Materials Physics and Mechanics 28 (2016) 72-76 Received: June 25, 2015

NON-STATIONARY MODEL OF MECHANICAL DIFFUSION FOR HALF-SPACE WITH ARBITRARY BOUNDARY CONDITIONS

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Abstract. A new approach to the solution of initial boundary value problems is proposed. It is based on defining integral relations connecting right sides of different types of boundary conditions. It is assumed that one of these solutions has been found. Right sides of boundary conditions of the other problem, being integral equation solutions, are defined through quadrature formulae. Then, solution of this problem assumes as Green's function convolution of the first problem with obtained solutions of integral equations. Non-stationary problem of elastic diffusion for half-space is used as an example.

1. Introduction

Complexity in solving non-stationary problems in continuum mechanics is associated with Laplace transform and further inverse Laplace transform. It depends, among others, on the type of boundary conditions. Under boundary conditions of definite types, it is allowed to use sine and cosine transform of space variable and Laplace time transform. Laplace transforms in this case are rational functions, which considerably simplifies their inverse, transform [1-3]. The disadvantage of this approach is limited area of application conditioned by peculiarities of boundary conditions.

This problem can be solved by determination of relations between boundary conditions of different types. In this case, these relations represent the system of 1-st kind Volterra integral equations. Any solved problem with definite boundary conditions becomes a benchmark and all the other problems will be solved through it. The proposed technique is demonstrated by an example of one-dimensional non-stationary problem of elastic diffusion for half-space.

2. Formulation of boundary value problem of elastic diffusion

Let's assume that we have homogeneous half-space, from the top limited by the surface $x_3 = 0$ (vector and tensor components are specified in Cartesian coordinate system $Ox_1x_2x_3$; Ox_3 axis is directed into half-space). One-dimensional physical and mechanical processes in the medium regardless temperature effects are described bounded elastic diffusion model [1-5]:

$$\rho \frac{\partial^2 u_3}{\partial t^2} = C_{3333} \frac{\partial^2 u_3}{\partial x_3^2} - \alpha_{33} \frac{\partial \eta}{\partial x_3}, \quad \frac{\partial \eta}{\partial t} = D_{33} \frac{\partial^2 \eta}{\partial x_3^2} - \Lambda_{3333} \frac{\partial^3 u_3}{\partial x_3^3};$$

$$\eta\big|_{x_3=0} = f_1^1(t), u_3\big|_{x_3=0} = f_2^1(t), \eta = O(1), u_3 = O(1)\,(x_3 \to \infty); \; u_3\big|_{t=0} = \frac{\partial u_3}{\partial t}\bigg|_{t=0} = \eta\big|_{t=0} = 0,$$

where t - time; u_3 - shift along axis Ox_3; $\eta = n - n_0$ - concentration increment; n_0 and n - initial and current substance concentration; C_{ijkl} - elastic constants' tensor components; ρ - medium density; α_{ij} - coefficients determined by the type of the crystal lattice so that $\alpha_{ij}\varepsilon_{ij}n$ value is the relative volume change demonstrating dependence of substance volume on substance concentration ε_{ij} - tensor deformation components; D_{ij} - self-diffusion coefficients; $\Lambda_{3333} = n_0\alpha_{33}D_{33}(RT_0)^{-1}$; R - universal gas constant; T_0 - initial temperature.

The following dimensionless values will further be used (in case of similar typeface these values are marked with asterisk that is omitted later):

$$x = \frac{x_3}{L}, \quad u = \frac{u_3}{L}, \quad \tau = \frac{ct}{L}, \quad \eta^* = \frac{\eta}{n_0}, \quad c^2 = \frac{C_{3333}}{\rho}, \quad \alpha = \frac{n_0\alpha_{33}}{C_{3333}}, \quad D = \frac{D_{33}}{cL},$$

$$\Lambda = \frac{\Lambda_{3333}}{n_0 cL}, \quad f_1^{1*}(\tau) = \frac{f_1^1(\tau)}{n_0}, \quad f_2^{1*}(\tau) = \frac{f_2^1(\tau)}{L} \quad (k = 1,2).$$

Then, dimensionless analogue of considered problem will have the following form:

$$\ddot{u} = u'' - \alpha\eta', \quad \dot{\eta} = D\eta'' - \Lambda u''' ; \tag{1}$$

$$\eta\big|_{x=0} = f_1^1(\tau), \quad u\big|_{x=0} = f_2^1(\tau), \quad \eta = O(1), \quad u = O(1) \quad (x \to \infty); \tag{2}$$

$$u\big|_{\tau=0} = \dot{u}\big|_{\tau=0} = \eta\big|_{\tau=0} = 0, \tag{3}$$

where a prime means derivative of space variable x, and point means derivative of time τ.

