Propagation of one-dimensional thermoelastodiffusive perturbations in a multicomponent layer

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Abstract. In this paper we present an algorithm for solving the unsteady problem of the one-dimensional thermoelastodiffusive perturbations propagation in a multicomponent layer. One-dimensional physicomechanical processes in the medium are described by a locally-equilibrium model, including the equations of medium motion, heat transfer and mass transfer. The required functions of displacement, temperature and concentration increments are sought in the integral form of convolution by time of the 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 by the spatial coordinate. The analysis of the Green's functions is done. The test calculation for finite and infinite velocities of perturbations propagation is performed.

1. Introduction

The materials creation with new exceptional properties and the technologies development for their production 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 [1–29]. A rather detailed review devoted to various problems of modelling thermomechanodiffusion processes in the 20th century is available in [30].

Most of the papers are devoted to solving static [4, 5], quasi-static [6–8] and stationary [9–12] 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 this paper we consider the one-dimensional unsteady thermoelastic diffusion problem for a homogeneous multicomponent layer. The locally-equilibrium model of coupled thermoelastic diffusion is used. The model describing perturbations propagation in continuum with finite speed and...
including equations of the elastic medium motion, heat transfer and mass transfer. The initial conditions are assumed to be zero.

The problem solution, similar to problems [24–28], is sought in the integral form, which is the convolution in time of the 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 by the spatial coordinate. As a result of the transformations, the Laplace images of the unknown functions harmonics are expressed as rational fractions with respect to the Laplace transform parameter. Their originals are found using known theorems and tables of operational calculus. This approach allows us to minimize the use of numerical algorithms and analyze the Green's functions.

2. Problem formulation

We consider a homogeneous \( N \)-component layer bounded by surfaces \( x_1 = 0 \) and \( x_2 = L \) (\( Ox_1, x_2, x_3 \) is a rectangular Cartesian coordinate system). The dimensionless local-equilibrium coupled thermoelastic diffusion model is used to describe perturbations propagating in a medium at a finite speed [2, 15, 19, 25, 29]. It includes: the equation of elastic medium motion, the heat transfer equation and \( N \) equations of the mass transfer (the primes denote derivatives with respect to the dimensionless spatial variable \( x \), the points denote derivatives with respect to the dimensionless time \( \tau \)):

\[
\ddot{u} = u^* - b_q \dot{q}^* - \sum_{q=1}^{N} \alpha_q \eta_q^*,
\]

\[
\dot{\theta} + \tau_\sigma \ddot{\theta} = \kappa \theta^* - b_t (\dot{u} + \tau_\tau \dot{u}'), - \sum_{q=1}^{N} \beta_q \left( \dot{\eta}_q + \tau_\tau \dot{\eta}_q' \right),
\]

\[
\dot{\eta}_q + \tau_\eta \ddot{\eta}_q = D_q \eta^*_q - A_q \theta^* - M_q \theta^* \quad (q = 1, N).
\]

Displacements, thermal and diffusion fluxes are given on the layer boundaries:

\[
[u|_{x=0} = f_{11}(\tau), \quad u|_{x=L} = f_{12}(\tau), \quad \theta|_{x=0} = f_{21}(\tau), \quad \theta|_{x=L} = f_{22}(\tau),
\]

\[
\left( A_q \theta^* + M_q \theta^* - D_q \eta^*_q \right)|_{x=0} = f_{q+1,1}(\tau), \quad \left( A_q \theta^* + M_q \theta^* - D_q \eta^*_q \right)|_{x=L} = f_{q+2,2}(\tau).
\]

The initial conditions are assumed to be zero:

\[
u|_{\tau=0} = \dot{u}|_{\tau=0} = \dot{\theta}|_{\tau=0} = \dot{\eta}_q|_{\tau=0} = \ddot{\eta}_q|_{\tau=0} \equiv 0.
\]

