are subjected to a zonal time-dependent concentration disturbance. The issue can be treated as an axisymmetric problem. The components of displacement and molar concentration are simplified as:

$$u_r=u_r(r,z,t),\quad u_\theta=0,\quad u_z=w(r,z,t) \tag{37}$$

$$c=c(r,z,t) \tag{38}$$

The initial and boundary conditions can be expressed as follows:
Initial conditions:

$$u_r(r,z,0)=w(r,z,0)=0,\quad \frac{\partial u_r(r,z,0)}{\partial t}=\frac{\partial w(r,z,0)}{\partial t}=0 \tag{39}$$

$$c(r,z,0)=0,\quad \frac{\partial c(r,z,0)}{\partial t}=0 \tag{40}$$

Boundary conditions:

$$\sigma_{zz}(r,0,t)=\sigma_{rz}(r,0,t)=0 \tag{41}$$

$$c(r,0,t)=c_0H(t)H(a-|r|) \tag{42}$$

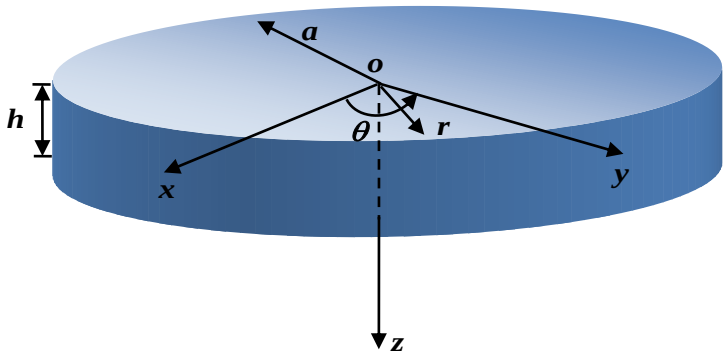


Fig. 2 The schematic model of the thick circular plate.

By using finite element method, the responses can be solved in time domain directly associating with the initial and boundary conditions. In the calculation, the finite element analysis model is sketched as shown in Fig. 3. The constants used for numerical calculation are taken as:

$$t = 0.05, \quad \tau = 0.02, \quad a = 0.5, \quad h = 1.5.$$

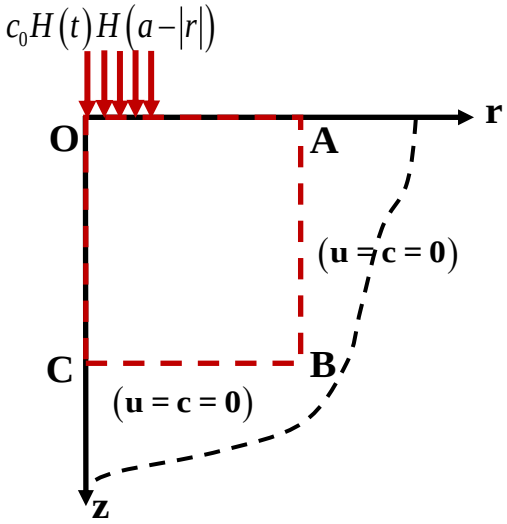


Fig. 3 Finite element analysis model

5.2.1 The effect of concentration-dependent elastic modulus

To investigate the influence of concentration-dependent elastic modulus on the nonlinear transient responses, three cases are discussed:

Case 1, $\chi_C = 0.00$ and $\chi_D = 0.00$;

Case 2, $\chi_C = 0.30$ and $\chi_D = 0.00$;

Case 3, $\chi_C = 0.60$ and $\chi_D = 0.00$.

in which $\chi_C > 0$ (i.e. $\chi_C = 0.30$ and 0.60) represents the enhanced elastic modulus. Fig. 4 displays the contours of the molar concentration in the thick circular plate for Case 1. It is found that the response region of molar concentration is limited in a finite area and the distribution of molar concentration is almost unchanged beyond this area. This means that the molar concentration diffuses at a finite speed. The molar concentration in Case 2 and Case 3 are almost the same: the response region of molar concentration is limited in finite areas.

