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Optimal Heating Algorithm for the Three-Dimensional Forced-Convection Problems

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A three-dimensional forced-convection optimal heating algorithm in determining the strength of the unknown optimal surface heating functions utilizing the conjugate gradient method and a general purpose commercial code CFX4.2 is applied successfully in the present study based on the desired surface temperature distributions at the final time of heating. Results obtained by using the conjugate gradient method to solve this three-dimensional optimal heating problem are justified based on the numerical experiments. Two different computational domains and two different desired temperature distributions are given, and the corresponding optimal heating functions are to be determined. Results show that the optimal heating functions can always be obtained with any arbitrary initial guesses of the boundary fluxes.

Nomenclature

Cp	=	heat capacity
f	=	body force
$J[q_i(S_i, t)]$	=	functional defined by Eq. (6)
$J_i'[q_i(S_i, t)]$	=	gradient of functional defined by Eq. (21)
k	=	thermal conductivity
$P_i^n(S_i, t)$	=	direction of descent defined by Eq. (8)
p	=	pressure
$q_i(S_i, t)$	=	unknown surface heating functions
$T(\Omega, t)$	=	estimated temperature
u, v, w	=	velocity in x, y, and z directions, respectively
$\mathbf{V}$	=	velocity vector
$Y(\Omega, t_f)$	=	desired temperature
β	=	search step size defined by Eq. (13)
γ_i	=	conjugate coefficients
$\Delta T_j(\Omega, t)$	=	sensitivity function defined by Eq. (10)
$\delta(\bullet)$	=	Dirac delta function
ε	=	convergence criteria
$\lambda(\Omega, t)$	=	Lagrange multiplier defined by Eq. (17)
μ	=	viscosity
ν	=	kinematic viscosity of fluid
ρ	=	density
Φ	=	viscous heating term
Ω	=	computational domain

Superscript

n	=	iteration index

I. Introduction

OPTIMAL heating for a given material to obtain the desired temperature distribution can be an objective in many industrial applications. One example would be in glass industry where glass nearing the final stages of certain manufacturing processes must be brought to a temperature that is as near uniform as possible to prevent unwanted inhomogeneities in the final article. Another example arises in the semiconductor manufacturing where the requirement of uniform temperature distribution of wafer is necessary. Moreover, rapid thermal process, that is, short time wafer heating, is also very important in the business. This also implies that the heating time is critical in reducing the thermal budget.

For many engineering applications it might often be necessary to find optimal heating functions such that the desired constraints can be satisfied. Such a system can be controlled either at the boundary (boundary heating) or through the spatial domain (distributed heating), or both.

The optimal heating problem for solid has been initiated by Butkovskii and Lerner.[1] Cavin and Tandon[2] considered a finite element method to numerical solutions of distributed parameter optimization problems. Meric[3,4] used the conjugate gradient method to find the optimal boundary control temperatures for a nonlinear system, that is, temperature-dependent thermal properties. There is also a vast amount of literature on such control systems, and a review can be found in Ray.[5]

Chen and Ozisik used a similar algorithm to determine the optimal heating sources for a slab[6,7] and for a cylinder[8] in a one-dimensional nonlinear optimal control problem. One should note that the nature of optimal heating problems is similar to the inverse problems[9–11] except that some additional constraints for the functional are required.

First, from the preceding review papers we learned that for the optimal heating problems considered in the literature[3,4,6–8] only constant final desired temperature is discussed. Second, there exist no explicit expressions for the determination of search step size. For example, in Ref. 4 the author stated only that the step size is determined by a one-dimensional minimization along the direction of search, and in Refs. 6–8 the authors claimed that they used the technique of cubic interpolation to determine the value of search step size. Those statements are both not clear and not efficient because no explicit formulation for the step size is given.

Recently, Huang[12] has solved a similar optimal heating problem using the conjugate gradient method as in Refs. 6–8 except that the heating functions are now the boundary heat fluxes and the desired temperature distributions are now functions of positions. To overcome the drawbacks as we have already mentioned, a general expression for the nonlinear optimal heating problem is derived. Moreover, an explicit expression for the determination of search step sizes is also derived with the help of the solutions of sensitivity problem.

All of the references just mentioned are one- or two-dimensional problems. More recently, Huang and Li[13] applied the technique used in Ref. 12 to a three-dimensional optimal heating problem for a solid, that is, optimal heating for heat conduction, and obtained good estimations.

The purpose of the present study is to extend the algorithm used in Refs. 12 and 13 to the optimal heating for a three-dimensional forced-convection problem in determining the optimal heating functions. To the authors' best knowledge, the problem of this kind has

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not been seen in the literature. The advantage of using the conjugate gradient method in the inverse problems lies in that it can estimate a huge number of unknown parameters at the same time; this can be seen in many literatures regarding inverse problems using the conjugate gradient method.

The conjugate gradient method derives from the perturbational principles and transforms the inverse problem to the solution of three problems, namely, the direct problem, the sensitivity problems, and the adjoint problem, which will be discussed in detail in text.

II. Direct Problem

To develop the methodology for use in simultaneously determining four unknown optimal boundary heating conditions for a three-dimensional forced-convection problem by CGM and CFX4.2, we consider the following example.

