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SHAPE SENSITIVITY AND OPTIMIZATION FOR TRANSIENT HEAT DIFFUSION PROBLEMS USING THE BEM

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ABSTRACT

A shape design sensitivity analysis (SDSA) of two-dimensional transient heat diffusion problems is proposed based on the BIE formulation. The adjoint variable method is used by using the Ionescu–Cazimir integral identity. The procedure is checked against the analytical solution in the case of a rod example, and by numerical comparisons with the finite differencing for a rectangular block under thermal shock and a plunger model. An optimal design problem is then formulated for the plunger and solved to obtain a realistic shape.

KEY WORDS Shape design sensitivity analysis Boundary integral equations Transient thermal problems

INTRODUCTION

The boundary element method (BEM) has been an attractive technique in many shape design sensitivity analyses (SDSAs) due to the accuracy on the boundary and the reduced number of unknowns. Choi and Kwak[1–3] have developed a general procedure for obtaining a shape sensitivity expression with the material derivative concept and adjoint variable method using the boundary integral equation formulation and applied it to two-dimensional potential and elasticity problems. The direct differentiation approach was proposed by Barone and Yang[4,5] for two- and three-dimensional elasticity problems. Choi and Choi[6] also presented the direct differentiation method for SDSA, in which they utilized the derivative of a boundary integral identity (BII) derived previously for the adjoint variable, and Choi and Kwak[7] proposed a unified approach for adjoint and direct method of SDSA.

Although considerable attention is focused on design sensitivity analysis in the fields of solids and structural mechanics, relatively little work is done on thermal problems. Haftka[8] proposed a design sensitivity analysis technique applicable to discretized system equations in finite elements for a steady state and a transient thermal problem. Park and Yoo[9] used a variational formulation to study SDSA for a steady state conduction problem using an adjoint system and equivalent BIE. Dems[10] derived first- and second-order sensitivities for a transient thermal problem using the adjoint load method and the direct differentiation. Meric[11] derived shape sensitivity formulae of thermoelastic problem using the adjoint approach based on the Lagrange multiplier. He used BEM as an analysis tool. Extending the method of Dems and Meric and using a mixed mutual energy functional, Tortorelli and Harber[12,13] presented a design sensitivity formula for transient heat conduction problems. They used FEM to perform the sensitivity calculation of an example, but no optimization was tried.

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Saigal and Chandra[14] developed a BEM formulation to determine design sensitivities for a steady state thermal problem through an implicit differentiation of discretized boundary integral equation. Kane *et al.*[15] employed a similar implicit differentiation and the particular integral technique to derive a pure boundary sensitivity formula that includes the rates of change of either steady or transient thermal response, and Kane and Wang[16] presented the shape design sensitivity formulation for nonlinear thermal problem using the implicit differentiation method. Recently Lee and Kwak[17,18] have extended the adjoint variable method of Choi and Kwak to two-dimensional and axisymmetric thermoelasticity problems and dealt with some numerical examples. Transient thermal problems are not yet studied in the frame of the boundary integral equation formulation.

In this paper, a SDSA formulation of transient thermal problems is developed using the material derivative concept and the adjoint variable method. An integral identity which represents a reciprocity of two arbitrary thermal systems is used to compose the adjoint systems. A general performance functional of domain and boundary integrals defined over a fixed time interval is considered for SDSA. A rod problem with analytic expressions is introduced to show the procedure of SDSA. Several numerical sensitivities calculated by the present method are compared with those by finite difference approach. The SDSA capability is then linked to a numerical optimization algorithm to find the optimum shape of a simplified plunger used in the glass forming of a TV bulb panel.

BOUNDARY INTEGRAL EQUATIONS

Consider a two-dimensional transient thermal problem for an isotropic and homogeneous solid body Ω of an arbitrary shape with a sufficiently smooth boundary Γ shown in *Figure 1*. The governing differential equations of the transient heat diffusion problem are written as:

$$q_i = -kT_{,i}$$

$$-q_{i,i} + Q = \rho C_\varepsilon \frac{\partial T}{\partial t} \tag{1}$$

where T is the temperature, q_i the ith component of the heat flux vector, t the time, Q the heat source intensity and k, ρ and C_ε denote the conductivity, the mass density and the specific heat at constant deformation, respectively. In this paper, the Einstein summation convention is used with the indices ranging from 1 to 2. The boundary conditions on the boundary $\Gamma = \Gamma_T + \Gamma_q + \Gamma_c$

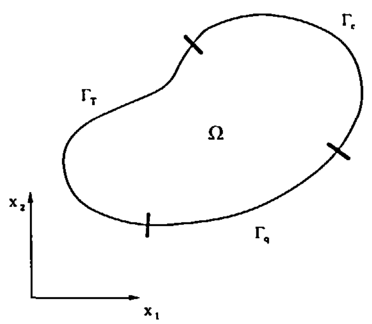

Figure 1 Two-dimensional diffusion problem

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are given as:

$$T(x,t) = \bar{T}(x,t) \qquad x \in \Gamma_T$$
$$q(x,t) \equiv -k\frac{\partial T}{\partial n} = \bar{q}(x,t) \qquad x \in \Gamma_q$$
$$q(x,t) = h(x,t)[T(x,t) - T_\infty(x,t)] \qquad x \in \Gamma_c \tag{2}$$

where n denotes the outward normal and q the normal heat flux. For the boundary conditions, temperature $\bar{T}(x,t)$ is prescribed on Γ_T, normal heat flux $\bar{q}(x,t)$ on Γ_q, and heat transfer coefficient $h(x,t)$ and surrounding temperature T_∞ on Γ_c. Since (1) is time-dependent, the initial conditions at $t = t_0$ must be prescribed as:

$$T(x,t_0) = T_0(x) \qquad x \in \Omega \tag{3}$$

where T_0 is a known initial temperature.

