The numerical manifold method for transient moisture diffusion in 2D functionally graded materials

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Abstract. Attributing to its unique dual cover systems, the numerical manifold method (NMM) provides a uniform framework for both continuous and discontinuous analysis. In this work, the NMM is developed to perform 2D transient moisture diffusion analysis in functionally graded materials (FGMs). The NMM discrete formulations are derived based on the governing equation, the boundary conditions and the modified variational principle, and then solved by the backward difference scheme. The accuracy of the proposed method is verified through a typical numerical example, and the influence of the material gradient of the FGMs on the moisture concentration field is also examined.

1. Introduction

Due to the use of two cover systems, that is, the mathematical cover (MC) and the physical cover (PC), the numerical manifold method (NMM) constructs a unified platform for both continuous and discontinuous analysis [1]. In the NMM, the MC may be independent of all domain boundaries, including the material interfaces and crack geometry (if any), which can facilitate the discretization, especially for problems involving discontinuity evolution (e.g., crack propagation). In the past years, many efforts have been put on the developments and applications of the NMM in different fields, e.g., in crack modeling [2-11], wave propagation [12, 13], fluid flow [14-16] and heat conduction [17, 18].

In this work, the NMM is further extended to model 2D transient moisture diffusion problems in the functionally graded materials (FGMs), whose material parameters such as the elastic modulus, the thermal conductivity and the moisture diffusion coefficient vary smoothly with the spatial location. For this purpose, the rest paper is addressed as follows. In Section 2, the governing equation, the boundary conditions and the initial condition are presented. In Section 3, the NMM discrete formulations for the present problem are derived. To validate the proposed method, a typical numerical example is analyzed in Section 4. Finally in Section 5, the concluding remarks are given.

2. Governing equations

Transient moisture diffusion in a 2D isotropic FGM body as shown in figure 1 is studied. The domain Ω is enclosed by the essential boundary Γ_C and the natural boundary Γ_f. The associated governing equation for this boundary and initial value problem (BIVP) is [19]

$$\frac{\partial}{\partial x}\left(D(x,y)\frac{\partial C(x,y,t)}{\partial x}\right)+\frac{\partial}{\partial y}\left(D(x,y)\frac{\partial C(x,y,t)}{\partial y}\right)+S(x,y,t)=\frac{\partial C(x,y,t)}{\partial t} \tag{1}$$

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where ∂ symbolizes the partial derivative. D is the spatially-varying moisture diffusivity of the FGMs, C is the moisture concentration, S is the moisture source and t is the time. (x, y) are the rectangular Cartesian coordinates.

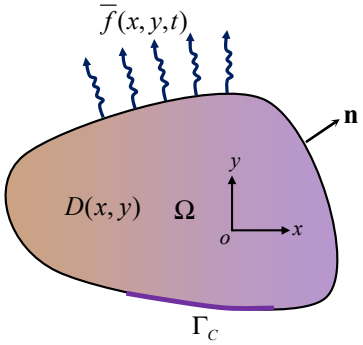


Figure 1. Transient moisture diffusion in an isotropic FGM body.

The corresponding boundary conditions are written as

$$C(x,y,t) = \overline{C}(x,y,t) \quad (\text{on } \Gamma_C) \tag{2}$$

$$-D(x,y)\frac{\partial C(x,y,t)}{\partial x}n_1 - D(x,y)\frac{\partial C(x,y,t)}{\partial y}n_2 = \overline{f} \quad (\text{on } \Gamma_f) \tag{3}$$

where $\overline{C}$ and $\overline{f}$ are, respectively, the prescribed moisture concentration on Γ_C and the applied moisture flux on Γ_f. $(n_1, n_2) = \mathbf{n}$ is the outward unit normal to the domain illustrated in figure 1.