For a duct domain Ω the initial temperature is equal to T_0. When $t > 0$, we assumed that there is an inlet fluid with velocity $\boldsymbol{V}$ and temperature T_{inlet} on inlet surface S_9 (see Fig. 1a). The optimal heating boundary conditions are applied from S_1 to S_4. The boundary conditions on the surfaces from S_5 to S_8 are all assumed insulated. The temperature distribution on outlet surface S_{10} is assumed fully developed. Figure 1a shows the geometry and the coordinates for the three-dimensional physical problem considered here. The wall thickness is neglected, and therefore the thermal conduction is also neglected in the present study.

The mathematical formulation of this three-dimensional forced-heat-convection problem is given by the following:

Continuity equation:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \qquad \text{in} \qquad \Omega, t>0 \tag{1}$$

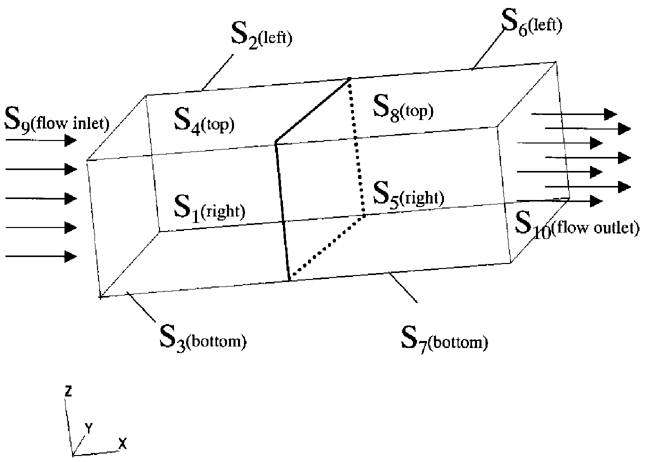

Fig. 1a Geometry and coordinates for test case 1.

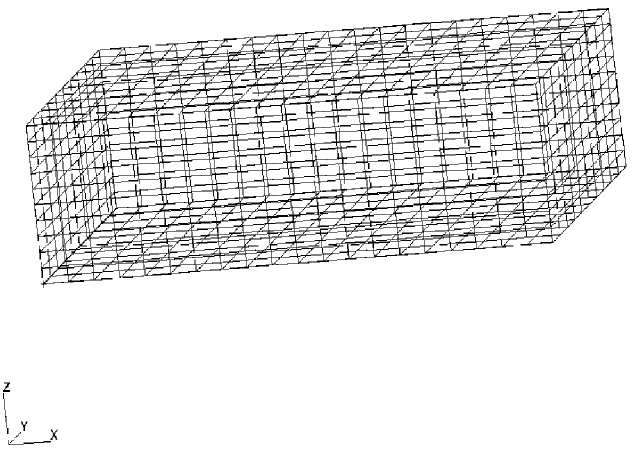

Fig. 1b Grid system for test case 1.

Momentum equation:

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z} = f_x-\frac{1}{\rho}\frac{\partial p}{\partial x}+\nu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right) \quad \text{in} \quad \Omega, t>0 \tag{2a}$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z} = f_y-\frac{1}{\rho}\frac{\partial p}{\partial y}+\nu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right) \quad \text{in} \quad \Omega, t>0 \tag{2b}$$

$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z} = f_z-\frac{1}{\rho}\frac{\partial p}{\partial z}+\nu\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right) \quad \text{in} \quad \Omega, t>0 \tag{2c}$$

Energy equation:

$$\rho C_p\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}+w\frac{\partial T}{\partial z}\right) = k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)+\mu\Phi \quad \text{in} \quad \Omega, t>0 \tag{3a}$$

subjected to the following boundary conditions:

$$k\frac{\partial T}{\partial n}=q_i(S_i,t)=\text{unknown} \qquad \text{on} \qquad S_1\sim S_4, t>0 \tag{3b}$$

$$\frac{\partial T}{\partial n}=0 \qquad \text{on} \qquad S_5\sim S_8, t>0 \tag{3c}$$

$$T=T_{\text{inlet}} \qquad \text{on} \qquad S_9, t>0 \tag{3d}$$

$$\frac{\partial T}{\partial n}=0 \qquad \text{on} \qquad S_{10}, t>0 \tag{3e}$$

$$T=T_0 \qquad \text{in} \qquad \Omega, t=0 \tag{3f}$$

Here Φ is given as

$$\Phi=2\left[\left(\frac{\partial u}{\partial x}\right)^2+\left(\frac{\partial v}{\partial y}\right)^2+\left(\frac{\partial w}{\partial z}\right)^2\right]+\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)^2 +\left(\frac{\partial w}{\partial y}+\frac{\partial v}{\partial z}\right)^2+\left(\frac{\partial w}{\partial x}+\frac{\partial u}{\partial z}\right)^2 \tag{4}$$

By defining the following notations,

$$\frac{\mathrm{D}T}{\mathrm{D}t}=\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}+w\frac{\partial T}{\partial z}\right) \tag{5a}$$

$$\nabla^2 T=\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right) \tag{5b}$$

Here $\mathrm{D}/\mathrm{D}t$ is the substantial derivative, and ∇^2 is the Laplace operator. The energy equation can be simplified as

$$\rho C_p\frac{\mathrm{D}T}{\mathrm{D}t}=k\nabla^2 T+\mu\Phi \qquad \text{in} \qquad \Omega, t>0 \tag{5c}$$

The solution for the preceding three-dimensional transient forced-convection problem in an irregular duct domain Ω is solved by calling CFX4.2 and its FORTRAN subroutine USRBCS in the main program. CFX 4.2 is available from AEA technology,[14] and the method of control volume is used to solve the direct problem. The direct problem considered here is concerned with the determination of the flow velocity field and fluid temperature when all of the boundary conditions at all boundaries are known.