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

\[
x = \frac{x_1}{L}, \quad u = \frac{u_1}{L}, \quad \tau = \frac{Ct}{L}, \quad C^2 = \frac{C_{1111}}{\rho}, \quad \alpha_q = \frac{\alpha_{11}^{(q)}}{C_{1111}}, \quad D_q = \frac{D_{11}^{(q)}}{CL}, \quad \tau_\sigma = \frac{Ct}{L}, \quad \tau_\eta = \frac{C_{11}^{(q)}}{L},
\]

\[
A_q = \frac{m^{(q)} n_0^{(q)} D_{11}^{(q)} \alpha_{11}^{(q)}}{\rho RT_0 CL}, \quad M_q = \frac{n_0^{(q)} D_{11}^{(q)} \ln(n_0^{(q)} / n_{0}^{(q)})}{\rho c_p LC}, \quad \kappa = \frac{\kappa_{11}}{\rho c_p LC}, \quad \beta_q = \frac{R \ln(n_0^{(q)} / n_{0}^{(q)})}{m^{(q)} c_0},
\]

\[
\theta = \frac{\theta^*}{T_0}, \quad b_u = \frac{b_{11} T_0}{C_{1111}}, \quad b_t = \frac{b_{12}}{\rho c_p}, \quad f_1(\tau) = \frac{f_{11}(t)}{L}, \quad f_2(\tau) = \frac{f_{22}(t)}{T_0}, \quad f_{q+2,2}(\tau) = \frac{f_{q,2,2}(t)}{n_0^{(q)} C}.
\]

Here \( t \) is time; \( u_1 \) is the displacement vector component; \( L \) is the layer thickness; \( \eta^{(q)} = n^{(q)} - n_0^{(q)} \) is a concentration increment; \( n_0^{(q)} \) and \( n^{(q)} \) are initial and actual concentrations (mass fractions); \( \tau_\sigma \) is the thermal relaxation time; \( \tau_\eta \) 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; \( \alpha_{11}^{(q)} \) is a coefficient characterizing the medium volumetric change due to diffusion; \( D_{11}^{(q)} \) is the self-diffusion coefficient; \( m^{(q)} \) is the molar mass; \( R \) is the universal gas constant; \( \theta^* = T - T_0 \) is a temperature increment; \( T_0 \)
and \( T \) are initial and actual temperatures; \( \kappa_{11} \) is the coefficient of thermal conductivity; \( \gamma^{(i)} \) is the activation 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]:

\[
u(x, \tau) = \sum_{k=1}^{N+2} [G_{ik}(x, \tau) * f_{i1}(\tau) + G_{ik}(1-x, \tau) * f_{i2}(\tau)],
\]

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

\[
G_{ik}|_{x=0} = \delta_ik, \quad G'_{ik}|_{x=0} = \delta_ik, \quad G_{ik}|_{x=1} = 0, \quad G'_{ik}|_{x=1} = 0,
\]

\[
\left( \Lambda_q G_{ik}^{\tau*} - D_q G_{q+i,2,kl} + M_q G_{ik}^{\tau*} \right)|_{x=0} = \delta_{q+i,2,kl}, \quad \left( \Lambda_q G_{ik}^{\tau*} - D_q G_{q+i,2,kl} + M_q G_{ik}^{\tau*} \right)|_{x=1} = 0.
\]

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) (\( \mathbb{L} \) is the transformation parameter, the upper index \( \mathbb{L} \) denotes the Laplace transformant):

\[
s^2G_{ik}^{\mathbb{L}} = G_{ik}^{\tau*} - h_{ik}G_{ik}^{\mathbb{L}} - \sum_{q=1}^{N} a_q \left( G_{q+i,2,kl}^{\mathbb{L}} \right),
\]

\[
s(1 + \tau \mathbb{L})G_{ik}^{\mathbb{L}} = \alpha G_{ik}^{\tau*} - s_{ik}(1 + \tau \mathbb{L})G_{ik}^{\mathbb{L}} - s(1 + \tau \mathbb{L})\sum_{q=1}^{N} \beta_q G_{q+i,2,kl}^{\mathbb{L}},
\]

\[
G_{ik}|_{x=0} = \delta_{ik}, \quad G_{ik}|_{x=1} = 0, \quad G'_{ik}|_{x=0} = 0, \quad G'_{ik}|_{x=1} = 0,
\]

\[
\left( \Lambda_q G_{ik}^{\tau*} - D_q G_{q+i,2,kl}^{\mathbb{L}} + M_q G_{ik}^{\mathbb{L}} \right)|_{x=0} = \delta_{q+i,2,kl}, \quad \left( \Lambda_q G_{ik}^{\tau*} - D_q G_{q+i,2,kl}^{\mathbb{L}} + M_q G_{ik}^{\mathbb{L}} \right)|_{x=1} = 0.
\]