Using the weighted residual method with the time dependent fundamental solution, the parabolic differential (1) together with (2) and (3) can be transformed into an integral equation formulation as follows[19,20]:

$$c(x_0)T(x_0,t_F) - \frac{\kappa}{k}\int_{t_0}^{t_F}\int_\Gamma T(x,t)\omega^*(x_0,x;t_F,t)\,d\Gamma(x)\,dt = -\frac{\kappa}{k}\int_{t_0}^{t_F}\int_\Gamma q(x,t)\theta^*(x_0,x;t_F,t)\,d\Gamma\,dt$$
$$+\int_\Omega \theta^*(x_0,x;t_F,t_0)T_0(x,t_0)\,d\Omega \qquad x_0 \in \Gamma \tag{4}$$

where $c(x_0)$ is the geometry-dependent quantity and $\kappa = k/\rho C_\varepsilon$, θ^* and ω^* are the diffusivity and the fundamental solutions, respectively. Here the fundamental solution θ^* and ω^* are of the form[19,20]:

$$\theta^* = \frac{1}{[4\pi\kappa(t_F - t)]^{d/2}}\exp\left[-\frac{r^2}{4\kappa(t_F - t)}\right]\nu(t_F - t) \qquad t \in [0, t_F]$$
$$\omega^* = -k\frac{\partial \theta^*}{\partial n} \tag{5}$$

where d is the dimensionality, $r = |x - x_0|$ is the Euclidian distance between the source point x_0 and the field point x and $\nu(x)$ is the unit step function, i.e. $\nu(x) = 0$ for $x < 0$ and $\nu(x) = 1$ for $x \geqslant 0$. Here the initial time is set to zero for brevity. Now an integral representation for the solutions of the heat diffusion equations is obtained. Discretizing (4) with a time integration process and applying the boundary conditions and the initial conditions, the histories of the state variables of the problems can be obtained[19,20].

While (4) is the direct BIE, one can obtain another integral equation by considering relations of arbitrary two thermal systems. An appropriate relation can be found in Ionescu-Cazimir's reciprocal theorem[21,22], which correlates two independent coupled thermoelastic states in terms of displacement, traction, temperature, heat flux, mechanical body force and heat source. Ignoring the coupled terms, the reciprocal theorem with zero initial conditions can be rewritten as:

$$\int_\Gamma [q \otimes T^* - T \otimes q^*]\,d\Gamma = \int_\Omega [Q \otimes T^* - T \otimes Q^*]\,d\Omega \tag{6}$$

where $[T, q, Q]$ and $[T^*, q^*, Q^*]$ are the states of any two independent thermal systems. The

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symbol $\otimes$ indicates a Riemann convolution integral where, for example,

$$
\begin{aligned}
q \otimes T^* &= \int_0^{t_F} q(x, t_F - t) T^*(x, t)\, \mathrm{d}t \\
&= \int_0^{t_F} q(x, t) T^*(x, t_F - t)\, \mathrm{d}t
\end{aligned} \tag{7}
$$

The integral identity (6) holds for any two systems which satisfy the governing equations. This integral identity will be utilized in the shape design sensitivity analysis of the transient thermal system.

SHAPE DESIGN SENSITIVITY ANALYSIS

Consider a general performance functional of the following form:

$$
\Phi = \int_0^{t_F} \int_\Omega \xi(T(x,t), q_i(x,t))\, \mathrm{d}\Omega\, \mathrm{d}t + \int_0^{t_F} \int_\Gamma \zeta(T(x,t), q(x,t))\, \mathrm{d}\Gamma\, \mathrm{d}t \tag{8}
$$

Using the material derivative concept[1], the variation of T is expressed as:

$$
\dot{T} = T' + T_{,j} V_j \tag{9}
$$

where the superscript $'$ means the partial derivative with respect to design and V means the design velocity as used in Reference 23. Decomposing the design velocity field on the boundary into the normal and tangential components, some relations are obtained as[2,17]:

$$
V_i = V_n n_i + V_s s_i \tag{10}
$$

$$
V_{k,k} - V_{i,j} n_i n_j = V_n H + V_{s,s} \tag{11}
$$

where n_i and s_i are the unit normal and tangential vector component of the boundary, respectively and H is the curvature of the boundary. Here, subscript s after a comma means differentiation in the tangential direction on the boundary. Taking the material derivative to the functional, Φ, with the design velocity V,

$$
\begin{aligned}
\Phi' &= \int_0^{t_F} \int_\Omega (\dot{\xi} + \xi V_{k,k})\, \mathrm{d}\Omega\, \mathrm{d}t + \int_0^{t_F} \int_\Gamma \{\dot{\zeta} + \zeta(V_{k,k} - V_{i,j} n_i n_j)\}\, \mathrm{d}\Gamma\, \mathrm{d}t \\
&= \int_0^{t_F} \int_\Omega \xi'\, \mathrm{d}\Omega\, \mathrm{d}t + \int_0^{t_F} \int_\Gamma \{\dot{\zeta} + \xi V_n + \zeta(V_{k,k} - V_{i,j} n_i n_j)\}\, \mathrm{d}\Gamma\, \mathrm{d}t
\end{aligned} \tag{12}
$$