III. Optimal Heating Problem

For the three-dimensional optimal heating problems the optimal heating functions $q_i(S_i, t)$ on S_i, $i = 1$–4, are regarded as being unknown, but everything else in the direct problem is known. In addition, the desired temperature distributions on some specified surface S_d within the domain Ω at final time t_f are considered available.

Let the desired temperature on S_d at final time t_f be denoted by $Y(S_d, t_f)$. Then this optimal heating problem can be stated as follows: by utilizing the preceding final desired temperature data $Y(S_d, t_f)$, estimate the strength of the optimal heating functions $q_i(S_i, t)$ on S_i, $i = 1$–4, over the specified space and time domain.

The solution of the present optimal heating problem is to be obtained in such a way that the following functional is minimized:

$$J\left[q_i^{n+1}(S_i,t)\right] = \int_{S_d} \left[T\left(S_d, t_f; q_i^{n+1}\right) - Y(S_d, t_f)\right]^2 \mathrm{d}S_d + \frac{1}{2}\sum_{i=1}^{4} \alpha_i \int_{S_i}\int_{t=0}^{t_f} q_i^{n+1}(S_i,t)^2\,\mathrm{d}t\,\mathrm{d}S_i$$
$$= \int_{\Omega} \left[T\left(\Omega, t_f; q_i^{n+1}\right) - Y(\Omega, t_f)\right]^2 \delta(S - S_d)\,\mathrm{d}\Omega + \frac{1}{2}\sum_{i=1}^{4} \alpha_i \int_{S_i}\int_{t=0}^{t_f} q_i^{n+1}(S_i,t)^2\,\mathrm{d}t\,\mathrm{d}S_i \tag{6}$$

Here $\delta(\bullet)$ is the Dirac delta function, and α_i, $i = 1$–4, are the given weighting coefficients with dimension $^{\circ}C^4 - m^4/W^2 - s$ such that Eq. (6) is dimensionally consistent. $T(\Omega, t_f)$ is the estimated or computed temperature at final time t_f. These quantities are determined from the solution of the direct problem already given by using the estimated heating function $q_i(S_i, t)$. If the value of functional J is less than the specified stopping criteria ε, stop the iterative process, and the optimal heating functions $q_i(S_i, t)$ are obtained; otherwise, continue the iteration until the stopping criteria is satisfied.

The first term on the right-hand side is the integration of the square of the deviation between the estimated and desired temperature on S_d at final time t_f. The summation terms are the integration with respect to time of the square of the heating functions $q_i(S_i, t)$ on S_i, $i = 1$–4, respectively, over the heating time t_f multiplied by the weighting coefficients α_i. Here, we consider the square of the heating functions because the quadratic form guarantees the existence of the minimum and avoids the cancellation effect between the positive and negative values. The weighting coefficients α_i, $i = 1$–4, are the design parameters that control the closeness of the estimated temperatures to the desired temperatures.

For example, $\alpha_i = 0$, $i = 1$–4, implies estimated temperatures close to the desired temperatures, but the estimated optimal heating functions might have oscillatory behavior. Therefore, a finite value for α_i is needed to damp such an oscillation. Moreover, the weighting coefficients α_i can also be used as the adjustment factors of the heating functions $q_i(S_i, t)$. When there exist some reasons such that the heating functions cannot be applied as what we have calculated, under this circumstance we should increase the value of weighting coefficients. As a result, the estimated heating functions will be damped, and the supplying rate of heat fluxes can be satisfied.

IV. Conjugate Gradient Method for Minimization

The following iterative process based on the conjugate gradient method[15] is now used for the estimation of heating functions $q_i(S_i, t)$ by minimizing the preceding functional $J[q_i(S_i, t)]$:

$$q_i^{n+1}(S_i,t) = q_i^n(S_i,t) - \beta^n P_i^n(S_i,t) \qquad n = 0, 1, 2, \ldots, i = 1\text{–}4 \tag{7}$$

where β^n is the search step size in going from iteration n to iteration $n+1$ and $P_i^n(S_i, t)$ are the directions of descent (i.e., search directions) given by

$$P_i^n(S_i,t) = J_i'^n(S_i,t) + \gamma_i^n P_i^{n-1}(S_i,t), \qquad i = 1\text{–}4 \tag{8}$$

which is a conjugation of the gradient directions $J_i'^n(S_i, t)$ at iteration n and the directions of descent $P_i^{n-1}(S_i, t)$ at iteration $n-1$. The conjugate coefficient is determined from

$$\gamma_i^n = \frac{\int_{S_i}\int_{t=0}^{t_f}\left[J_i'^n(S_i,t)\right]^2 \mathrm{d}t\,\mathrm{d}S_i}{\int_{S_i}\int_{t=0}^{t_f}\left[J_i'^{n-1}(S_i,t)\right]^2 \mathrm{d}t\,\mathrm{d}S_i} \quad \text{with} \quad \gamma_i^0 = 0, i = 1\text{–}4 \tag{9}$$

To perform the iterations according to Eq. (7), we need to compute the step sizes β^n and the gradient of the functional $J_i'^n(S_i, t)$. To develop expressions for the determination of these two quantities, a "sensitivity problem" and an "adjoint problem" are constructed as described next.