To further discuss the influence of concentration-dependent elastic modulus on molar concentration, the distributions of molar concentration along *z*-axis and *r*-axis are presented in Fig. 5 (a) and (b), respectively. As shown in Fig. 5 (a), it is seen that the jump of molar concentration along *z*-axis at the diffusive wave front is not affected by the change of elastic modulus. Similarly, Fig. 5 (b) shows that the distribution of molar concentration along *r*-axis for Case 1 agrees well with that for Case 2 and 3. In addition, the molar concentration keeps constant within $0 \le r \le 0.5$, which is consistent with the boundary conditions at the upper surface of the thick circular plate.

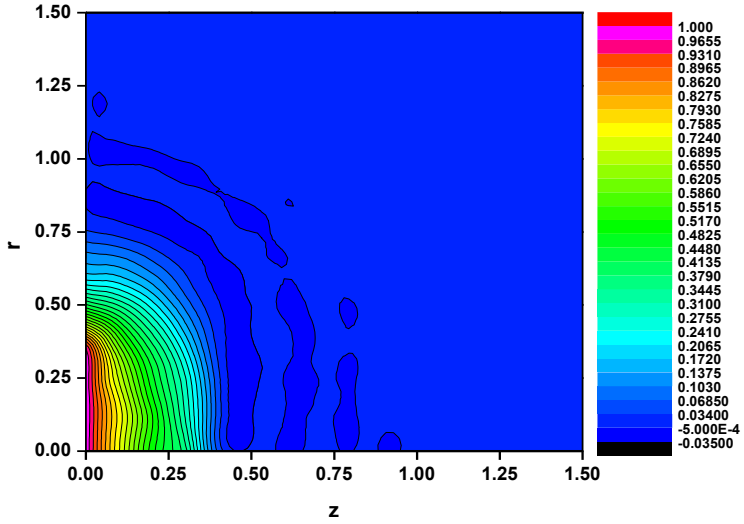
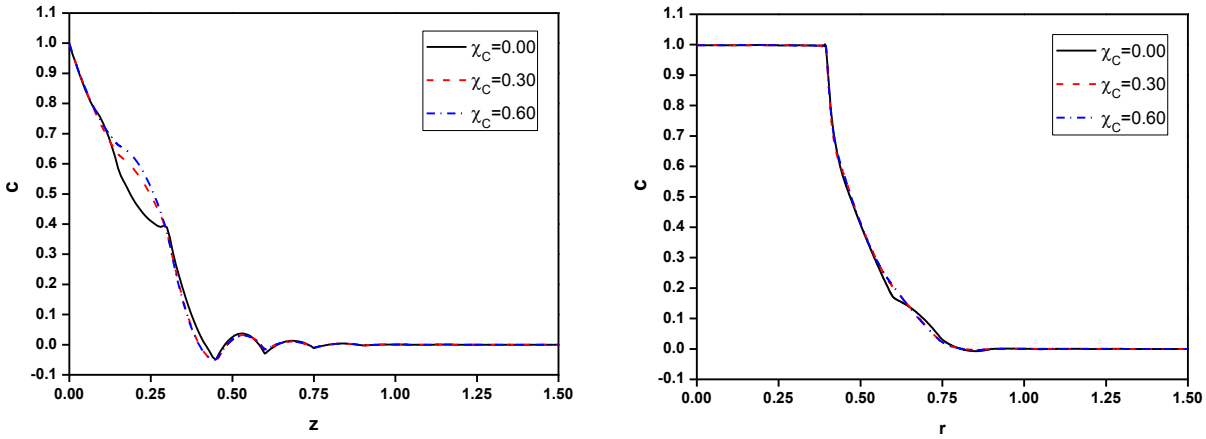


Fig. 4 The contours of molar concentration in Case 1



(a) (b)

Fig. 5 The distribution of molar concentration along (a) *z*-axis (b) *r*-axis.