Note that the time is independent of the design changes. Expanding $\dot{\xi}$ and $\dot{\zeta}$ with their arguments and using the integration by parts, (12) can be rewritten as:

$$
\begin{aligned}
\Phi' = &\int_0^{t_F} \int_\Omega \left[\frac{\partial \xi}{\partial T} + k\left(\frac{\partial \xi}{\partial q_i}\right)_{,i} \right] \dot{T}\, \mathrm{d}\Omega\, \mathrm{d}t + \int_0^{t_F} \int_\Gamma \left[\left(\frac{\partial \zeta}{\partial T} - k \frac{\partial \xi}{\partial q_i} n_i \right) \dot{T} + \frac{\partial \zeta}{\partial q} \dot{q} \right] \mathrm{d}\Gamma\, \mathrm{d}t \\
&- \int_0^{t_F} \int_\Omega \left[\frac{\partial \xi}{\partial T} T_{,j} V_j + \frac{\partial \xi}{\partial q_i} q_i(T_{,j} V_j) \right] \mathrm{d}\Omega\, \mathrm{d}t + \int_0^{t_F} \int_\Gamma [(\xi + \zeta H) V_n + \zeta V_{s,s}]\, \mathrm{d}\Gamma\, \mathrm{d}t
\end{aligned} \tag{13}
$$

The purpose of sensitivity analysis is to explicitly express $\dot{T}$ and $\dot{q}$ in terms of design velocity, V, or shape variation. To this end adjoint systems are introduced in conjunction with (6). Before taking the material derivative of (6), some formulae are introduced as follows:

$$
\dot{n}_i = (V_s H - V_{n,s}) s_i \tag{14}
$$

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$$\dot{q}^* \equiv \dot{q}^*(T^*) = q^*(T^{*\prime}) - kT^*_{,nn}V_n + q^*_{,s}(T^*)V_s + kT^*_{,s}V_{n,s} \tag{15}$$

$$kT^*_{,nn} + k(T^*_{,s})_{,s} + k\frac{\partial T^*}{\partial n}H = k\nabla^2 T^* = \rho C_\varepsilon \frac{\partial T^*}{\partial t} - Q^* \tag{16}$$

$$T^*_{,j}V_j = -\frac{q^*}{k}V_n + T^*_{,s}V_s \tag{17}$$

$$\sum\langle\{T\otimes q^*\}V_s + T\otimes(kT^*_{,s})V_n\rangle = 0 \tag{18}$$

where $\langle . \rangle$ denotes a jump term, which appears from the integration by parts through a discontinuous point[6]. Since the state $(T^{*\prime}, q^*(T^{*\prime}), Q^{*\prime})$, with partial derivatives also satisfies the governing differential equations, the integral identity of (6) is applicable as follows:

$$\int_\Gamma [q\otimes T^{*\prime} - T\otimes q^*(T^{*\prime})]\,\mathrm{d}\Gamma = \int_\Omega [Q\otimes T^{*\prime} - T\otimes Q^{*\prime}]\,\mathrm{d}\Omega \tag{19}$$

Using (14)–(19) and some simplifications, one can obtain the variation of the integral identity as follows:

$$\begin{aligned} &-\int_\Omega \dot{T}\otimes Q^*\,\mathrm{d}\Omega + \int_\Gamma [\dot{T}\otimes q^* - \dot{q}\otimes T^*]\,\mathrm{d}\Gamma \\ &= -\int_\Omega (T_{,j}V_j)\otimes Q^*\,\mathrm{d}\Omega + \int_\Gamma [T_{,s}\otimes q^* - q_{,s}\otimes T^*]V_s\,\mathrm{d}\Gamma \\ &+ \int_\Gamma \left[T\otimes\left(\rho C_\varepsilon \frac{\partial T^*}{\partial t}\right) - Q\otimes T^* + T_{,s}\otimes(kT^*_{,s}) + q\otimes T^*H - \frac{1}{k}q\otimes q^*\right]V_n\,\mathrm{d}\Gamma \\ &+ \sum\langle\{q\otimes T^*\}V_s\rangle \end{aligned} \tag{20}$$

Comparing (20) with (13) for eliminating $\dot{T}$ and $\dot{q}$, we can introduce an adjoint system as:

$$k\nabla^2 T^* + Q^* = \rho C_\varepsilon \frac{\partial T^*}{\partial t} \qquad x\in\Omega \tag{21}$$

$$Q^*(x,t) = -\left\{\frac{\partial\xi(x,t_F - t)}{\partial T} + k\left(\frac{\partial\xi(x,t_F - t)}{\partial q_i}\right)_{,i}\right\} \qquad x\in\Omega \tag{22}$$

$$T^*(x,t) = -\frac{\partial\zeta(x,t_F - t)}{\partial q} \qquad x\in\Gamma_T \tag{23}$$

$$q^*(x,t) = \left\{\frac{\partial\zeta(x,t_F - t)}{\partial T} - k\frac{\partial\xi(x,t_F - t)}{\partial q_i}n_i\right\} \qquad x\in\Gamma_q \tag{24}$$

$$q^*(x,t) = h(x,t_F - t)\left[T^*(x,t) + \frac{\partial\zeta(x,t_F - t)}{\partial q}\right] + \left\{\frac{\partial\zeta(x,t_F - t)}{\partial T} - k\frac{\partial\xi(x,t_F - t)}{\partial q_i}n_i\right\} \qquad x\in\Gamma_c \tag{25}$$

where $t\in[0, t_F]$. Substituting (2) and (22)–(25) into (20) and (13), respectively, the desired sensitivity