In the previous studies by Chen and Ozisik,[6–8] they used the technique of cubic interpolation to determine the value of search step size. This technique is actually not efficient because it does not have any theoretical base of optimization. For this reason the rate of convergence can become very slow. This matter has been discussed by Huang.[12]

To overcome this drawback, we then derive in the following section an explicit expression of the search step size for the optimal heating functions $q_i(S_i, t)$ with the help of the solution of sensitivity problems.

V. Sensitivity Problem and Search Step Size

Because the problem involves four unknown heating functions $q_i(S_i, t)$, in order to derive the sensitivity problem for each unknown function, we should perturb the unknown functions one at a time.

It is assumed that when $q_i(S_i, t)$ undergoes a variation $\Delta q_i(S_i, t)\delta(i - j)$, $T(x, y, z, t)$ is perturbed by ΔT_j. Here $j = 1$–4 represents four sensitivity problems. Then, replacing in the direct problem $q_i(S_i, t)$ by $q_i(S_i, t) + \Delta q_i(S_i, t)\delta(i - j)$ and $T(x, y, z, t)$ by $T(x, y, z, t) + \Delta T_j$, subtracting from the resulting expressions the direct problem, and neglecting the second-order terms, the following sensitivity problems for the sensitivity function ΔT_j are obtained:

$$\rho C_P \frac{\mathrm{D}\Delta T_j(x,y,z,t)}{\mathrm{D}t} = k\nabla^2(\Delta T_j) \quad \text{in} \quad \Omega(x,y,z) \qquad j = 1\text{–}4, t > 0 \tag{10a}$$

$$\frac{\partial \Delta T_j(x,y,z,t)}{\partial n} = \Delta q_1(S_1,t)\delta(1-j) \quad \text{on} \quad S_1, t > 0 \tag{10b}$$

$$\frac{\partial \Delta T_j(x,y,z,t)}{\partial n} = \Delta q_2(S_2,t)\delta(2-j) \quad \text{on} \quad S_2, t > 0 \tag{10c}$$

$$\frac{\partial \Delta T_j(x,y,z,t)}{\partial n} = \Delta q_3(S_3,t)\delta(3-j) \quad \text{on} \quad S_3, t > 0 \tag{10d}$$

$$\frac{\partial \Delta T_j(x,y,z,t)}{\partial n} = \Delta q_4(S_4,t)\delta(4-j) \quad \text{on} \quad S_4, t > 0 \tag{10e}$$

$$\frac{\partial \Delta T_j(x,y,z,t)}{\partial n} = 0 \quad \text{on} \quad S_5 \sim S_8, t > 0 \tag{10f}$$

$$\Delta T_j(x,y,z,t) = 0 \quad \text{on} \quad S_9, t > 0 \tag{10g}$$

$$\frac{\partial \Delta T_j(x,y,z,t)}{\partial n} = 0 \quad \text{on} \quad S_{10}, t > 0 \tag{10h}$$

$$\Delta T_j(x,y,x,t) = 0 \quad \text{in} \quad \Omega, \quad \text{for} \quad t = 0 \tag{10i}$$

The preceding four ($j = 1$–4) sensitivity problems are similar to the direct problem, and CFX4.2 can also be used to solve these sensitivity problems.

The functional $J[q_i^{n+1}(S_i, t)]$ for iteration $n+1$ is obtained by rewriting Eq. (6) as

$$J\left[q_i^{n+1}(S_i,t)\right] = \int_{\Omega}\left[T\left(\Omega, t_f; q_i^n - \beta^n P_i^n\right) - Y(\Omega, t_f)\right]^2 \times \delta(S - S_d)\,\mathrm{d}\Omega + \frac{1}{2}\sum_{i=1}^{4}\alpha_i \int_{S_i}\int_{t=0}^{t_f}\left(q_i^n - \beta^n P_i^n\right)^2 \mathrm{d}t\,\mathrm{d}S_i \tag{11}$$

where we replaced $q_i^{n+1}(S_i, t)$ in Eq. (6) by the expression given by Eq. (7). If the estimated temperatures $T(\Omega, t_f; q_i^n - \beta^n P_i^n)$ are linearized by a Taylor expansion, Eq. (11) takes the form

$$J\left[q_i^{n+1}(S_i,t)\right] = \int_\Omega \Big[T\big(\Omega, t_f; q_i^n\big) - \beta^n \sum_{j=1}^4 \Delta T_j P_i^n \delta(i-j) - Y(\Omega, t_f)\Big]^2 \delta(S - S_d)\,\mathrm{d}\Omega + \frac{1}{2}\sum_{i=1}^4 \alpha_i \int_{S_i}\int_{t=0}^{t_f} \big(q_i^n - \beta^n P_i^n\big)^2 \,\mathrm{d}t\,\mathrm{d}S_i \tag{12}$$

