

SOLUTION OF DUAL PHASE LAG EQUATION BY MEANS OF THE BOUNDARY ELEMENT METHOD USING DISCRETIZATION IN TIME

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Abstract. The dual phase lag equation describing the temperature field in a 3D domain is considered. This equation supplemented by boundary and initial conditions is solved by means of the boundary element method using discretization in time, while at the same time the Dirichlet and Neumann boundary conditions are taken into account. Numerical realization of the BEM for the constant boundary elements and constant internal cells is presented. The example of computations concerns the temperature field distribution in a heated domain. The conclusions connected with the proper choice of time step and discretization of the domain considered are formulated.

Introduction

The dual phase lag equation describes a number of thermal problems, among others the heat transfer in microscale [1, 2] or thermal phenomena occurring in living organisms subjected to strong external heat sources [3, 4]. So far, this equation supplemented by boundary and initial conditions solved mainly by using the finite difference method [5-7].

In the paper the algorithm based on the boundary element method using discretization in time is proposed. At the first stage the derivatives with respect to time are replaced by the differential quotients and next to the obtained in this way equation a weighted residual criterion is applied. In this criterion, the weight function, called a fundamental solution, is known which allows one to derive boundary integral equation. To solve this equation the numerical algorithm for constant boundary elements and constant internal cells is presented.

An example of computations concerns the temperature field distribution in heated cube the dimensions of which are expressed in nanometers. The influence of the time step and the number of boundary elements on the results of the calculations is discussed. In the final part of the paper the conclusions are formulated.

1. Formulation of the problem

The dual-phase-lag equation has the following form

$$c \left[\frac{\partial T(x,t)}{\partial t} + \tau_q \frac{\partial^2 T(x,t)}{\partial t^2} \right] = \lambda \nabla^2 T(x,t) + \lambda \tau_T \frac{\partial \nabla^2 T(x,t)}{\partial t} + Q(x,t) + \tau_q \frac{\partial Q(x,t)}{\partial t} \quad (1)$$

where c is the volumetric specific heat, λ is the thermal conductivity, τ_q is the relaxation time, τ_T is the thermalization time, $Q(x,t)$ is the source term, T is the temperature, x are the spatial co-ordinates and t is the time.

This equation is supplemented by the boundary conditions

$$\begin{aligned} x \in \Gamma_1: \quad T(x,t) &= T_b(x,t) \\ x \in \Gamma_2: \quad q(x,t) &= q_b(x,t) \end{aligned} \quad (2)$$

and initial ones

$$t=0: \quad T(x,t) = T_p, \quad \left. \frac{\partial T(x,t)}{\partial t} \right|_{t=0} = 0 \quad (3)$$

where $T_b(x,t)$ is the known boundary temperature, $q_b(x,t)$ is the known boundary heat flux and T_p is the initial temperature.

It should be pointed out that using the dual phase lag model the following form of second type boundary condition should be considered

$$(x,y) \in \Gamma_2: \quad q_b(x,t) + \tau_q \frac{\partial q_b(x,t)}{\partial t} = -\lambda \left[\frac{\partial T(x,t)}{\partial n} + \tau_T \frac{\partial}{\partial t} \left(\frac{\partial T(x,t)}{\partial n} \right) \right] \quad (4)$$

where n is the normal outward vector and $\partial(\cdot)/\partial n$ is the normal derivative.

2. Boundary element method using discretization in time

Let $T^f = T(x, f \Delta t)$, where Δt is the time step. Then, for time $t^f = f \Delta t$ ($f \geq 2$) the following approximate form of equation (1) resulting from the introduction of adequate differential quotients can be proposed

$$\begin{aligned} c \left(\frac{T^f - T^{f-1}}{\Delta t} + \tau_q \frac{T^f - 2T^{f-1} + T^{f-2}}{(\Delta t)^2} \right) &= \\ = \lambda \nabla^2 T^f + \frac{\lambda \tau_T}{\Delta t} (\nabla^2 T^f - \nabla^2 T^{f-1}) + Q + \tau_q \frac{\partial Q}{\partial t} \end{aligned} \quad (5)$$

or

$$\nabla^2 T^f - BT^f + C\nabla^2 T^{f-1} + DT^{f-1} + ET^{f-2} + F = 0 \quad (6)$$

where

$$B = \frac{c(\Delta t + \tau_q)}{\lambda \Delta t (\Delta t + \tau_T)}, \quad C = -\frac{\tau_T}{\Delta t + \tau_T}, \quad D = \frac{c(\Delta t + 2\tau_q)}{\lambda \Delta t (\Delta t + \tau_T)} \quad (7)$$

$$E = -\frac{c \tau_q}{\lambda \Delta t (\Delta t + \tau_T)}, \quad F = \frac{\Delta t (Q + \tau_q \partial Q / \partial t)}{\lambda (\Delta t + \tau_T)}$$

Using the weighted residual method criterion (WRM) [8] one obtains

$$\int_{\Omega} \left(\nabla^2 T^f - BT^f + C\nabla^2 T^{f-1} + DT^{f-1} + ET^{f-2} + F \right) T^*(\xi, x) d\Omega = 0 \quad (8)$$

where $T^*(\xi, x)$ is the fundamental solution and for the 3D objects oriented in a rectangular co-ordinate system it is a function of the form

$$T^*(\xi, x) = \frac{1}{4 \pi r} \exp(-r \sqrt{B}) \quad (9)$$

where r is the distance between source point ξ and field point x .