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formula in terms of V can be obtained as follows:

$$\Phi' = -\int_\Omega (T_{,j}V_j)\otimes Q^*\,\mathrm{d}\Omega - \int_0^{t_F}\int_\Omega \left[\frac{\partial\xi}{\partial T}T_{,j}V_j + \frac{\partial\xi}{\partial q_i}q_i(T_{,j}V_j)\right]\mathrm{d}\Omega\,\mathrm{d}t$$
$$+\int_0^{t_F}\int_\Gamma [(\xi+\zeta H)V_n + \zeta V_{s,s}]\,\mathrm{d}\Gamma\,\mathrm{d}t + \int_\Gamma [T_{,s}\otimes q^* - q_{,s}\otimes T^*]V_s\,\mathrm{d}\Gamma$$
$$+\int_\Gamma\left[T\otimes\left(\rho C_\varepsilon\frac{\partial T^*}{\partial t}\right) - Q\otimes T^* + T_{,s}\otimes(kT^*_{,s}) + q\otimes T^*H - \frac{1}{k}q\otimes q^*\right]V_n\,\mathrm{d}\Gamma$$
$$+\sum\langle\{q\otimes T^*\}V_s\rangle \tag{26}$$

In this expression, the time histories of primary and adjoint variables being obtained, Φ' can be evaluated easily by standard Guassian quadrature. Note that the adjoint systems introduced have the same governing equations as the primal system. Hence we need not calculate the system matrices of the adjoint system. However, it is evident from (22)–(25) that the primal and adjoint systems cannot be solved simultaneously because the primal variables must be known for the boundary conditions and the source intensity of the adjoint systems from the final time in reverse order.

As an analytical example, consider a rod of length l with the initial temperature of 0°C. The temperature at one end, $x = 0$ is suddenly changed to $T = T_1$ while at the other end $x = l$ is kept zero. The transient heat conduction without heat loss from its surface is considered with the following temperature functional,

$$\Phi = T(x_0, t_0) = \int_0^{t_F}\int_0^l T(x,t)\delta(x-x_0)\delta(t-t_0)\,\mathrm{d}x\,\mathrm{d}t \tag{27}$$

where $0 < x_0 < l$, $0 < t_0 < t_F$. The point x_0 is moving to $x_{0\tau} = x_0 + \tau V(x)$ where τ is a time-like parameter[1] and t_0 fixed. Considering rod length l as a design variable, $V(0) = 0$ and $V(l) = \delta l$. In the domain, it is possible to select $V(x) = x\delta l/l\,(0 \leqslant x \leqslant l)$; that is, points on the rod move to the right proportionally. The analytic solution of the temperature is[24]:

$$T(x,t) = T_1\left[1 - \frac{x}{l} - \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin\frac{n\pi x}{l}\mathrm{e}^{-\kappa n^2\pi^2 t/l^2}\right] \tag{28}$$

If the design sensitivity of the temperature point $x_0 = l/2$ is desired, since x_0 moves to $x_{0\tau} = x_0 + \tau V(x) = (l + \tau\delta l)/2$, from (27) and (28):

$$\Phi(\tau) = T_1\left[1 - \frac{(l+\tau\delta l)}{2l} - \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin\frac{n\pi(l+\tau\delta l)}{2l}\mathrm{e}^{-\kappa n^2\pi^2 t/l^2}\right] \tag{29}$$

Taking the variation of the temperature functional of (29) with respect to τ and evaluating the result at $\tau = 0$:

$$\Phi' \equiv \left.\frac{\mathrm{d}\Phi}{\mathrm{d}\tau}\right|_{\tau=0} = -\frac{T_1\mathrm{d}l}{2l}\left[1 + 2\sum_{n=1}^{\infty}\frac{1}{n}\cos\frac{n\pi}{2}\mathrm{e}^{-\kappa n^2\pi^2 t_0/l^2}\right] \tag{30}$$

If the present method is used, taking the material derivative of (27):

$$\Phi' = \int_0^{t_F}\int_0^l \dot{T}(x,t)\delta(x-x_0)\delta(t-t_0)\,\mathrm{d}x\,\mathrm{d}t \tag{31}$$

Consider the following adjoint system:

$$Q^*(x,t) = -\delta(x-x_0)\delta(t-(t_F-t_0))$$
$$T^*(x,t) = 0, \qquad x = 0, l \tag{32}$$

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Substituting (32) into (6) and taking the material derivative of the resulting equation, one obtains:

$$\int_0^l \dot{T} \otimes Q^* \,\mathrm{d}x = \int_0^l \frac{\mathrm{d}T}{\mathrm{d}x} V(x) \otimes Q^* \,\mathrm{d}x \tag{33}$$

Comparing (33) and (31), one can finally obtain the sensitivity formula as:

$$\Phi' = -\int_0^l \frac{\mathrm{d}T}{\mathrm{d}x} V(x) \otimes Q^* \,\mathrm{d}x \tag{34}$$

Substituting (32) and the design velocity expression into (34), one can obtain the sensitivity of Φ, the same as the exact expression (30).

NUMERICAL EXAMPLES AND DISCUSSIONS

For illustrating the validity of the shape design sensitivity formulations, two numerical examples are taken. The first example is a rectangular block under a thermal shock at time zero and another one is a plunger being used in forming a TV bulb. To obtain the solutions of the primal and the adjoint systems appearing in the sensitivity expression using the BEM, the discretization of (4) is necessary along both the boundary and time with some interpolation functions. Using a time marching scheme and itegrating the discretized equation with special consideration on the evaluation of the singular integral, one obtain finally the system of linear algebraic equations which can be solved easily, for example, by the Gaussian elimination. In this study the equations are approximated by using constant values for each time step and linear interpolations in space. A restarting time marching scheme[19] is adopted to take advantage of avoiding domain discretization when the initial temperature field is harmonic.