Equation (12) is differentiated with respect to β^n and equating them equal to zero, that is, $\partial J[q_i^{n+1}(S_i,t)]/\partial\beta^n = 0$, to obtain the following expression for β^n:

$$\beta^n = \frac{\sum_{j=1}^4 \left[\int_\Omega 2(T-Y)\Delta T_j \delta(S-S_d)\right]\mathrm{d}\Omega + \sum_{i=1}^4 \alpha_i \int_{S_i}\int_{t=0}^{t_f} q_i^n p_i^n \,\mathrm{d}t\,\mathrm{d}S_i}{\sum_{j=1}^4 \left[\int_\Omega 2(\Delta T_j)^2 \delta(S-S_d)\right]\mathrm{d}\Omega + \sum_{i=1}^4 \alpha_i \int_{S_i}\int_{t=0}^{t_f} \left(p_i^n\right)^2 \mathrm{d}t\,\mathrm{d}S_i} \tag{13}$$

where $T(\Omega, t_f; q_i^n)$ is the solution of the direct problem by using estimate $q_i(S_i, t)$ at the final time t_f. The sensitivity functions $\Delta T_j[\Omega, t; P_i^n \delta(i-j)]$ are taken as the solutions of problem (10) at time t by letting $\Delta q_i = P_i^n$.

VI. Adjoint Problem and Gradient Equation

To obtain the adjoint problem, Eq. (5c) is multiplied by the Lagrange multiplier (or adjoint function) λ_1, and the resulting expression is integrated over the time and corresponding space domains. Then, the result is added to the right-hand side of Eq. (6) to yield the following expression for the functional $J[q_i(S_i, t)]$:

$$J[q_i(S_i,t)] = \int_\Omega [T(\Omega,t_f) - Y(\Omega,t_f)]^2 \delta(S-S_d)\,\mathrm{d}\Omega + \frac{1}{2}\sum_{i=1}^4 \alpha_i \int_{S_i}\int_{t=0}^{t_f} q_i(S_i,t)^2\,\mathrm{d}t\,\mathrm{d}S_i + \int_\Omega\int_{t=0}^{t_f}\lambda_1 \times \left[k\nabla^2 T(\Omega,t) + \mu\Phi - \rho C_P \frac{\mathrm{D}T(\Omega,t)}{\mathrm{D}t}\right]\mathrm{d}t\,\mathrm{d}\Omega \tag{14}$$

First, for $j = 1$ the variation $\Delta J_j = \Delta J_1$ is obtained by perturbing $q_i(S_i, t)$ by $q_i(S_i, t) + \Delta q_i(S_i, t)\delta(i-1)$ and $T(\Omega, t)$ by $T(\Omega, t) + \Delta T_1$ in Eq. (14), subtracting from the resulting expression the original Eq. (14), and neglecting the second-order terms. We thus find

$$\Delta J_1[q_i(S_i,t)] = \int_\Omega 2[T(\Omega,t_f) - Y(\Omega,t_f)]\Delta T_1 \delta(S-S_d)\,\mathrm{d}\Omega + \alpha_1 \int_{S_1}\int_{t=0}^{t_f} q_1(S_1,t)\Delta q_1\,\mathrm{d}t\,\mathrm{d}S_1 + \int_\Omega\int_{t=0}^{t_f}\lambda_1(\Omega,t) \times \left[k\nabla^2 \Delta T_1(\Omega,t) - \rho C_P \frac{\mathrm{D}\Delta T_1(\Omega,t)}{\mathrm{D}t}\right]\mathrm{d}t\,\mathrm{d}\Omega \tag{15}$$

where $\delta(\bullet)$ is the Dirac delta function.

In Eq. (15) the domain integral term containing the Laplace operator is reformulated based on the following Green's second identity:

$$\int_\Omega \lambda_1(\Omega,t)\nabla^2\Delta T_1(\Omega,t)\,\mathrm{d}\Omega = \int_S \lambda_1(\Omega,t)\frac{\partial\Delta T_1}{\partial n}\,\mathrm{d}S - \int_S \Delta T_1(\Omega,t)\frac{\partial\Delta\lambda_1}{\partial n}\,\mathrm{d}S + \int_\Omega \Delta T_1(\Omega,t)\nabla^2\Delta\lambda_1(\Omega,t)\,\mathrm{d}\Omega \tag{16a}$$

The domain integral term containing substantial derivative is reformulated based on the Reynolds second transport theorem,

$$\int_\Omega \lambda_1(\Omega,t)\frac{\mathrm{D}\Delta T_1(\Omega,t)}{\mathrm{D}t}\,\mathrm{d}\Omega = \frac{\mathrm{D}}{\mathrm{D}t}\int_\Omega \lambda_1\Delta T_1\,\mathrm{d}\Omega - \int_\Omega \Delta T_1(\Omega,t)\frac{\mathrm{D}\lambda_1}{\mathrm{D}t}\,\mathrm{d}\Omega = \int_\Omega \frac{\partial(\lambda_1\Delta T_1)}{\partial t}\,\mathrm{d}\Omega + \int_S \lambda_1\Delta T_1(V\bullet n)\,\mathrm{d}S - \int_\Omega \Delta T_1(\Omega,t)\frac{\mathrm{D}\lambda_1}{\mathrm{D}t}\,\mathrm{d}\Omega \tag{16b}$$