One can check that the fundamental solution fulfills the equation

$$\nabla^2 T^*(\xi, x) - BT^*(\xi, x) = -\delta(\xi, x) \quad (10)$$

where $\delta(\xi, x)$ is the Dirac function.

On the basis of formula (9) the heat flux resulting from fundamental solution $q^*(\xi, x) = -\lambda \partial T^*(\xi, x) / \partial n$ can be calculated in analytical way, namely

$$q^*(\xi, x) = \frac{\lambda d}{4 \pi r^2} \exp(-r \sqrt{B}) \left(\frac{1}{r} + \sqrt{B} \right) \quad (11)$$

where

$$d = \sum_{e=1}^3 (x_e - \xi_e) \cos \alpha_e \quad (12)$$

while $\cos \alpha_e$ are the directional cosines of the normal boundary vector.

Applying the second Green formula to the first component of criterion (8) and taking into account the fundamental solution property (10) one obtains the following integral equation

$$\begin{aligned}
& B(\xi)T(\xi, t^f) + \frac{1}{\lambda} \int_{\Gamma} T^*(\xi, x) Z^f d\Gamma = \\
& = -\frac{1}{\lambda} \int_{\Gamma} q^*(\xi, x) T^f d\Gamma + \int_{\Omega} (C \nabla^2 T^{f-1} + DT^{f-1} + ET^{f-2} + F) T^*(\xi, x) d\Omega
\end{aligned} \tag{13}$$

where $Z^f = -\lambda \partial T^f / \partial n$ and $B(\xi) \in (0, 1]$ is the coefficient dependent on the location of point ξ .

It should be pointed out that the boundary condition (4) can be approximated as follows

$$q_b^f + \tau_q \left. \frac{\partial q_b}{\partial t} \right|_{t=t^f} = -\lambda \left[\frac{\partial T^f}{\partial n} + \frac{\tau_T}{\Delta t} \left(\frac{\partial T^f}{\partial n} - \frac{\partial T^{f-1}}{\partial n} \right) \right] \tag{14}$$

or

$$Z^f = -\lambda \frac{\partial T^f}{\partial n} = -\frac{\lambda \tau_T}{\Delta t + \tau_T} \frac{\partial T^{f-1}}{\partial n} + \frac{\Delta t}{\Delta t + \tau_T} \left(q_b^f + \tau_q \left. \frac{\partial q_b}{\partial t} \right|_{t=t^f} \right) \tag{15}$$

In numerical realization of the BEM the boundary Γ is divided into N boundary elements, while the interior Ω is divided into L internal cells. For the constant boundary elements and constant internal cells the following approximation of equation (13) appears

$$\sum_{j=1}^N G_{ij} Z_j^f = \sum_{j=1}^N H_{ij} T_j^f + \sum_{l=1}^L P_{il} (C \nabla^2 T_l^{f-1} + DT_l^{f-1} + ET_l^{f-2} + F) \tag{16}$$

where

$$G_{ij} = \frac{1}{\lambda} \int_{\Gamma_j} T^*(\xi_i, x) d\Gamma_j \tag{17}$$

and

$$H_{ij} = \begin{cases} \int_{\Gamma_j} q^*(\xi_i, x) d\Gamma_j, & i \neq j \\ -0.5, & i = j \end{cases} \tag{18}$$

while

$$P_{il} = \int_{\Omega_l} T^*(\xi_i, x) d\Omega_l \tag{19}$$

Introducing the boundary conditions (2) (cf. formula (15)) into the linear algebraic equations (16) one obtains the equations for the unknown Z^f on the boundary Γ_1

and unknown T^f on the boundary Γ_2 . After solving the system of equations (16), the temperatures T^f at the internal points ξ_i are calculated using the formula

$$T_i^f = \sum_{j=1}^N H_{ij} T_j^f - \sum_{j=1}^N G_{ij} Z_j^f + \sum_{l=1}^L P_{il} (C \nabla^2 T_l^{f-1} + D T_l^{f-1} + E T_l^{f-2} + F) \quad (20)$$

3. Results of computations

The micro-domain (cube) of dimensions $50 \text{ nm} \times 50 \text{ nm} \times 50 \text{ nm}$ made of gold is considered. On the upper surface the Dirichlet condition $T_b = 500 \text{ K}$ is assumed, on the remaining surfaces the Neumann condition $q_b = 0$ is accepted. Initial temperature is equal to $T_p = 300 \text{ K}$. The following input data are introduced: thermal conductivity $\lambda = 315 \text{ W/(mK)}$, volumetric specific heat $c = 2.5 \text{ MJ/(m}^3\text{K)}$, relaxation time $\tau_q = 8.5 \text{ ps}$, thermalization time $\tau_T = 90 \text{ ps}$, source function $Q = 0$.