A rectangular block under a thermal shock

As a simple first example, a rectangular block under sudden heating is considered. The convection boundary condition is imposed on Γ_3, and the temperature on Γ_1 is elevated suddenly to 100°C and the others are insulated as shown in *Figure 2*. The initial temperature of the block is 0°C. The functionals to be considered here are defined as:

$$\Phi_1 = \int_0^{t_F} \int_{\Gamma_3} T^2 \,\mathrm{d}\Gamma \,\mathrm{d}t \tag{35}$$

$$\Phi_2 = \int_0^{t_F} \int_{\Gamma_3} h \cdot (T - T_\infty) \,\mathrm{d}\Gamma \,\mathrm{d}t \tag{36}$$

Here Φ_2 means the sum of heat extracted through the boundary Γ_3. The y-coordinate of design boundary Γ_3 is elected as the design variable. Fixing the end points of the design boundary Γ_3, we obtain the sensitivity formula of the functionals from (26) as follows:

$$\Phi_i' = \int_{\Gamma_3} \left[T \otimes \rho C_\varepsilon \frac{\partial T^*}{\partial t} + T_{,s} \otimes (k T^*_{,s}) - \frac{1}{k} q \otimes q^* \right] V_n \,\mathrm{d}\Gamma \qquad i = 1, 2 \tag{37}$$

From (22)–(25) the boundary conditions of the adjoint systems are obtained. For numerical computation of the sensitivity, the problem is modelled using 44 linear elements as shown in *Figure 3*. The design boundary is represented with piecewise linear segments and the design variables chosen are the y-coordinate of the nodal points. The design velocity is generated linearly over neighbouring 4 elements as shown in *Figure 3*. The material constants are set to unity for convenience and the final time t_F is set to 1 sec. The time increment is chosen as $\Delta t = 0.001$ sec.

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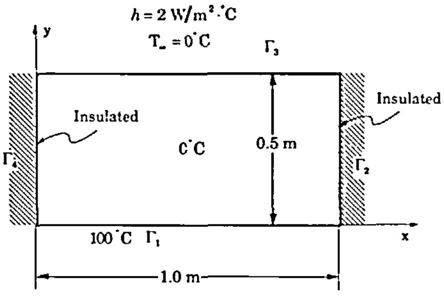

Figure 2 A rectangular block under thermal shock

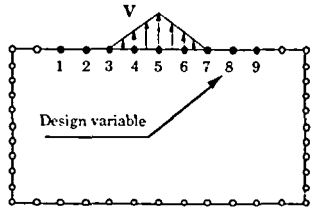

Figure 3 A BEM model with design variables and a typical design velocity for the rectangular block problem

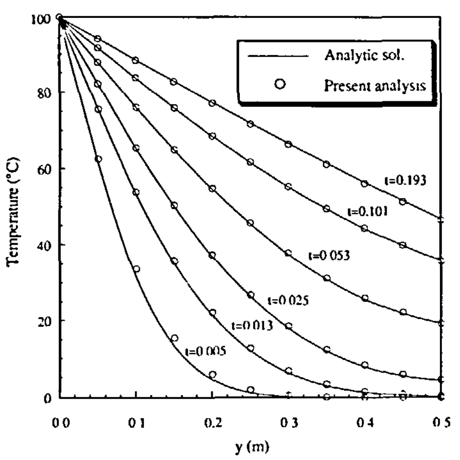

Figure 4 Temperature response of the rectangular block on boundary Γ_2

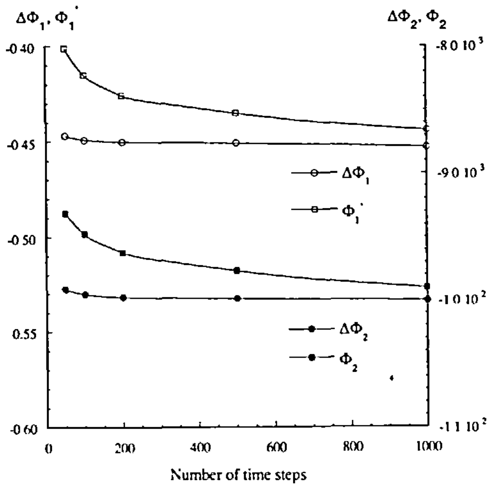

Figure 5 Sensitivity results of Φ_1 and Φ_2 for the first design variable

Figure 4 shows the temperature history calculated using a BEM code along the boundary Γ_2 and the results show excellent agreement with those obtained from the analytic solution in the text of Carslaw and Jaeger[24]. For comparison of the results of the sensitivity analysis with those of the finite difference method, we defined $\Delta\Phi \equiv \Phi_m - \Phi_i$ where Φ_m and Φ_i are the functional values at the modified and the initial design, respectively. The numerical results with 0.1% perturbation of a design variable at the initial configuration are listed in *Tables 1* and *2* for the temperature and flux functional, respectively. Owing to the symmetric behaviour of the results, only 5 design variables are perturbed. Fairly good results are observed. The differences with those of FDM happen to be the same for all the design perturbation. In *Figure 5* it is shown for the first design variable that they become smaller as smaller time steps are adopted. To know an asymptotic behaviour of sensitivity solutions with respect to time step, the Richardson extrapolation[25] solutions using the two data on the right in *Figure 5* with an assumption of $O(\Delta t)$ error are obtained. The ratios of solutions of the present method to the finite differencing are 99.48% and 100.16% for Φ_1 and Φ_2, respectively. This shows convergence of the sensitivity solutions.

