Unsteady one-dimensional thermoelastic cross-diffusion perturbations in a layer

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Abstract. In the paper we present an algorithm for solving the unsteady problem of the thermoelastodiffusion perturbations propagation in a multicomponent layer. One-dimensional physicomechanical processes in the medium are described by the locally equilibrium model, including the equations of elastic medium motion, heat transfer and mass transfer with cross-diffusion effects. The unknown functions of displacement, temperature and concentration increments are sought in the integral form of convolution by time of the surface Green’s functions and boundary conditions. To find the Green’s functions, we use the integral Laplace transform with respect to time and the Fourier expansion into series by the spatial coordinate. It allows us to reduce the problem to system of linear algebraic equations. The originals of the Fourier series coefficients are found using known theorems and tables of operational calculus. Thus, the use of numerical algorithms is minimized and the surface Green’s functions are found. Calculation example is presented.

1. Introduction

The materials creation and their production technologies development require not only an advanced experimental base, but also accurate math models describing complex physical processes. One way to modify and refine math models is to take into account such phenomena as the coupling of various interacting physical fields. An example of such a coupling is the thermoelastic diffusion model of the mechanical, thermal, and diffusive fields interaction.

The research direction relevance is confirmed by the presence of many papers by scientists from around the world [1–4]. Most of the papers are devoted to solving static [5,6], quasi-static [7–9] and stationary [10–12] thermomechanical diffusion problems. However, the unsteady one-dimensional [13–15] and two-dimensional problems [16–20] of thermomechanical diffusion are the most interesting and complex. But in these papers the solution reduces to the integral Laplace transform with respect to time and its inversion is associated with great mathematical difficulties. For this reason, in most of the above works, algorithms and ready packages of computational mathematics and mechanics are used to find the originals [21–23].

In the paper we consider the one-dimensional unsteady thermoelastic problem with cross-diffusion effects for a isotropic multicomponent layer. The linear locally-equilibrium model of coupled thermoelastic diffusion is used [24–29].
2. Problem formulation

The mathematical problem formulation of the coupled thermoelastic cross-diffusion in a rectangular Cartesian coordinate system \( \Omega_{x_1x_2x_3} \) along an axis \( x_i \) is the system of motion, heat transfer, and \( N \) mass transfer equations [2, 15, 19, 25, 29]:

\[
\ddot{u} = u^* - b_2 \dot{\vartheta} - \sum_{q=1}^{N} \alpha_q \dot{n}_q, \\
\dot{\vartheta} + \tau_\gamma \ddot{\vartheta} = \kappa \dot{\vartheta} - b_1 (\dot{u}^* + \tau_\gamma \dot{u}^*), \\
\dot{n}_q + \tau_\gamma \dot{n}_q = \sum_{p=1}^{N} D_{qp} \eta_p^* - \Lambda_q \eta^* - M_q \dot{\vartheta}^* \\
\quad(q = 1, N).
\]

(1)

Here the primes denote derivatives with respect to the dimensionless spatial variable \( \tilde{x} \); the points denote derivatives with respect to the dimensionless time \( \tau \); \( q \) is component number of the medium. Displacements, thermal and diffusion fluxes are given on the layer boundaries:

\[
u_{x_i} |_{x_i = 0} = f_{x_i}(\tau), \quad \vartheta |_{x_i = 0} = f_{x_i}(\tau), \quad \left( \Lambda_q \eta^* + M_q \dot{\vartheta}^* - \sum_{p=1}^{N} D_{qp} \eta_p^* \right) |_{x_i = 0} = f_{x_i+2} \quad (i = 1, 2).
\]

(2)

The initial conditions are assumed to be zero:

\[
u_i = 0, \quad \vartheta = 0, \quad (\eta_i^*) = 0, \quad (\eta_i^*) |_{x_i = 0} = \eta_i |_{x_i = 0} = 0.
\]

(3)