The boundary conditions of the sensitivity problem given by Eqs. (10b–10h) are utilized. The vanishing of the integrands containing ΔT_1 leads to the following adjoint problem for the determination of $\lambda_1(x, y, z, t)$:

$$\rho C_p \frac{\mathrm{D}\lambda_1}{\mathrm{D}t} + k\nabla^2(\lambda_1) = 0 \qquad \text{in} \qquad \Omega, t > 0 \tag{17a}$$

$$\frac{\partial\lambda_1}{\partial n} = 0 \qquad \text{on} \qquad S_1 \sim S_8, t > 0 \tag{17b}$$

$$\lambda_1 = 0 \qquad \text{on} \qquad S_9, t > 0 \tag{17c}$$

$$-k\frac{\partial\lambda_1}{\partial n} = \lambda_1\rho C_p \boldsymbol{V}\bullet\boldsymbol{n} \qquad \text{on} \qquad S_{10}, t > 0 \tag{17d}$$

$$\lambda_1 = 2(T-Y)\delta(S-S_d) \qquad \text{in} \qquad \Omega, t = t_f \tag{17e}$$

The adjoint problems are different from the standard initial value problems in that the final time conditions at time $t = t_f$ are specified instead of the customary initial condition. However, this problem can be transformed to an initial value problem by the transformation of the time variables as $\tau = t_f - t$. Then CFX 4.2 can be used to solve the preceding adjoint problem.

Finally, the following integral term is left:

$$\Delta J_1 = \int_{S_1}\int_{t=0}^{t_f} [k\lambda_1(S_1,t) + \alpha_1 q_1]\Delta q_1\,\mathrm{d}t\,\mathrm{d}S_1 \tag{18}$$

From definition,[15] the functional increment can be presented as

$$\Delta J_1 = \int_{S_1}\int_{t=0}^{t_f} (J_1'\Delta q_1)\,\mathrm{d}t\,\mathrm{d}S_1 \tag{19}$$

A comparison of Eqs. (18) and (19) leads to the following expression for the gradient of functional J_1':

$$J_1'[q_1(S_1,t)] = k\lambda_1(S_1,t) + \alpha_1 q_1(S_1,t) \tag{20}$$

Similarly, to derive the adjoint problems for the case $j =$ 2–4, Eq. (5c) is multiplied by the Lagrange multiplier (or adjoint function) $\lambda_j(\Omega, t)$, $j = 2$–4, and follows the same procedure as already described. Eventually, we found that the adjoint equation for $\lambda_j(\Omega, t)$ is identical to that for $\lambda_1(\Omega, t)$. This implies that the adjoint equation needs to be solved only once because $\lambda_1(\Omega, t) = \lambda_j(\Omega, t)$. For this reason we will use $\lambda(\Omega, t)$ to represent $\lambda_j(\Omega, t)$, $j = 1$–4, for the rest of this paper.

Finally, the general expression of gradient equation for $q_i(S_i, t)$ can be obtained as

$$J_i'[q_i(S_i,t)] = k\lambda(S_i,t) + \alpha_i q_i(S_i,t) \qquad i = 1\text{–}4 \tag{21}$$

VII. Computational Procedure

The computational procedure for the solution of this three-dimensional forced-convection optimal heating problem can be summarized as follows:

Suppose heating functions $q_i^n(S_i, t)$, $i = 1$–4 are available at iteration n:

Step 1) Solve the direct problem given by Eq. (3) for $T(\Omega, t)$.

Step 2) Examine the stopping criterion ε. Continue if not satisfied.

Step 3) Solve the adjoint problem given by Eq. (17) for $\lambda(\Omega, t)$.

Step 4) Compute the gradient of the functional $J_i'[q_i(S_i, t)]$, $i = 1$–4, from Eq. (21).

Step 5) Compute the conjugate coefficients γ_i^n and the direction of descent $P_i^n(S_i, t)$ from Eqs. (9) and (8), respectively.

Step 6) Set $\Delta q_i(S_i, t) = P_i^n(S_i, t)$, and solve the sensitivity problems given by Eq. (10) for $\Delta T_j(\Omega, t)$, $j = 1$–4, respectively.

Step 7) Compute the search step size β^n from Eq. (13).

Step 8) Compute the new estimation for $q_i^{n+1}(S_i, t)$ on S_i, $i = 1$–4, from Eq. (7) and return to step 1.

In the present study the value of stopping criteria ε is assigned as the value of functional when the functional can hardly decrease. One would expect that as the value of weighting coefficients increases the value of ε will also increase.

VIII. Results and Discussions

The objective of this study is to show the validity of the CGM in estimating the optimal surface heating functions $q_i(S_i, t)$ on S_i, $i = 1$–4 for a three-dimensional forced-convection problem with no prior information on the functional form of the heating functions.

To illustrate the ability of the conjugate gradient method in predicting $q_i(S_i, t)$ with optimal heating analysis from the knowledge of desired final time temperature distribution on surface S_d, we consider following one regular and one irregular domain where the desired temperature distributions are in different forms.