The initial condition for this BIVP is

$$C(x,y,t)\big|_{t=0} = C_0(x,y) \tag{4}$$

3. The NMM for transient moisture diffusion in FGMs

3.1. NMM discretization procedure

In the NMM, domain discretization is a key step. Firstly, an MC formed by a certain number of mathematical patches (MPs) is built. Theoretically, the MC may be inconsistent with all domain boundaries as long as it can cover the whole domain, and the MP is composed of user-defined mathematical elements. Secondly, the physical patches (PPs) are obtained through the intersection of the MPs and the domain. The union of all PPs then establishes the PC. Lastly, the manifold elements (MEs) are generated through the common parts of as many as possible PPs.

3.2. NMM approximation

Based on the above discretization, the NMM approximation of the moisture concentration field in a certain ME E is expressed as

$$C^h(x,y,t) = \sum_{I=1}^{N} w_I(x,y)C_I(x,y,t) \tag{5}$$

where N is the amount of PPs forming E and $w_I(x,y)$ is the weight function defined on the MP containing the Ith PP. $C_I(x,y)$ is the local function defined on the Ith PP, and for continuous problems, it is often taken as

$$C_I(x,y,t)=\mathbf{P}(x,y)\mathbf{a}_I(x,y,t) \tag{6}$$

where $\mathbf{a}_I$ is the vector of unknowns defined on the Ith PP and $\mathbf{P}(\mathbf{x})$ is the row vector of polynomial basis being

$$\mathbf{P}(x,y)=\left[1,\ x,\ y,\ x^2,\ xy,\ y^2,\ ...\right] \tag{7}$$

3.3. NMM discrete equations

Utilizing the governing equation(equation (1)), boundary conditions (equations (2)-(3)), the NMM approximation (equation (5)) and the modified variational principle, the NMM discrete formulations for the transient moisture diffusion in the FGMs are deduced as

$$\mathbf{M}\dot{\mathbf{C}}+\mathbf{K}\mathbf{C}=\mathbf{F} \tag{8}$$

where $\mathbf{C}$ and $\dot{\mathbf{C}}$ are, respectively, the column vector of all unknowns and their first derivatives with respect to time. $\mathbf{M}$, $\mathbf{K}$ and $\mathbf{F}$ represent, respectively, the coefficient matrix, the moisture diffusion matrix and the equivalent moisture load vector. In the NMM, these matrices are calculated ME by ME and their values on the ME E are

$$\mathbf{M}^E=\int_{\Omega^E}\left(w_I\mathbf{P}\right)^{\mathrm{T}}\left(w_I\mathbf{P}\right)d\Omega \tag{9}$$

$$\mathbf{K}^E=\int_{\Omega^E}\mathbf{B}^{\mathrm{T}}D\mathbf{B}d\Omega+\int_{\Gamma_C^E}\left(w_I\mathbf{P}\right)^{\mathrm{T}}\lambda\left(w_I\mathbf{P}\right)d\Gamma \tag{10}$$

$$\mathbf{F}^E=\int_{\Omega^E}\left(w_I\mathbf{P}\right)^{\mathrm{T}}Sd\Omega+\int_{\Gamma_C^E}\left(w_I\mathbf{P}\right)^{\mathrm{T}}\lambda\overline{T}d\Gamma-\int_{\Gamma_f^E}\left(w_I\mathbf{P}\right)^{\mathrm{T}}\overline{f}d\Gamma \tag{11}$$

where the superscript $\mathbf{T}$ represents the matrix transpose. Ω^E, Γ_C^E and Γ_f^E are, respectively, the domain, the essential boundary and the natural boundary associated with E. λ is the penalty for the approximate treatment of the essential boundary condition in equation (2) because of the inconsistence between the MC and the domain boundaries. The matrix $\mathbf{B}$ is

$$\mathbf{B}=\left[\mathbf{B}_1\quad\mathbf{B}_2\quad ...\quad\mathbf{B}_I\quad ...\quad\mathbf{B}_N\right] \tag{12}$$

with

$$\mathbf{B}_I=\begin{bmatrix}\left(w_I\mathbf{P}\right)_{,x}\\ \left(w_I\mathbf{P}\right)_{,y}\end{bmatrix} \tag{13}$$

where the subscript $,x$ and $,y$ denote, respectively, the partial differential with respect to x and y.