In (1) – (3) and further dimensionless quantities are used (if the symbol coincide, then the dimensional value is indicated by an asterisk; \( \psi = 1, 2 \)):

\[
x = \frac{x_1}{L}, \quad u = \frac{u_1}{L}, \quad \tau = \frac{\tau_1}{L}, \quad C^2 = \frac{C_{1111}}{\rho}, \quad \alpha_q = \frac{\alpha_q^{(q)}}{C_{1111}}, \quad D_{qp} = \frac{D_{qp}^{(qp)}}{CL}, \quad \tau_\gamma = \frac{\tau_\gamma}{\kappa}, \quad \alpha_q = \frac{\alpha_q^{(q)}}{C_{1111}}, \quad \Lambda_q = \frac{m_q n_0^{(q)} D_{11}^{(qp)} \alpha_1}{\rho R T_0 C_L}, \quad \beta_q = \frac{R \ln \left( \frac{n_0^{(q)} \gamma^{(q)}}{n_0^{(q)}} \right)}{m_q c_0}, \\
\dot{\vartheta} = \frac{T}{T_0}, \quad \beta_q = \frac{b_{11} T_0}{C_{1111}}, \quad \eta_i = \frac{\rho c_0}{m_q}, \quad f_{x_i}(\tau) = \frac{f_{x_i}^{(q)}}{L}, \quad f_{x_i}(\tau) = \frac{L f_{x_i}^{(q)}}{T_0}, \quad f_{x_i+2}(\tau) = \frac{f_{x_i+2}^{(q)}}{T_0}.
\]

(4)

Here \( t \) is time; \( u \) is the displacement vector component; \( L \) is the layer thickness; \( \eta_i^{(q)} = n_i^{(q)} - n_0^{(q)} \) is a concentration increment; \( n_0^{(q)} \) and \( n_i^{(q)} \) are initial and actual concentrations (mass fractions); \( \tau_1 \) is the thermal relaxation time; \( \tau_\gamma^{(q)} \) is the diffusion relaxation time; \( C_{1111} \) is the elastic constant; \( \rho \) is the mass density; \( b_{11} \) is a temperature constant characterizing thermal deformations; \( \alpha_q^{(q)} \) is a coefficient characterizing the medium volumetric change due to diffusion; \( D_{11}^{(qp)} \) is the diffusion coefficient; \( m_q^{(q)} \) is the molar mass; \( R \) is the universal gas constant; \( \dot{\vartheta}^* = T - T_0 \) is a temperature increment; \( T_0 \) and \( T \) are initial and actual temperatures; \( \gamma^{(q)} \) is the actvity coefficient; \( c_0 \) is the specific heat at constant concentration and deformation.
3. Solution algorithm

We represent the solution of problem (1) – (3) in the form of convolutions by time [24–28]:

\[ u(x, \tau) = \sum_{k=1}^{N+2} \left[ G_{ik}(x, \tau) \ast f_{k_1}(\tau) + G_{ik}(1-x, \tau) \ast f_{k_2}(\tau) \right], \]

\[ \vartheta(x, \tau) = \sum_{k=1}^{N+2} \left[ G_{2k}(x, \tau) \ast f_{k_1}(\tau) - G_{2k}(1-x, \tau) \ast f_{k_2}(\tau) \right], \]

\[ \eta_q(x, \tau) = \sum_{k=1}^{N+2} \left[ G_{q+2,k}(x, \tau) \ast f_{k_1}(\tau) - G_{q+2,k}(1-x, \tau) \ast f_{k_2}(\tau) \right], \]

where \( G_{ik}(x, \tau) \) are the Green's functions of problem (1) – (3) and \( i, k = 1, N+2 \). They are solutions of problem involving equations (1), initial conditions (3) and the following boundary conditions:

\[ G_{ik} |_{x=0} = \delta_{ik} \delta(\tau), \quad G_{2k} |_{x=0} = \delta_{2k} \delta(\tau), \quad \left( \Lambda q G_{ik}^* + M_q G_{2k}^* - \sum_{p=1}^{N} D_{qp} G_{p+2,k}^* \right) |_{x=0} = \delta_{q+2,k} \delta(\tau), \]

\[ G_{ik} |_{x=1} = 0, \quad G_{2k} |_{x=1} = 0, \quad \left( \Lambda q G_{ik}^* + M_q G_{2k}^* - \sum_{p=1}^{N} D_{qp} G_{p+2,k}^* \right) |_{x=1} = 0. \]