3. Transition to equivalent boundary conditions

To solve (1) - (3) problem let's consider auxiliary (benchmark) problem, determined by equations (1), initial conditions (3) and boundary conditions (second members of the second equations coincide here and in (2)):

$$\left(\Lambda u'' - D\eta'\right)\big|_{x=0} = f_1^2(\tau), \quad u\big|_{x=0} = f_2^2(\tau), \quad \Lambda u'' - D\eta' = O(1), \quad u = O(1) \quad (x \to \infty). \tag{4}$$

Its solution is found in works [1-3] and has the following integral form (asterisk means time convolution):

$$u = \sum_{k=1}^{2} G_{2k} * f_k^2, \quad \eta = \sum_{k=1}^{2} G_{1k} * f_k^2, \tag{5}$$

where $G_{1k} = \eta, G_{2k} = u \ (k = 1,2)$ - are Green's functions of problem (1), (3), (4), i.e. solution of two problems (k - is their number), comprising equations (1), initial conditions (3) and the following boundary conditions:

$$G_{1k}\big|_{x=0} = \delta_{1k}\delta(\tau), \quad G_{2k}\big|_{x=0} = \delta_{2k}\delta(\tau), \quad G_{1k} = O(1), \quad G_{2k} = O(1) \quad (x \to \infty),$$

where $\delta(\tau)$ - Dirac delta function; δ_{ik} - Kronecker symbol, $i = 1,2$.

Assuming that solution of benchmark problem satisfies equations $\eta(0,\tau) = f_1^1(\tau)$ and considering that $f_2^2(\tau) = f_2^1(\tau)$, we come to Volterra equations as convolution kind affecting functions $f_1^2(\tau)$:

$$G_{11}(0,\tau) * f_1^2(\tau) = \varphi(\tau), \ \varphi(\tau) = f_1^1(\tau) - G_{12}(0,\tau) * f_2^1(\tau). \tag{6}$$

We taking into account Green's function symmetry properties defined in [1-3].

The main complexity when solving the system (6) is the fact that functions $G_{11}(0,\tau)$ have singularity if $\tau = 0$. To study singularity features we will do the following. In the Laplace transform set the Green's function $G_{11}(x,\tau)$ is the following [1-3]:

$$G_{1k}^{L}=\frac{2}{\pi}\int_0^\infty G_{1k}^{LF}\cos\lambda x d\lambda,\; G_{11}^{LF}=\frac{s^2+\lambda^2}{P(\lambda,s)},\quad P(\lambda,s)=\left(s^2+\lambda^2\right)\left(s+D\lambda^2\right)-\alpha\Lambda\lambda^4. \tag{7}$$

The following transformation is made in formula (7) for function G_{11}^{LF} :

$$G_{11}^{LF}=\frac{s^2+\lambda^2}{P(\lambda,s)}=\frac{1}{s+D\lambda^2}+\frac{\alpha\Lambda\lambda^4}{Q(\lambda,s)},\quad Q(\lambda,s)=\left(s+D\lambda^2\right)P(\lambda,s).$$

Then function $G_{11}^{L}(x,s)$ has the following form:

$$G_{11}^{L}=\frac{2}{\pi}\int_0^\infty \frac{\cos\lambda x}{s+D\lambda^2}d\lambda+\frac{2\alpha\Lambda}{\pi}\int_0^\infty \frac{\lambda^4\cos\lambda x}{Q(\lambda,s)}d\lambda.$$

Its original has the following form:

$$G_{11}(x,\tau)=\sqrt{\frac{1}{D\pi\tau}}e^{-\frac{x^2}{4D\tau}}+\frac{2\alpha\Lambda}{\pi}\int_0^\infty \tilde{G}_{11}^{F}(\lambda,\tau)\cos\lambda x d\lambda,$$

$$\tilde{G}_{11}^{F}(\lambda,\tau)=e^{\gamma\tau}\left(A_1\cos\beta\tau-A_2\sin\beta\tau\right)+A_3e^{s_3\tau}+A_4e^{-D\lambda^2\tau}.$$

Here s_1, s_2 are complex and s_3 is the real root of polynomial $P(\lambda,s)$, $\gamma=\operatorname{Re}s_1<0$, $\beta=\operatorname{Im}s_1$, $s_2=\bar{s}_1$, $s_3<0$; coefficients A_q $\left(q=\overline{1,4}\right)$ are determined in the following formulae (where the prime means s derivative):

$$A_1=2\operatorname{Re}\frac{\lambda^4}{Q'(\lambda,s_1)},\; A_2=2\operatorname{Im}\frac{\lambda^4}{Q'(\lambda,s_1)},\; A_3=\frac{\lambda^4}{Q'(\lambda,s_3)},\; A_4=\frac{\lambda^4}{Q'\left(\lambda,-D\lambda^2\right)}.$$