3.4. Solving strategy

To solve the linear system of ordinary differential equations (see equation (8)), the unconditionally stable and non-oscillating Euler backward difference scheme is adopted. Accordingly, by dividing the total computation time t_{total} into n intervals, i.e., $[t_0,t_1],[t_1,t_2],\cdots,[t_i,t_{i+1}],\cdots,[t_{n-1},t_n]\,(t_0=0,t_n=t_{\text{total}})$, and supposing that the vector $\mathbf{C}$ at t_i (denoted as $\mathbf{C}_i$) is known and the time step size is Δt, its value at t_{i+1}, i.e., $\mathbf{C}_{i+1}$, can be computed by

$$\left(\frac{\mathbf{M}}{\Delta t}+\mathbf{K}_{i+1}\right)\mathbf{C}_{i+1}=\mathbf{F}_{i+1}+\frac{\mathbf{M}}{\Delta t}\mathbf{C}_i \tag{14}$$

where $\mathbf{C}_0$ is determined by the initial condition in equation (4).

4. Numerical example

Consider the transient moisture diffusion in a square FGM plate of unit width illustrated in figure 2, where the associated material property, the moisture source, the boundary conditions and the initial condition are also presented with γ the material gradient. Accordingly, the exact solution to the moisture concentration is

$$C(x,y,t)=\exp(-\gamma y+t) \tag{15}$$

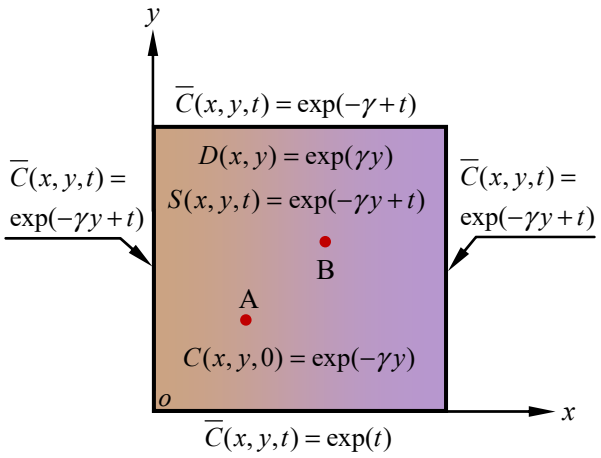


Figure 2. Transient moisture diffusion in a square FGM plate.

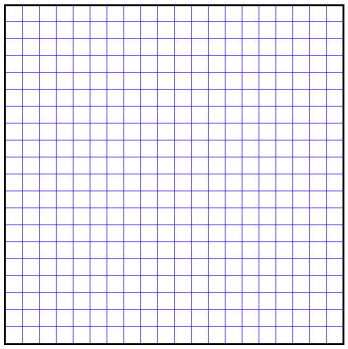
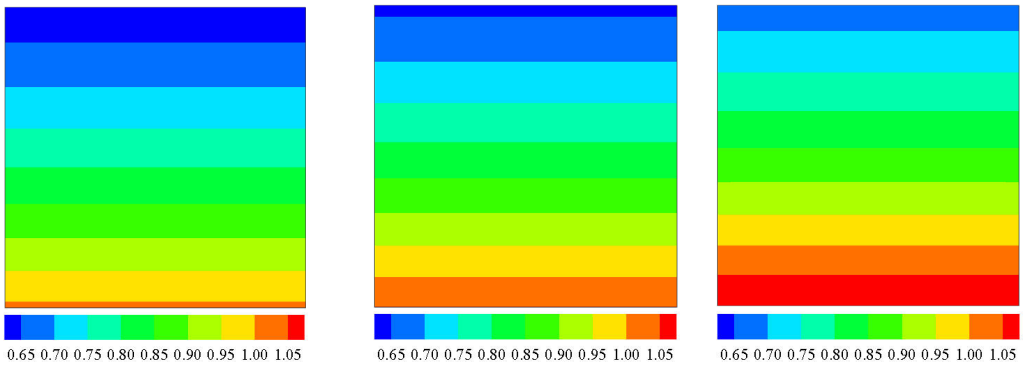


Figure 3. Discretized domain when h=0.05.