Here \( \delta(\tau) \) is the Dirac delta function and \( \delta_{ik} \) is the Kronecker symbol.

In this case, we need to find the Green's functions. We apply the integral Laplace transform by time to (1) and (6) taking into account (3) and (5) (« s » is the transformation parameter, the upper index « L » denotes the Laplace transformant):

\[ s^2 G_{ik}^L = G_{ik}^{l,*} - b_q G_{2k}^{l,*} - \sum_{q=1}^{N} \alpha_q G_{q+2,k}^{l,*}, \]

\[ s \left( 1 + \tau \gamma \right) G_{2k}^L = \kappa G_{2k}^{l,*} - s b_q \left( 1 + \tau \gamma \right) G_{ik}^{l,*} - s \left( 1 + \tau \gamma \right) \sum_{q=1}^{N} \beta_q G_{q+2,k}^{l,*}, \]

\[ s \left( 1 + \tau \gamma \right) G_{q+2,k}^L = \sum_{p=1}^{N} D_{qp} G_{p+2,k}^{l,*} - \Lambda q G_{ik}^{l,*} - M_q G_{2k}^{l,*}. \]

\[ G_{ik}^L |_{x=0} = \delta_{ik}, \quad G_{2k}^L |_{x=0} = \delta_{2k}, \quad \left( \Lambda q G_{ik}^{l,*} + M_q G_{2k}^{l,*} - \sum_{p=1}^{N} D_{qp} G_{p+2,k}^{l,*} \right) |_{x=0} = \delta_{q+2,k}, \]

\[ G_{ik}^L |_{x=1} = 0, \quad G_{2k}^L |_{x=1} = 0, \quad \left( \Lambda q G_{ik}^{l,*} + M_q G_{2k}^{l,*} - \sum_{p=1}^{N} D_{qp} G_{p+2,k}^{l,*} \right) |_{x=1} = 0. \]

Further, we represent the images of the Green's functions in the incomplete Fourier series form:

\[ G_{ik}^L(x, s) = \sum_{n=1}^{\alpha} G_{ik,n}(s) \sin(\lambda_n x), \quad G_{ik}^{l,*}(x, s) = \frac{G_{ik,n}(s)}{2} + \sum_{n=1}^{\alpha} G_{ik,n}(s) \cos(\lambda_n x) \quad (l \neq 1), \quad \lambda_n = \pi n. \]

To find the coefficients of the expansion:

\[ G_{ik,n}(s) = \int_0^1 G_{ik}^L(x, s) \sin(\lambda_n x) dx, \quad G_{ik,n}^{l,*}(s) = \int_0^1 G_{ik}^{l,*}(x, s) \cos(\lambda_n x) dx, \]

we multiply the first equation in (7) by \( \sin(\lambda_n x) \), and the rest by \( \cos(\lambda_n x) \). Then integrate by parts over the variable \( x \) in the interval from 0 to 1 taking into account (8). As result we obtain the following system of linear algebraic equations [24–28]:

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The solution of the system (9) has the form:

\[
G_{l+2}^{I} = 2b_y, \quad G_{l+1}^{I} = -2\frac{\kappa}{\omega}, \quad G_{l+2,0}^{I} = -2\frac{\beta_1}{\chi_q}, \quad G_{l+2,2,0}^{I} = 2\frac{1}{\chi_q},
\]

\[
G_{l+3}^{I} = \frac{P_{l}^{I} (\lambda_n, s)}{P(\lambda_n, s)} (n \geq 1).
\]

Here \( P \) is the determinant of homogeneous system (9), \( P_{l}^{I} \) is the determinants obtained from \( P \) by replacing its \( i \)-th column with the right side of the system (9) by Cramer's Rule.