Fig. 6 displays the distribution of axial displacement along *z*-axis at $r=0$. It is observed that the magnitude of axial displacement along *z*-axis increases when the elastic modulus is positive growth with molar concentration. Notably, the jump of displacement at elastic wave front moves forward when χ_C increases. It implies that the elastic wave travels faster with the increase of concentration-dependent elastic modulus.

The distributions of radial and axial displacement at *z*=0 along *r*-axis are illustrated graphically in Fig. 7 (a) and (b), respectively. Fig. 7 (a) shows that the peak value of radial displacement along r-axis becomes smaller with the increase of χ_C. However, the magnitudes of axial displacement along *r*-axis near on the upper surface increases when χ_C becomes larger. Therefore, it is obtained that concentration-dependent effect on elastic modulus plays an important role in determining the distribution of displacement.

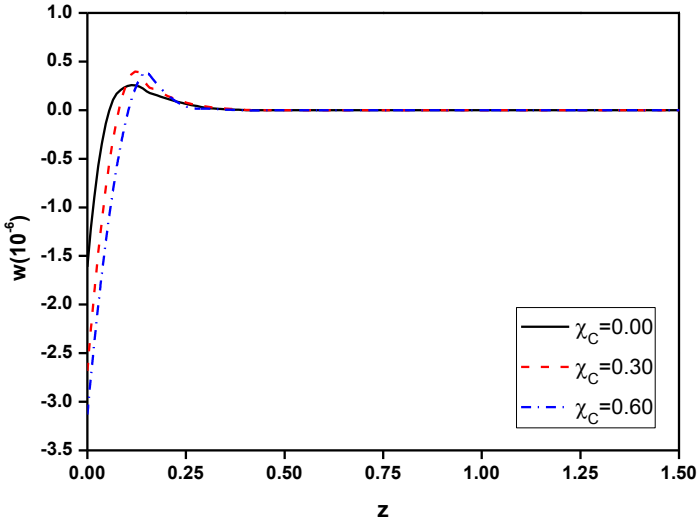
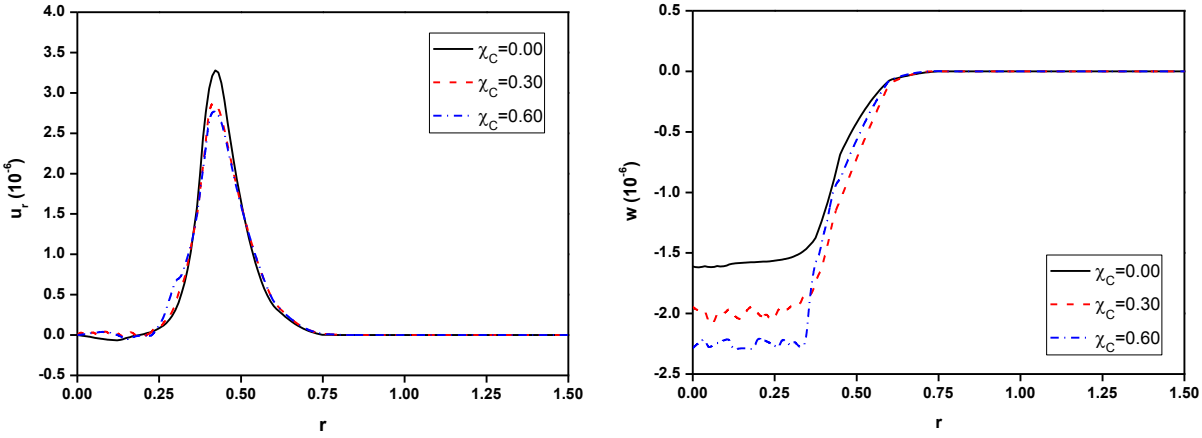


Fig. 6 The distribution of axial displacement along z-axis.