The boundary is divided into N constant boundary elements (squares) and L constant internal cells (cubes). It is assumed that $h = l/n$, where l is the length of the side of the cube, n is the natural number and then $N = 6n^2$, $L = n^3$. The fragment of Delphi code in which the boundary and internal nodes coordinates are defined is presented in [9].

In Figure 1 the heating curve at the central point of cube for a different number of boundary elements and internal cells ($n = 10$, $n = 15$, $n = 20$) under the assumption that time step is equal to $\Delta t = 0.2 \text{ ps}$ is presented. As it can be seen, for $n = 10$ (600 boundary elements and 1000 internal cells) the results are not satisfactory, while for $n = 15$ and $n = 20$ the temperatures are almost the same.

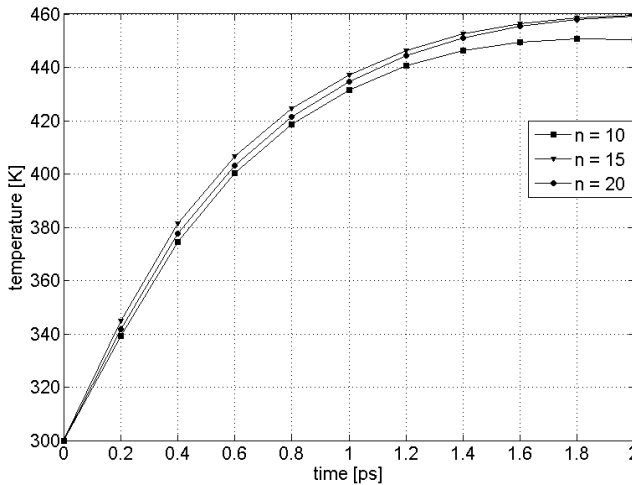


Fig. 1. Heating curve at the central point for different mesh density

An important problem is the proper choice of the time step. Figure 2 shows that when the time step is too small (here $\Delta t = 0.1$ ps), even for a dense mesh the results are incorrect.

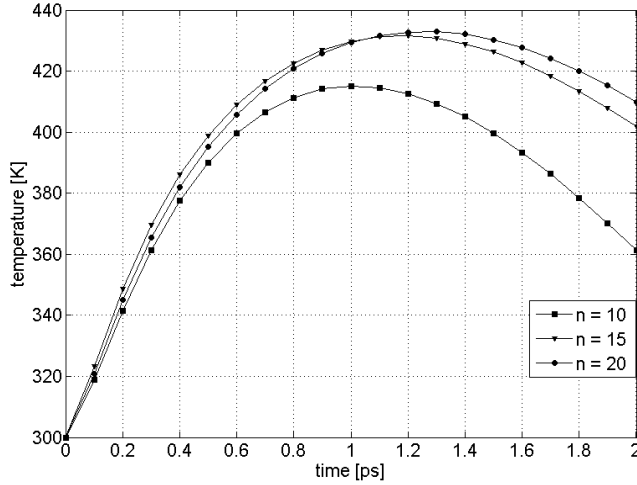


Fig. 2. Heating curve at the central point for different mesh density and to small of a time step

It should be pointed out that for the assumed boundary and initial conditions in reality heat transfer takes place only in the z -direction (1D problem). In Figure 3 the temperature profiles along the axis z for correctly chosen values of n and Δt , this means $n = 20$ and $\Delta t = 0.2$ ps, respectively, are shown.

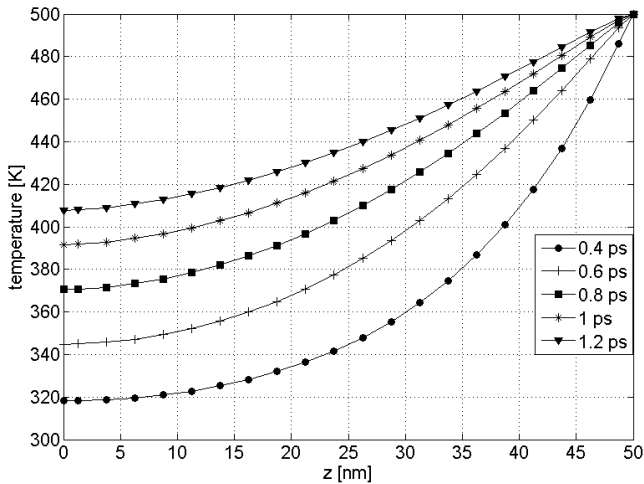


Fig. 3. Temperature profiles ($n = 20$, $\Delta t = 0.2$ ps)

Conclusions

To solve a dual phase lag equation, the boundary element method using discretization in time is proposed. The calculations show that this method gives good results under the assumption that the time step and the number of internal and boundary elements are well chosen.

Since the application of a very large number of boundary elements and internal cells significantly increases the computation time to solve the dual phase lag equation, the other variants of the boundary element method should therefore also be developed, for example, the general boundary element method [10].

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