One of the advantages of using the conjugate gradient method is that the initial guesses of the unknown control functions $q_i^n(S_i, t)$ can be chosen arbitrarily. In all of the test cases considered here, the initial guesses of control functions used to begin the iteration are taken as $q_i^0(S_i, t) = 0.0$.

We now present the numerical experiments in determining $q_i^n(S_i, t)$ by the optimal control analysis.

A. Numerical Test Case 1

The geometry for the test case 1 is shown in Fig. 1a, which represents a rectangular duct and the aspect ratio is 0.5. The inlet and outlet flows are perpendicular to the vertical inlet S_9 and outlet S_{10}, respectively. The grids along the y and z directions are taken as 10, whereas along the x direction is taken as 20. The number of desired temperature on surface S_d, where S_d is on the $y - z$ plane, is thus $10 \times 10 = 100$, and a time step $\Delta t = 1$ s is used. The grid system for test case 1 is shown in Fig. 1b.

The parameters that were used in the present study are taken as $\boldsymbol{V} = u = 0.1$ m/s, $k = 1$ W/(m^2-°C), $\rho = 1$ kg/m^3, $Cp = 1$ kj/(kg-°C), $\mu = 1$ kg/(m-s), $T_{\text{inlet}} = 0$°C, $T_0 = 0$°C, and without body forces. Those numbers did not represent any physical meanings; they are just some numbers to perform the test cases for optimal control problem. The heating functions $q_i^n(S_i, t)$ are applied on surface S_1, S_2, S_3, and S_4, whereas S_5, S_6, S_7, and S_8 are all assumed insulated.

The desired temperature distribution at final time t_f on surface $S_d = S(10, J, K)$ is assumed constant and is given as

$$Y(10, J, K, t_f) = 8°\text{C} \qquad 1 \leqq J \leqq 10, \qquad 1 \leqq K \leqq 10 \tag{22}$$

where I, J, and K represent the index of discrete position in domain Ω; J and K represent the grid index on surface S_d.

The optimal heating problem is examined first by using a different period of heating time. It is assumed that the heating process is to be completed at a time equal to 12 s and 20 s, respectively, using $\alpha_i = 0.0$.

For $t_f = 12$ s a total of 4800 unknown discreted heat fluxes are to be determined at the same time in the present study. If the stopping criterion ε is set as $\varepsilon = 20$, after four iterations the solutions for optimal heating functions $q_i(S_i, t)$ can be obtained.

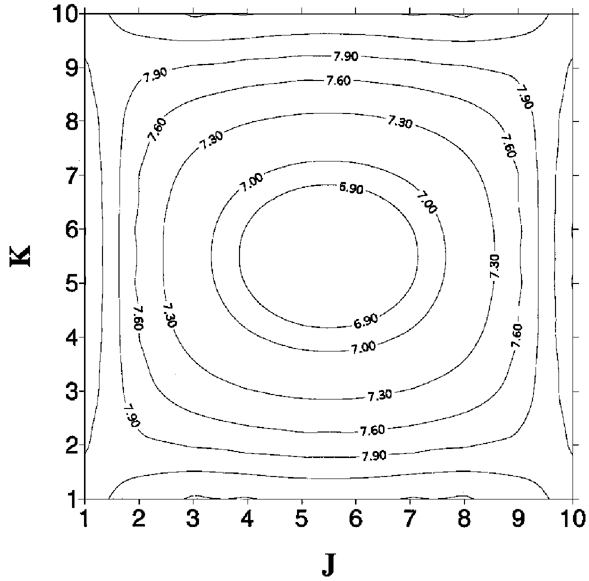

Fig. 2 Estimated temperatures $T(10, J, K, 12)$ for $Y(10, J, K, 12) = 8.0$ and $\alpha_i = 0.0$ in test case 1.

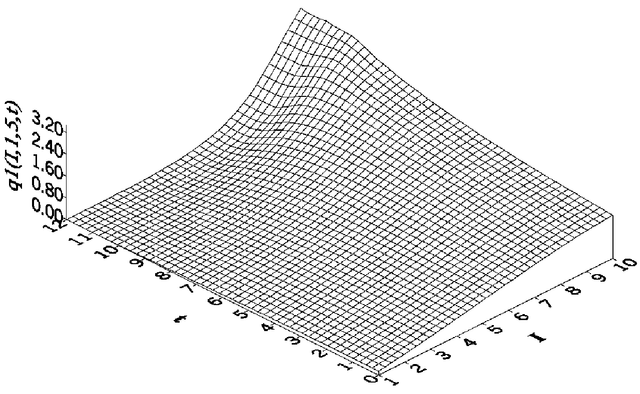

Fig. 3a Estimated boundary heating flux $q_1(I, 1, 5, t)$ with $t_f = 12$ and $\alpha_i = 0.0$ in test case 1.