Function $G_{11}(0,\tau)$ in the vicinity of $\tau=0$ has integrable singularity of order $(-1/2)$. in this case, following [7], let's multiply equation (6) by $d\tau/(\xi-\tau)^{1/2}$ and integrate from 0 to ξ. As a result, we obtain the following equation:

$$\int_0^\xi K(\xi-t)f_1^2(t)dt=\Phi(\xi), \tag{8}$$

where

$$K(\zeta)=\int_0^\infty\int_0^\zeta \frac{G_{11}(0,\zeta-\tau)}{\tau^{1/2}}d\tau d\lambda=\sqrt{\frac{\pi}{D}}+\frac{2}{\pi}\int_0^\infty A_1\left[e^{-\gamma\zeta}\cos(\beta\zeta)I_1+e^{-\gamma\zeta}\sin(\beta\zeta)I_2\right]d\lambda-$$
$$-\frac{2}{\pi}\int_0^\infty A_2\left[e^{-\gamma\zeta}\sin(\beta\zeta)I_1-e^{-\gamma\zeta}\cos(\beta\zeta)I_2\right]d\lambda+\frac{2}{\pi}\int_0^\infty A_3e^{s_3\zeta}I_3d\lambda+\frac{2}{\pi}\int_0^\infty A_4e^{-D\lambda^2\zeta}I_4d\lambda, \tag{9}$$

$$I_1(\zeta)=\operatorname{Re}\left[\sqrt{\frac{\pi}{-\gamma+i\beta}}\operatorname{erfi}\left(\sqrt{(-\gamma+i\beta)\zeta}\right)\right],\; I_3(\zeta)=\sqrt{\frac{\pi}{-s_3}}\operatorname{erfi}\left(\sqrt{-s_3\zeta}\right),\quad \operatorname{erfi}(\zeta)=\frac{2}{\sqrt{\pi}}\int_0^\zeta e^{z^2}dz,$$

$$I_2(\zeta)=\operatorname{Im}\left[\sqrt{\frac{\pi}{-\gamma+i\beta}}\operatorname{erfi}\left(\sqrt{(-\gamma+i\beta)\zeta}\right)\right],\; I_4(\zeta)=\sqrt{\frac{\pi}{D\lambda^2}}\operatorname{erfi}\left(\sqrt{D\lambda^2\zeta}\right),\quad \Phi(\xi)=\int_0^\xi\frac{\varphi(\tau)d\tau}{(\xi-\tau)^{1/2}},$$

while kernel $K(\zeta)$ doesn't have singularity at zero and $\Phi(0)=0$.

Improper integrals, located in (9), can be determined numerically. For this purpose, let's transform them in the following way:

$$\int_0^\infty f(\lambda,\tau)d\lambda=\int_0^a f(\lambda,\tau)d\lambda+\int_a^\infty f(\lambda,\tau)d\lambda,$$

where a is any intermediate point; $f(\lambda,\tau)$ is any integrand in (9).

The first integral is calculated by means of any quadrature formula (for example, midpoint quadrature formula). The second integral is converted into post gap integral $[0, a]$ by substitution of variables $\lambda = a^2/(a-\nu)$. Then it is also calculated numerically [1, 2]. Since the second integral converges very slowly, a parameter should be rather large. However, taking into account small subinterval on the one hand and arithmetic power of PC on the other hand, it is assumed that $a = 100$.

We use quadrature formulas for solution of (8). Range $[0, T]$ of time variable τ is split into N intervals by dots $\tau_i = ih$ with steady subinterval $h = T/N$ and mesh functions $y_i = f_1^2(\tau_i)$ and $K_i = K(\tau_i)$ are introduced. With $\tau = \tau_i$, each of the integrals in (8) is approximately substituted with the sum corresponding to the midpoint quadrature rule:

$$\int_0^{\tau_i} K(\tau_i - t) f_1^2(t) dt \approx hS_{i-1/2} + hK_{1/2} y_{i-1/2}, \quad S_{i-1/2} = \sum_{j=1}^{i-1} K_{i-j+1/2} y_{j-1/2},$$

where the nodes are defined in the following formulae:

$$\tau_{i-1/2} = \frac{\tau_{i-1} + \tau_i}{2} = h\left(i - \frac{1}{2}\right), \quad \tau_{i-j+1/2} = \tau_i - \tau_{j-1/2} = h\left(i - j + \frac{1}{2}\right), \quad i = \overline{1, N}.$$

As a result, we obtain recurring sequence of linear equations ($i \geq 1$):

$$Ay_{i-1/2} = b_{i-1/2}, \; A = K_{1/2}, \; b_{i-1/2} = \Phi(\tau_{i-1/2})/h - S_{i-1/2}, \; i \geq 1.$$

Its solution has the following form $y_{i-1/2} = b_{i-1/2}(K_{1/2})^{-1}$.