(a) (b)

Fig. 7 The distributions of (a) radial and (b) axial displacements along *r*-axis.

5.2.2 The effect of concentration-dependent diffusivity

To study the effects of concentration-dependent diffusivity on the transient responses, the following three cases are investigated:

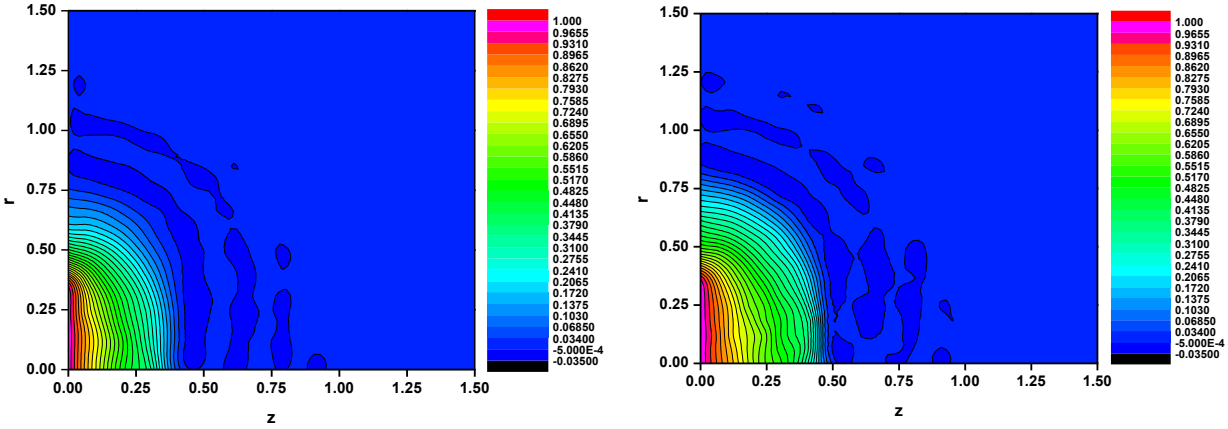
Case 4, $\chi_C = 0.00$ and $\chi_D = 0.00$;

Case 5, $\chi_C = 0.00$ and $\chi_D = 0.80$;

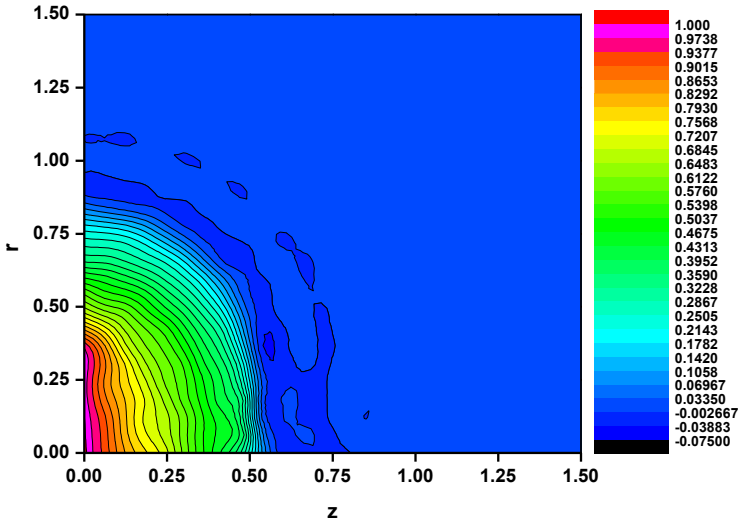
Case 6, $\chi_C = 0.00$ and $\chi_D = 1.60$.

in which $\chi_D > 0$ (i.e. $\chi_D = 0.80$ and 1.60) represents the increased diffusivity. The value of diffusion coefficient is increased when the concentration dependency is considered. This suggests the capability of mass transfer is increased. Therefore, the molar concentration response region should be expanded. The contours of molar concentration in the circular plate are depicted in Fig. 8 for Case 4, Case 5 and Case 6. As shown in Fig. 8, the response region of molar concentration is expanding with the

increase of χ_D.