In the NMM modeling, an MC formed by square mathematical elements with its size h =0.05 is adopted (the size of the MC is defined as the side length of the mathematical element) and the final discretization is given in figure 3, which contains 441 PPs and 400 MEs. What's more, the polynomial basis in equation (6) is chosen to be constant and the penalty λ in equation (10) and (11) is chosen as 1.0×10^{10}.

In the computation, the influence of the material gradient γ on the moisture concentration is mainly studied. Three graded parameters with $\gamma=0.5$, 1.0 and 2.0 are, respectively, studied at $\Delta t=0.001$. The simulated moisture concentrations at $t=0.01, 0.05$ and 0.1 when $\gamma=0.5$ are, respectively, plotted in figure 4(a) ~ (c), from which we can observe that the time-varying moisture concentrations change only in the vertical direction, conforming to the rules obtained from equation

(15). Further, the calculated moisture concentrations by the NMM at point A (0.3, 0.3) and B (0.6, 0.6) are, respectively, illustrated in figure 5(a) and 5(b), together with the exact solutions. From figure 5, we can conclude that the present results are in excellent agreement with the theoretical ones. Moreover, we can also find that the moisture concentration decreases with γ at a given instant and point.



(a) (b) (c)

Figure 4. Distribution of moisture concentration field: (a) t=0.01, (b) t=0.05 and (c) t=0.1

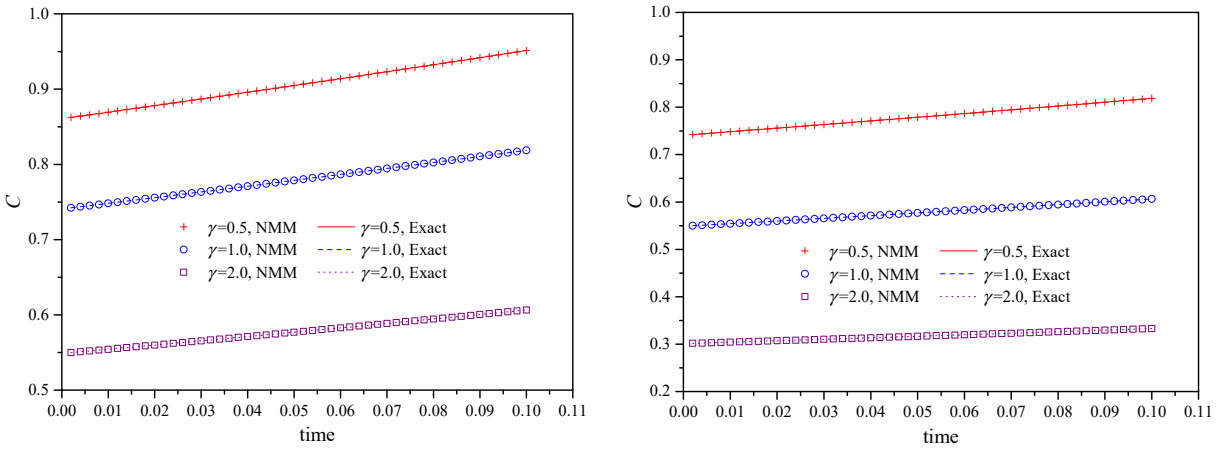


Figure 5. The computed moisture concentrations at different time and material gradient: (a) point A and (b) point B

5. Concluding remarks

In this work, the numerical manifold method was further developed to model transient moisture diffusion in 2D FGMs. The fundamental equations of this BIVP are presented. The NMM discrete formulations and their solving scheme are also provided. To verify the proposed method, a typical example is studied on uniform MC composed of square mathematical elements. It is found that the present solutions match well with the reference ones. Besides, the effect of the material gradient on the distribution of moisture diffusions is also tested.

For the present continuous moisture diffusion problems, the superiority of the NMM is mainly in the discretization aspect, that is, the MC may be nonconforming with all domain boundaries. Actually, due to the use of bi-cover systems, the extension of the NMM to discontinuous analysis in FGMs involving hygro-thermo-mechanical coupling effect is more challenging and the work is on.

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