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

\[
G_{ik}^{\mathbb{L}}(x, s) = \sum_{n=1}^{\infty} G_{nk}^{\mathbb{L}}(s) \sin \lambda_n x, \quad G_{ik}^{\tau*}(x, s) = \frac{G_{ik}^{\mathbb{L}}(s)}{2} + \sum_{n=1}^{\infty} G_{nk}^{\mathbb{L}}(s) \cos \lambda_n x,
\]

To find the coefficients of the expansion

\[
G_{nk}^{\mathbb{L}}(s) = 2 \int_0^1 G_{nk}^{\mathbb{L}}(x, s) \sin \lambda_n x dx, \quad G_{nk}^{\mathbb{L}}(s) = 2 \int_0^1 G_{nk}^{\mathbb{L}}(x, s) \cos \lambda_n x dx,
\]

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]:

3.
\[ k_n G_{1n}^L - b_n \lambda_n G_{2n}^L - \lambda_n \sum_{q=1}^N \alpha_q G_{q,2n}^L = 2 \lambda_n \delta_{1k}, \]

\[ b_q \omega \lambda_q G_{1n}^L + k_{2n} G_{2n}^L + \omega \sum_{q=1}^N \beta_q G_{q,2n}^L = 2 \left( b_q \omega \delta_{1k} - \kappa \delta_{2k} \right), \tag{10} \]

\[ \Lambda_q \lambda_n^{2} G_{1n}^L + M_q \lambda_n^{2} G_{2n}^L - k_{q+2,n} G_{q+2,2n}^L = 2 \left( \Lambda_q \lambda_n^{2} \delta_{1k} - \delta_{q+2,k} \right), \]

where \( k_{1n} = s^2 + \lambda_n^{2}, \quad k_{2n} = \omega + \kappa \lambda_n^{2}, \quad k_{q+2,n} = \chi_q + D_q \lambda_n^{2}, \quad \omega = s(1 + \tau, s), \quad \chi_q = s(1 + \tau, s). \)

Solution of the system (10) has the form:

\[
G_{210}^L = 2b_r, \quad G_{220}^L = -2 \frac{K}{\omega}, \quad G_{22q+2,0}^L = -2 \frac{B_q}{\chi_q}, \quad G_{q+2,q+2,0}^L = 2 \frac{1}{\chi_q}, \quad \]

\[
G_{i,n}^L = \frac{P_i \left( \lambda_n, s \right)}{P \left( \lambda_n, s \right)} \quad (i = 1, 2), \quad G_{q+2,2n}^L = \frac{Q_{q+2,k} \left( \lambda_n, s \right)}{Q \left( \lambda_n, s \right)}, \quad n \geq 1. \tag{11} \]

Here \( P \) is the determinant of homogeneous system (10), \( P_{ik} \) is the determinants obtained from \( P \) by replacing its \( i \)-th column with the right side of the system (10) by Cramer’s Rule:

\[
P = \left( k_{1n} k_{2n} + b_n b_r \omega \lambda_n^{2} \right) \Pi - \omega \lambda_n^{6} \sum_{q=1}^N \Lambda_q \sum_{p=1}^N M p \Pi q + \]

\[ + \lambda_n^{2} \sum_{q=1}^N \left[ \omega \left( \beta_q M_q k_{1n} + b_r \alpha_q M_q \lambda_n^{2} + \beta_q M_q k_{2n} \lambda_n^{2} \right) - \alpha_q \lambda_q \lambda_n^{2} \right] \Pi q, \]

\[ P_{11} = 2 \lambda_n \left( k_{2n} + b_r \omega \lambda_n^{2} \right) \Pi + 2 \omega \lambda_n^{4} \sum_{q=1}^N M_q \sum_{p=1}^N \Lambda p \Pi q + \]

\[ + 2 \omega \lambda_n^{6} \sum_{q=1}^N \left[ \alpha_q M_q, b_r + \beta_q M_q, b_\lambda \lambda_q \right] - k_{2n} \alpha_q \lambda_q \Lambda q \right] \Pi q, \]