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Table 1 Design sensitivity of Φ_1 for the rectangular block problem

Design var. No.	Φ_1 ($\times 10^4$)	$\Delta\Phi$	Φ'	$\left(\frac{\Phi'}{\Delta\Phi}\right) \times 100$
1	0.222766	−0.453213	−0.444166	98.00
2	0.222766	−0.453712	−0.444098	97.88
3	0.222766	−0.453834	−0.444013	97.84
4	0.222766	−0.453877	−0.443966	97.82
5	0.222766	−0.453888	−0.443915	97.81

Table 2 Design sensitivity of Φ_2 for the rectangular block problem

Design var. No.	Φ_1 ($\times 10^2$)	$\Delta\Phi$ ($\times 10^{-1}$)	Φ' ($\times 10^{-2}$)	$\left(\frac{\Phi'}{\Delta\Phi}\right) \times 100$
1	0.919832	−0.100046	−0.990285	98.98
2	0.919832	−0.100179	−0.990189	98.84
3	0.919832	−0.100214	−0.990063	98.79
4	0.919832	−0.100227	−0.989993	98.77
5	0.919832	−0.100231	−0.989971	98.77

A plunger problem

The plunger considered here is a two-dimensional model of a precisely shaped die, which forms the panel of a TV bulb from a block of molten glass. The inside surface of the plunger shown in *Figure 6* is cooled by water. It is known[26] that a primary factor affecting the surface quality of the product is the variation of temperature on the contacting surface with the workpiece. Hence the objective of this problem is to design a cooling boundary for minimizing the temperature variation along the cavity boundary, Γ_3. Thus the following performance functionals are considered,

$$\Phi_3 = \int_{t_0}^{t_F} \int_{\Gamma_3} (T_{,s})^2 \, d\Gamma \, dt \tag{38}$$

$$\Phi_4 = \int_{0}^{t_F} \int_{\Gamma_3} q \, d\Gamma \, dt \tag{39}$$

It is seen that the sensitivity formula derived previously cannot be applied directly to the functional Φ_3 because the integrand contains temperature gradient instead of temperature. Therefore some additional work is necessary to treat the function Φ_3.

Take now the material derivative of (38) to obtain:

$$\Phi'_3 = \int_{t_0}^{t_F} \int_{\Gamma 3} 2T_{,s}\dot{T}_{,s} \, d\Gamma \, dt + R(\mathbf{V}) \tag{40}$$

where $R(\mathbf{V})$ is a collection of terms which are explicit in terms of design velocity $\mathbf{V}$ as follows:

$$R(\mathbf{V}) = \int_{t_0}^{t_F} [2T_{,s}(q(V_{n,s} + V_s H) - T_{,k}V_{k,s}) + (T_{,s})^2(V_{k,k} - V_{i,j}n_i n_j)] \, d\Gamma \, dt \tag{41}$$

The integral in (40) has $\dot{T}_{,s}$ instead of $\dot{T}$. The following idea[2] is used to substitute it by an

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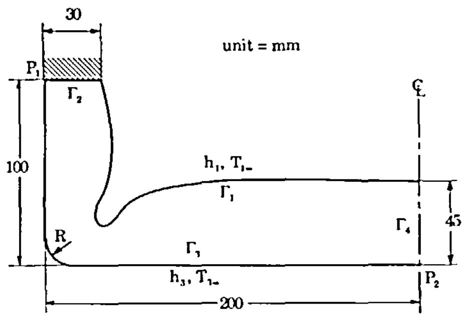

Figure 6 A plunger shape design problem

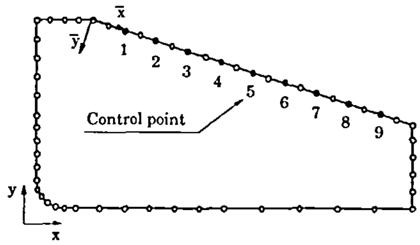

Figure 7 A BE model and control points of the plunger

equivalent $\partial\zeta/\partial T$ appearing in (24). It can be calculated by a weighted residual method as follows:

$$\int_{\Gamma_3} 2T_{,s}W_{,s}\,\mathrm{d}\Gamma = \int_{\Gamma_3} \lambda W \mathrm{d}\Gamma \tag{42}$$

where W is an arbitrary weighting function with C^0 continuity and $\lambda \equiv \partial\zeta/\partial T$. Now obtaining the equivalent λ from (42), the boundary conditions of the adjoint system for the functional Φ_3 are given as:

$$\begin{aligned}
&Q^*(x,t) = 0 && x \in \Omega \\
&q^*(x,t) = 0 && x \in \Gamma_2, \Gamma_4 \\
&q^*(x,t) = h[T^*(x,t)] && x \in \Gamma_1 \\
&q^*(x,t) = \begin{cases} h[T^*(x,t)] + \lambda(x, t_F - t) & x \in \Gamma_3, 0 \leqslant t \leqslant t_F - t_0 \\ h[T^*(x,t)] & x \in \Gamma_3, t_F - t_0 < t \leqslant t_F \end{cases}
\end{aligned} \tag{43}$$

Noting that the design velocity on the boundary Γ_3 is zero, the desired sensitivity formula for Φ_3 is obtained as follows:

$$\Phi_3' = \int_{\Gamma_1} \left[T \otimes \rho C_\varepsilon \frac{\partial T^*}{\partial t} + T_{,s} \otimes (kT^*_{,s}) + q \otimes T^*H - \frac{1}{k} q \otimes q^* \right] V_n \mathrm{d}\Gamma + \sum \langle \{q \otimes T^*\} V_s \rangle \tag{44}$$