The solution in the images is obtained. Further we need to go to the originals domain.

Let \( s_{m} = s (\lambda_n) \in \mathbb{C}, \quad j = 1, 2N + 4 \) are the simple zeros of the polynomial \( P \). Then the originals of the Green’s functions images (10) are [24]:

\[
G_{ik} (x, \tau) = \sum_{n=1}^{2N+4} G_{ik} (\tau) \sin (\lambda_n x), \quad G_{2k} (x, \tau) = \frac{G_{2k,0} (\tau)}{2} + \sum_{n=1}^{2N+4} G_{2k,0} (\tau) \cos (\lambda_n x),
\]

\[
G_{q+2,k} (x, \tau) = \frac{G_{q+2,k,0} (\tau)}{2} + \sum_{n=1}^{2N+4} G_{q+2,k,0} (\tau) \cos (\lambda_n x);
\]

where

\[
G_{ik} = \sum_{j=1}^{2N+4} \frac{P_{j}^{I} (\lambda_n, s_{m})}{P(\lambda_n, s_{m})} \exp (s_{m} \tau) (i, k = 1, 2N + 2);
\]

\[
G_{210} = 2b_y \delta (\tau), \quad G_{220} = -2\kappa \left[ 1 - \exp \left( -\frac{\tau}{\tau_y} \right) \right],
\]

\[
G_{2q+2,0} = -2\beta_q \left[ 1 - \exp \left( -\frac{\tau}{\tau_q} \right) \right], \quad G_{q+2,q+2,0} = 2\left[ 1 - \exp \left( -\frac{\tau}{\tau_q} \right) \right].
\]

The prime in (12) denotes the derivative with respect to the parameter \( s \).

Finally, we need to substitute the Green’s functions (11), (12) into convolutions (5) to find the unknown functions of displacement and increments.

In a similar way we can find a solution for the half-space. In this case, it is necessary to set the unknown functions boundedness at infinity and use Fourier transforms instead of expanding into Fourier series [26, 28]. Fourier transformation inversion will be performed numerically.

4. Calculation example

The layer material for example is duralumin \( (q = 1: 95\% - Al; \quad q = 2: 5\% - Cu) \). Its thickness \( L \) is 1 mm and the initial temperature \( T_0 \) is 600 K. In this case, the following dimensionless quantities obtained with the formulas (4) will correspond to the layer [15, 30–32]:
We set in the boundary conditions (2) that:

1) both boundaries of the layer are heat-insulated and rigidly fixed: \( f_{11}(\tau) = f_{12}(\tau) = f_{21}(\tau) = f_{22}(\tau) = 0 \); 
2) on the upper boundary of the layer \( (x = 0) \) the diffusion flux is the Heaviside function, and at the lower boundary \( (x = 1) \) it is absent: \( f_{31}(\tau) = 10^{-15} \cdot H(\tau) \), \( f_{32}(\tau) = 0 \).

Then we obtain the following results of the convolutions (5) shown on the figures 1–4.

**Lines:** solid is \( \tau = 1 \cdot 10^{12} \), dotted is \( \tau = 3 \cdot 10^{12} \), dashed is \( \tau = 5 \cdot 10^{12} \).

5. Conclusion

The algorithm for solving a one-dimensional unsteady thermoelastic cross-diffusion problem for a multicomponent layer is proposed. The main advantage of this approach is the ability to analytically...
find originals of the Green’s functions. In calculation example shown that it is necessary to take into account the cross-diffusion effects in solving problems of coupled thermoelastic diffusion problems for a multicomponent medium.

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