\[ P_{12} = -2 \omega \lambda_n \left( b_n \Pi + \lambda_n^{2} \sum_{q=1}^N \alpha_q M_q \Pi q \right), \quad P_{1, q+2} = 2 \lambda_n \left( k_{2n} \alpha_q - \omega b_n b_q \right) \Pi q + \omega \lambda_n^{4} \sum_{q=1}^N M_q \Pi q, \]

\[ P_{21} = 2 \omega \left( s^2 b_r \Pi + s^2 \lambda_n^{2} \sum_{q=1}^N \beta_q M_q, \Pi q - \lambda_n^{2} \sum_{q=1}^N \Lambda_p \Pi q \right), \]

\[ P_{22} = 2 \omega \left( \lambda_n^{4} \sum_{q=1}^N \alpha_q, \delta_q, \Pi q - k_{1n} \Pi q \right), \quad P_{2, q+2} = -2 \omega \left( k_{1n} \beta_q + b_r \alpha_q \lambda_n^{2} \right) \Pi q + \lambda_n^{4} \sum_{q=1}^N M_q \Pi q, \]

\[ Q_{q+2,l} = \lambda_n^{2} \left( \Lambda_q \lambda_n^{2} P_{l+1} + M_q P_{q+2, l} \right) - 2 \delta_q \lambda_n^{2} \Lambda_q P + 2 \delta_q \lambda_n^{2} P \left( l = 1, N + 2 \right), \quad Q_q = k_{q+2, n} P, \]

\[ \Pi = \prod_{r=1}^N k_{r+2}, \quad \Pi_q = \prod_{r=1}^N k_{r+2}, \quad \Pi_{q, p} = \left( \alpha_q \beta_p - \alpha_p \beta_q \right) \prod_{r=1}^N k_{r+2}. \]

**Remark.** If \( N = 1 \) then \( \Pi_q = 1 \) and \( \Pi_{q, p} = 0. \) If \( N = 2 \) then \( \Pi_{q, p} = \alpha_q \beta_p - \alpha_p \beta_q. \)

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

Let \( s_{j,n} = s_j \left( \lambda_n \right) \in \mathbb{C} \quad (j = 1, 2N + 4) \) are the simple zeros of the polynomial \( P; \)

\( s_{2N+5, n}, s_{2N+6, n} \in \mathbb{C} \) are the additional zeros of the polynomial \( Q_q \) due to \( k_{q+2, n} \). Then the originals of the Green’s functions images (9) are [24]:

4
\[ G_{kh} (x, \tau) = \sum_{n=1}^{\infty} G_{1kn}(\tau) \sin \lambda_n x, \quad G_{2k} (x, \tau) = \frac{G_{2kn}(\tau)}{2} + \sum_{n=1}^{\infty} G_{2kn}(\tau) \cos \lambda_n x, \]
\[ G_{q2,k} (x, \tau) = \frac{G_{q2,kn}(\tau)}{2} + \sum_{n=1}^{\infty} G_{q2,kn}(\tau) \cos \lambda_n x; \]

where
\[ G_{1kn}(\tau) = \sum_{j=1}^{2N+1} A_{1kn}^{(j)} \exp(s_{\mu j} \tau) + \delta_{j,q+2} \left[ A_{1kn}^{(2(N+5))} \exp(s_{2N+5,0} \tau) + A_{1kn}^{(2(N+6))} \exp(s_{2N+6,0} \tau) \right] (i, k = 1, N + 2); \]
\[ G_{210} = 2b_2 \delta(\tau), \quad G_{220} = -2k \left[ 1 - \exp\left( -\frac{\tau}{\tau_f} \right) \right], \]
\[ G_{2,q+2,0} = -2\beta_q \left[ 1 - \exp\left( -\frac{\tau}{\tau_q} \right) \right], \quad G_{q+2,q+2,0} = 2 \left[ 1 - \exp\left( -\frac{\tau}{\tau_q} \right) \right]. \]