A simplified geometry and boundary conditions of the plunger are depicted in *Figure 6*. Because of the symmetry, a half of the plunger is considered. It is not unrealistic to model the cooling boundary Γ_1 as a convection boundary and the cavity boundary Γ_3 as another convection boundary to simplify the problem. For numerical calculations k, κ, h_1, $T_{l\infty}$, h_3 and $T_{3\infty}$ are 27.52×10^{-3} W/mm°C, 12.03 mm²/sec, 3.15×10^{-4} W/mm²°C, 0°C, 2.88×10^{-4} W/mm²°C, 1000°C, respectively. And the temperature at $t = 0$ and the final time of the functionals are 0°C and 50 sec, respectively. Two cases of t_0 for the functional Φ_3 are tested; one with 0 sec and the other 40 sec.

The initial design selected is shown in *Figure 7*. The design boundary Γ_1 is represented by the composite cubic splines with free end conditions at both ends of Γ_1 and two linear boundary elements are used in discretization of a spline segment. Nine $\bar{y}$-coordinates in *Figure 7* which control the splines are selected as design variables. For the solutions of the primal and adjoint system, the model is discretized by 56 elements. Note that (42) should be solved before obtaining the solutions for the adjoint system. By using the same shape function for the weighting function, W, as that of boundary elements, an equivalent λ is calculated at every time step. The sensitivity

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Table 3 Design sensitivity of Φ_3 with $t_0 = 0$ sec for the plunger problem ($\Delta t = 1$ sec, $\Delta b = 0.01$ mm)

Design var. No.	Φ_1 ($\times 10^5$)	$\Delta\Phi$ ($\times 10^{-2}$)	Φ' ($\times 10^{-2}$)	$\left(\frac{\Phi'}{\Delta\Phi}\right) \times 100$
1	0.208397	−17.3619	−19.7019	113.48
2	0.208397	−1.93948	−2.01833	104.07
3	0.208397	−0.570300	−0.618541	108.46
4	0.208397	−0.226555	−0.254400	112.29
5	0.208397	−0.306475	−0.342355	111.71
6	0.208397	−0.353653	−0.391304	110.65
7	0.208397	−0.329000	−0.356145	108.25
8	0.208397	−0.163643	−0.174226	106.47
9	0.208397	0.174278	0.209943	102.46

Table 4 Design sensitivity of Φ_3 with $t_0 = 0$ sec for the plunger problem ($\Delta t = 0.5$ sec, $\Delta b = 0.01$ mm)

Design var. No.	Φ_1 ($\times 10^5$)	$\Delta\Phi$ ($\times 10^{-2}$)	Φ' ($\times 10^{-2}$)	$\left(\frac{\Phi'}{\Delta\Phi}\right) \times 100$
1	0.213446	−17.3701	−18.9218	108.93
2	0.213446	−1.88960	−1.83053	96.87
3	0.213446	−0.550800	−0.558640	101.42
4	0.213446	−0.209781	−0.215984	102.96
5	0.213446	−0.284895	−0.296759	104.16
6	0.213446	−0.326990	−0.338933	103.65
7	0.213446	−0.310749	−0.315385	101.49
8	0.213446	−0.173736	−0.172094	99.05
9	0.213446	0.145671	0.191650	131.50

results with 0.01 mm perturbation of each design variable for the performance functionals defined by (38) and (39) are calculated for time steps 1 and 0.5 sec and are found all similar in trend and percentage difference to those shown in *Tables 3* and *4*. The notations are the same as in the previous example. Several time steps are tested for each functional and the results summarized in *Figures 8* and *9*. It is seen that the magnitude of time step has much influence on the numerical results. The Figures also show the converging trend of those by the finite differencing.

SHAPE OPTIMIZATION AND DISCUSSIONS

The plunger model described in the previous section is taken as a shape optimal design problem. The objective is to find the shape of the boundary Γ_1 of the plunger that gives the temperature distribution of the cavity boundary Γ_3 as uniform as possible under some design variable constraints. Thus, the shape optimization problem can be defined as follows.

Find the shape of Γ_1 such that:

$$\begin{aligned} &\textit{min} \quad \Phi_3, \\ &\textit{subject to} \quad b_i^L \leqslant b_i \leqslant b_i^U \qquad i = 1, \ldots, m \end{aligned} \tag{45}$$

where b_i is the ith design variable, m is the number of design variables, b_i^L and b_i^U are lower and upper limits of the ith design variable, respectively. In this optimization formulation the functional

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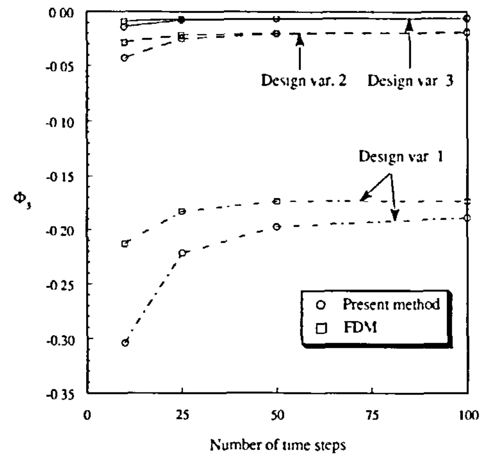

Figure 8 Sensitivity results of Φ_3 with $t_0 = 0\,\text{sec}$ ($\Delta b = 0.01$ mm)