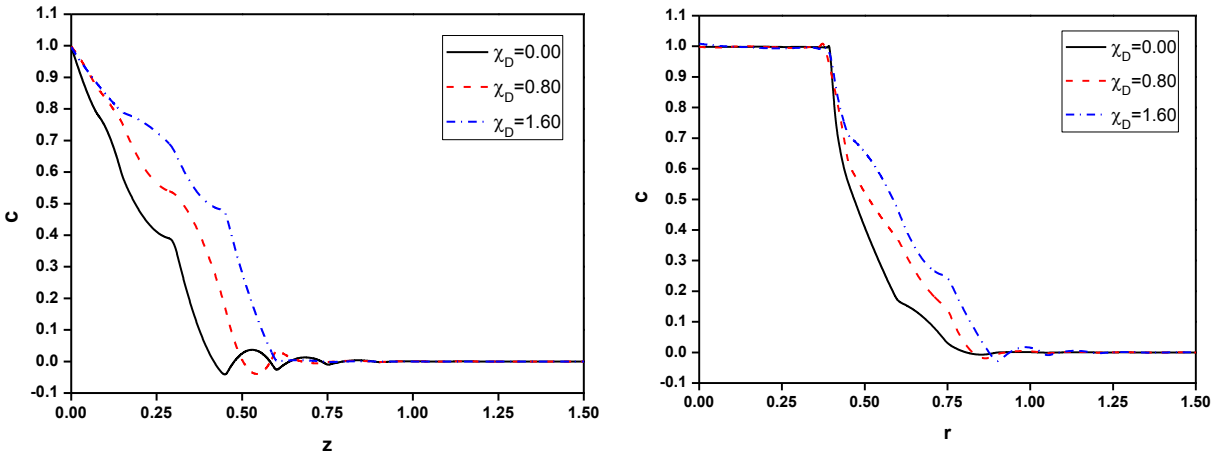
(a) $\chi_C = 0.00, \quad \chi_D = 0.00$ (b) $\chi_C = 0.00, \quad \chi_D = 0.80$



(c) $\chi_C = 0.00, \quad \chi_D = 1.60$.

Fig. 8 The contours of molar concentration in the thick circular plate.

Fig. 9 (a) and (b) presents the distributions of molar concentration along *z*-axis and *r*-axis, respectively. From Fig. 9 (a), it is indicated that the jump of molar concentration at diffusive wave front moves forward with increasing χ_D. This implies that the larger the diffusivity is, the faster the diffusive travels. As shown in Fig. 9(b), the magnitude of molar concentration becomes much larger when χ_D is increasing.



(a) (b)

Fig. 9 The distribution of molar concentration along (a) *z*-axis (b) *r*-axis.

The distribution of axial displacement along *z*-axis at $r = 0$ is presented in Fig. 10. It is shown that the peak value of axial displacement at the upper surface of the plate is increases significantly with the increasing χ_D. One can also find that the jump of displacement at elastic wave front moves forward when the concentration-dependent effect on diffusivity is considered. It means that the propagation of elastic wave is accelerated when the diffusivity is increasing.