The coefficients \( A_{1kn}^{(j)} \) are found by the formulas \( k = 1, N + 2 \), the prime denotes the derivative with respect to the parameter \( s \):
\[ A_{1kn}^{(j)} = \frac{P_{1k} (\lambda_n, \nu \mu)}{P'(\lambda_n, \nu \mu)}, \quad A_{2kn}^{(j)} = \frac{P_{2k} (\lambda_n, \nu \mu)}{P'(\lambda_n, \nu \mu)} \quad (j = 1, 2N + 4); \]
\[ A_{q+2,kn}^{(j)} = \frac{Q_{q+2,k} (\lambda_n, \nu \mu)}{Q'(\lambda_n, \nu \mu)} \quad (q = 1, N; \quad j = 1, 2N + 6). \]

Finally, we need to substitute the Green’s functions (12), (13) 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 is aluminum \( (N = 1) \). Its thickness \( L = 10^{-3} m \) and the initial temperature \( T_0 = 600 \text{ K} \). The data on the relaxation times values in available publications vary greatly. Based on the sources [15, 31–33] and taking into account \( t_{\eta}^{(1)} \gg t_f \), for the calculation example we guess \( t_{\eta}^{(1)} = 200 \text{ sec} \) and \( t_f = 0.002 \text{ sec} \). In this case, the following dimensionless quantities obtained with the formulas (4) will correspond to the aluminum layer [15, 31–33]:
\[ M_1 = -3.00 \cdot 10^{-13}, \quad \Lambda_1 = 1.39 \cdot 10^{-17}, \quad D_1 = 1.36 \cdot 10^{-14}, \quad \alpha_1 = 4.64 \cdot 10^{-6}, \quad \tau_f = 1.27 \cdot 10^4, \]
\[ \tau_1 = 1.27 \cdot 10^9, \quad \kappa = 3.63 \cdot 10^9, \quad b_u = 1.37 \cdot 10^{-2}, \quad b_f = 1.01, \quad \beta = -2.78 \cdot 10^{-3}. \]

We set in the boundary conditions (2) that:
- both boundaries of the layer are heat-insulated and rigidly fixed:
\[ f_{11} (\tau) = f_{21} (\tau) = f_{12} (\tau) = f_{22} (\tau) = 0; \quad (14) \]
- 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:
\[ f_{33} (\tau) = 10^{-14} \cdot H (\tau), \quad f_{32} (\tau) = 0. \]
\[ (15) \]
Figure 1. Dependence of displacement $u$ on the layer depth $x$.

Figure 2. Dependence of concentration increment $\eta_1$ on the layer depth $x$.

Figure 3. Dependence of temperature increment $\vartheta$ on the layer depth $x$.

The calculations results of the convolution (5) taking into account (14), (15) and (12) are presented on Figures 1 – 3. They show the spatial and temporal distributions of displacements, temperature increments and concentration increments that demonstrate the relations of the corresponding fields for given surface disturbances.

In the calculation, only one hundred terms of the series were used. A further increase in the terms number does not lead to any significant changes in the obtained results. It should also be noted that for $\tau_r = \tau_l = 0$ the graphs at such time intervals practically do not differ from those presented above and coincide with the results obtained earlier in [24, 26, 28].

Further, we consider that accounting for non-zero relaxation times gives a large contribution to the problem final solution at small time intervals ($\tau \sim \tau_r \sim 10^9$) for intense surface disturbances. To distinctly demonstrate this phenomenon, we will use conditions (14) and multiply the diffusion flux in condition (15) by 100: $f_{31}(\tau) = 10^{-12} \cdot H(\tau)$. Figures 4 – 6 clearly show the difference in the solutions obtained for non-zero ($\tau_r = 1.27 \cdot 10^9$ and $\tau_l = 1.27 \cdot 10^9$ are solid lines) and zero ($\tau_r = 0$ and $\tau_l = 0$ are pointed lines) relaxation times.

When constructing the Figures 1 – 3, only 100 terms of the Fourier series were used. For the Figures 4 – 6, 1000 terms were used. Further number increasing of the terms does not lead to any visible changes on graphs.
5. Conclusion
The algorithm for solving a one-dimensional unsteady thermoelastic diffusion problem for a multicomponent layer is proposed. It can be used to refine and verify the numerical solutions of more complex unsteady thermomechanical diffusion problems. The main advantage of this approach is the ability to analytically find originals of the Green's functions and analyze them. The effectiveness of the method is demonstrated on a concrete calculating example. The necessity of taking into account the finite speeds of thermal and diffusion perturbations propagation in the high-intensity processes simulations is demonstrated.

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