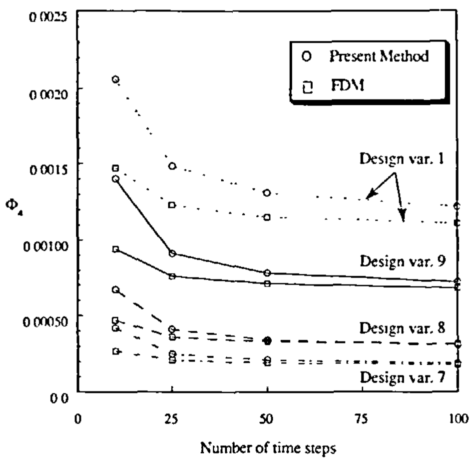

Figure 9 Sensitivity results of Φ_4 ($\Delta b = 0.01$ mm)

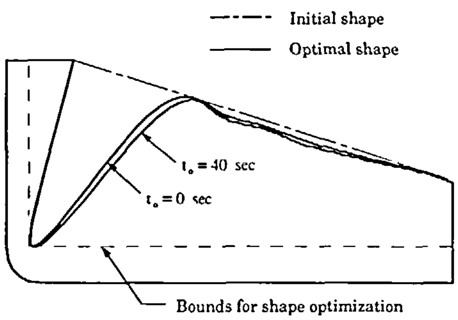

Figure 10 Initial and optimal shape of the plunger problem

Φ_4 defined in the previous section is not included as a constraint because the amount of heat extracted from molten material is considered not so critical to the surface quality.

The optimization routine IDESIGN[27] is used on a HP720 engineering workstation. The primal and the adjoint systems are analysed using the same model as shown in *Figure 7*. In this case the sensitivity is calculated with the cubic spline representation of Γ_1. On the design boundary from two to eight boundary elements are used on discretization of a spline segment in proportion to the distortion of the segment during the iterations. The model is discretized by 70 elements. The time step is chosen as $\Delta t = 2\,\text{sec}$ referring to *Figures 8* and *9*. With this time step which corresponds to 25 in the Figures, computational efficiency can be gained although the accuracy of sensitivity is somewhat limited. *Figure 10* shows the initial design, the optimal shape obtained and the bounds of the design variables. It is seen that the first design variable reached the upper bound and the last 6 design variables are almost fixed due to small magnitude of these sensitivities in relative sense. The cost function has reduced in 2 iterations from 2.04×10^4 to 1.52×10^4 $(^\circ\text{C/mm})^2$ for the case with $t_0 = 0\,\text{sec}$, and from 5.65×10^3 to 3.72×10^3 for $t_0 = 40\,\text{sec}$, which show 25.6 and 34.2% decrease of the objective, respectively. *Figure 11* shows the temperature responses of the initial and the final designs along the cavity boundary Γ_3 where the objective functional is defined. We can find the critical region at the corner zone and the peak temperature

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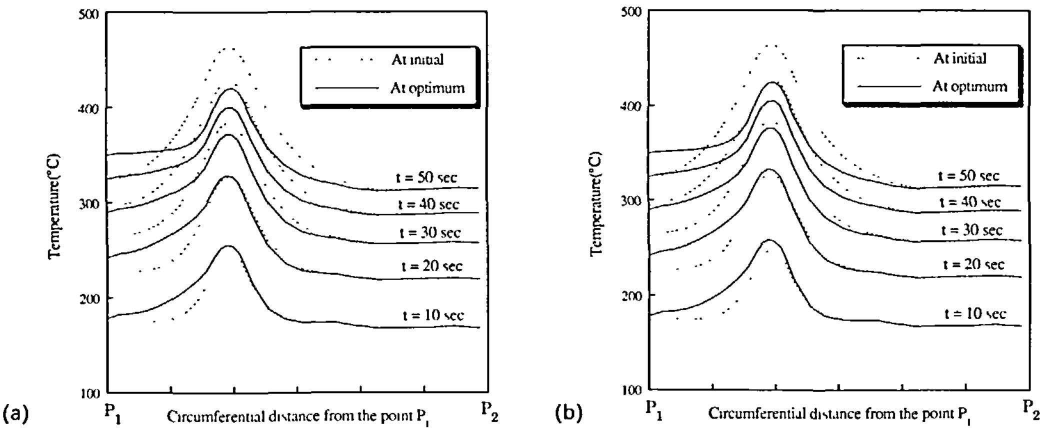

Figure 11 Temperature responses of the initial and the optimum shape on boundary Γ_3. (a) $t_0 = 0$ sec; (b) $t_0 = 40$ sec

there is not lowered much partially due to the tight design variable constraint. The general optimal shape conforms well with the intuition and current design. To be realistic, a three-dimensional model with a more realistic boundary conditions may be necessary and is a challenge for future work.

CONCLUSIONS

A procedure and resulting formula for the shape design sensitivity analysis of two-dimensional transient heat diffusion problems using the BIE formulation have been presented. It is based on the material derivative concept and the adjoint variable method. The Ionescu-Cazimir integral identity is introduced to correlate the primal system and the adjoint systems. The adjoint systems introduced are affected by the primal variables with a reverse sequence of time. The procedure of SDSA is illustrated through a rod example with analytic expressions. The accuracy of the proposed formulation is demonstrated through numerical implementation. The sensitivities are calculated for a rectangular block and a plunger problem and compared with those by the finite difference method, showing good agreement. Optimum shape is obtained for the plunger problem by applying the derived sensitivity formula to an iterative optimization algorithm. The applicability of the formulation is well shown with this non-trivial numerical example.

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