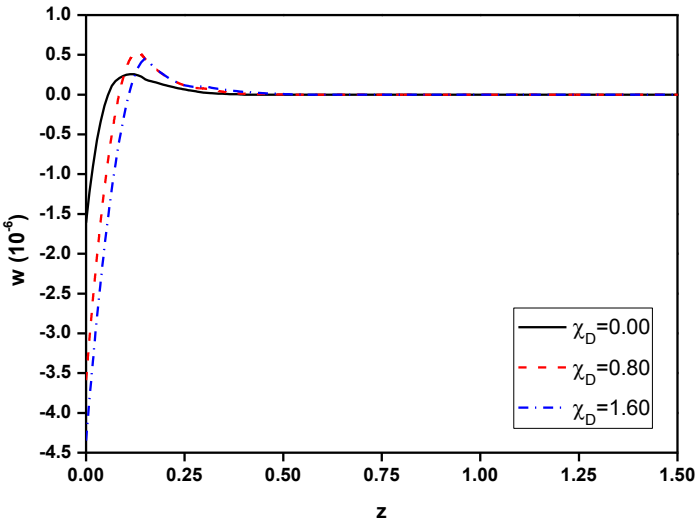
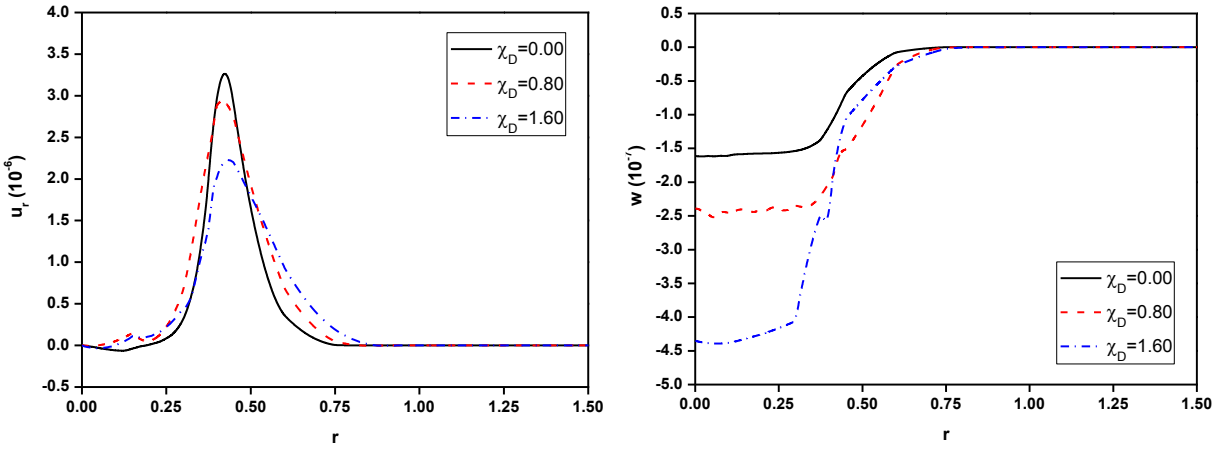


Fig. 10 The distribution of displacement along *z*-axis.

Fig. 11 displays the distributions of radial and axial displacement on upper surface along *r*-axis, respectively. Fig. 11(a) shows that the peak value of radial displacement along *r*-axis decreases with the increase of χ_D. From Fig. 11(b), it is seen that the magnitude of axial displacement on upper surface of the plate increases steeply with increasing χ_D.



(a) (b)

Fig. 11 The distributions of (a) radial and (b) axial displacements along *r*-axis.

6 CONCLUSIONS

With the aids of the principle of virtual work, the finite element formulation of the problem is obtained. The corresponding nonlinear finite element governing equations are solved in time domain directly. As a numerical example, transient response of a thick circular plate with concentration- dependent material properties under concentration shock loading is studied. From numerical results, the following conclusions can be reached:

1) The concentration-dependent effect on elastic modulus shows a significant influence on displacement and stress. When $\chi_C > 0$, the increase of concentration-dependent elastic modulus results in: (a) The elastic wave travels faster; (b) The magnitude of displacement at the upper surface of the thick circular plate becomes larger; (c) The peak values of stress around the elastic wave front increase; (d) Molar concentration is unaffected by the changes of concentration-dependent elastic modulus.

2) With the increase of concentration-dependent diffusivity for $\chi_D > 0$, it is found that: (a) The velocity of diffusive wave increases and diffusive wave front moves forward; (b) The magnitude of molar concentration, displacement and stress increase.

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