Thus, having found the solution of equation (8) and substituted it in equation (5), we obtain the solution of initial problem (1) - (3).

4. Example

Let's consider (1) - (3) problem, with boundary conditions in the following form:

$$\eta|_{x=0} = f_1^1(\tau) = H(\tau), \quad u|_{x=0} = 0,$$

where $H(\tau)$ is Heaviside function.

The material of half-space is aluminium with the following properties:

C_{3333}=$1.26 \cdot 10^{11}$ H/m^2, T_0=773 K, $\rho = 2700$ kg/m^3, D_{33}= $7.73 \cdot 10^{-14}$ m^2/s, L =1 m .

The results of numerical calculation of equation (8) at the number of points of division $N_x = 1000$ by variable x and $N_t = 100$ by time τ are shown on Fig. 1.

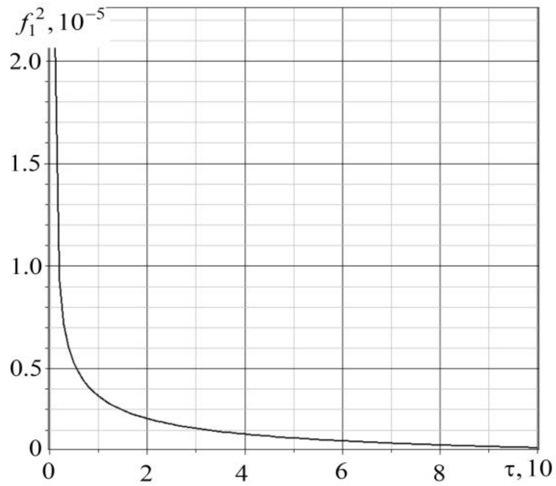

Fig. 1. Quantitative solution for $f_1^2(\tau)$.

Midpoint quadrature formula is also used for convolutions in (5). The results of calculations for displacement and concentration increment in different points of the layer are shown on Figs. 2 and 3.

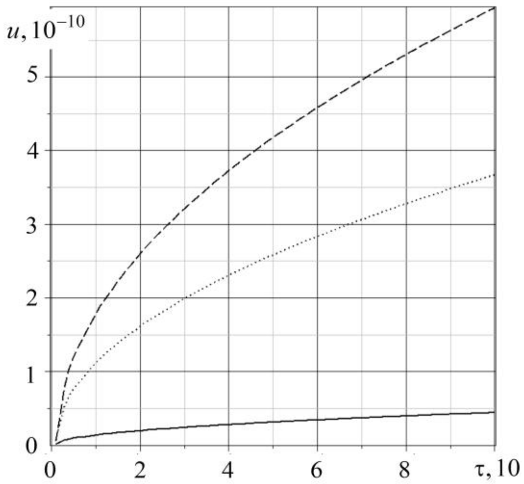

Fig. 2. Dependence of displacement on time: $x = 0.05$ is solid line, $x = 0.5$ is dotted line, $x = 1$ is dashed line.

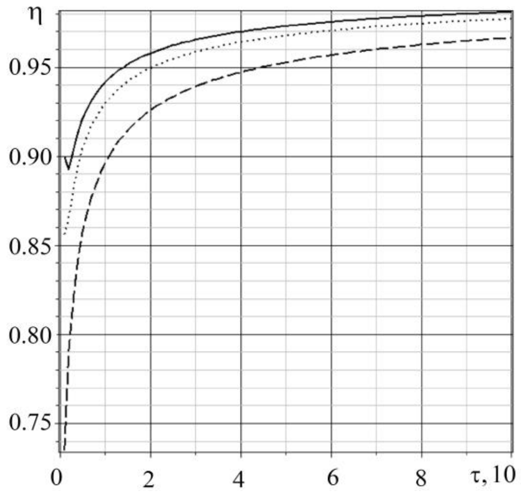

Fig. 3. Dependence of concentration increment on time: $x = 10^{-6}$ is solid line, $x = 10^{-5}$ is dotted line, $x = 2 \cdot 10^{-5}$ is dashed line.

It should be noted that in case of halving of subintervals diagrams almost have no differences.

Acknowledgement

Financial support for this work has been provided by Russian Foundation for Basic Research (project 14-08-01161).

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