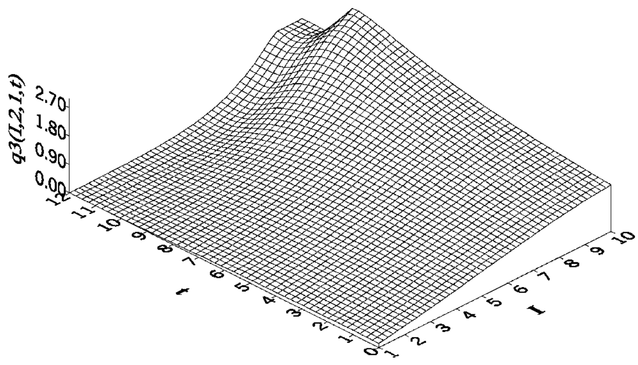

Fig. 3b Estimated boundary heating flux $q_3(I, 2, 1, t)$ with $t_f = 12$ and $\alpha_i = 0.0$ in test case 1.

It is difficult to show all of the estimated heating functions here because of the limitation of pages. For this reason we will show only a portion of the results. Figure 2 shows the contour plot for the estimated final temperature distributions $T(I, J, K, 12)$ on $I = 10$. Figures 3a and 3b show the estimated optimal heating functions $q_1(I, 1, 5, t)$ and $q_3(I, 2, 1, t)$, respectively. Here $q_1(I, 1, 5, t)$ represents the optimal heating along the x direction (i.e., $I = 1$ to 10) on S_1 (i.e., $J = 1$) at $K = 5$ with time, and $q_3(I, 2, 1, t)$ indicates the optimal heating along the x direction (i.e., $I = 1$ to 10) on S_3 (i.e., $K = 1$) at $J = 2$ with time.

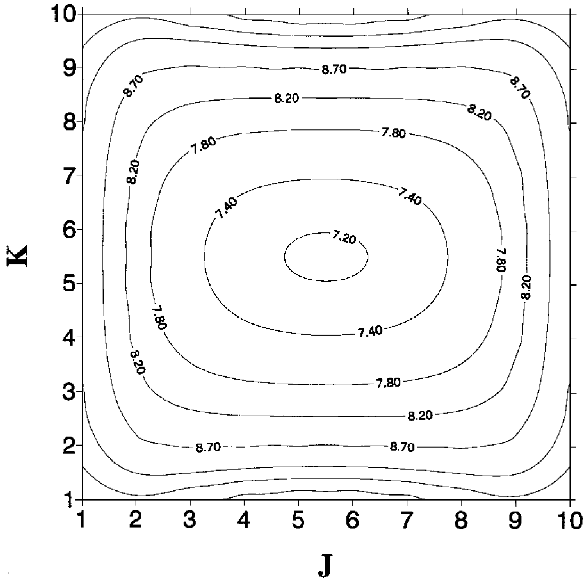

Fig. 4 Estimated temperatures $T(10, J, K, 20)$ for $Y(10, J, K, 20) = 8.0$ and $\alpha_i = 0.0$ in test case 1.

It is obvious from Fig. 3 that the estimated heating functions are all very stable as a constant heat flux but exhibit drastic change near $I = 10$ and final time. This implies that we might have difficulties in controlling such functions near $I = 10$ at final time. However the estimated final temperature distribution is satisfied with the desired distribution because the average error for the desired and estimated temperature at $t_f = 12$ is calculated as ERR = 6.69%, where the definition for ERR is given here:

$$\text{ERR\%} = \sum_{I=S_d}\left[\sum_{J=1}^{10}\sum_{K=1}^{10}\left|\frac{T(I,J,K,t_f)-Y(I,J,K,t_f)}{Y(I,J,K,t_f)}\right|\right] \div (10\times 10)\times 100\% \tag{23}$$

Similarly, for $t_f = 20$ a total of 8000 discrete heating fluxes should be calculated. The stopping criterion ε is set as $\varepsilon = 30$, and after four iterations the optimal heating functions $q_i(S_i, t)$ can be determined.

The estimated final temperature distribution $T(I, J, K, 12)$ on $I = 10$ is shown in Fig. 4. The estimated optimal heating functions $q_1(I, 1, 5, t)$ and $q_3(I, 2, 1, t)$ are shown in Figs. 5a and 5b, respectively. Again, the estimated heating functions have drastic changes near $I = 10$ and final time. The average error for the desired and estimated temperature at $t_f = 20$ is ERR = 8.44%.

From the preceding two test cases we found that the average error for estimated temperatures for a long heating time process is larger than that for short time heating. This test is to show the ability of the present algorithm in determining the optimal heating functions for different heating time.

Besides Eq. (18), one can also evaluate the ability of the optimal heating by comparing the predicted mean temperature with the desired temperature. The predicted mean temperatures for $t_f = 12$ and 20 s cases are 7.56 and 8.22, respectively, that is, 5.5 and 2.8% error when comparing with the desired temperature.

To examine the effectiveness of the weighting coefficients α_i to the control functions, we consider the following numerical experiment in which the calculating conditions are the same as the preceding conditions for short time heating (i.e., $t_f = 12$ s) except that $\alpha_i = 100$, $i = 1$–4, is used.

We do not expect that the value of functional J be decreased to a small number because there is a large weighting on the square of the heating functions $q_i(S_i, t)$. For this reason the difference between estimated and desired temperatures can be increased, but at the same time the oscillatory behavior for control functions can also be decreased.

The stopping criterion ε is set as $\varepsilon = 850$; after only two iterations, the optimal heating functions $q_i(S_i, t)$ can be determined.

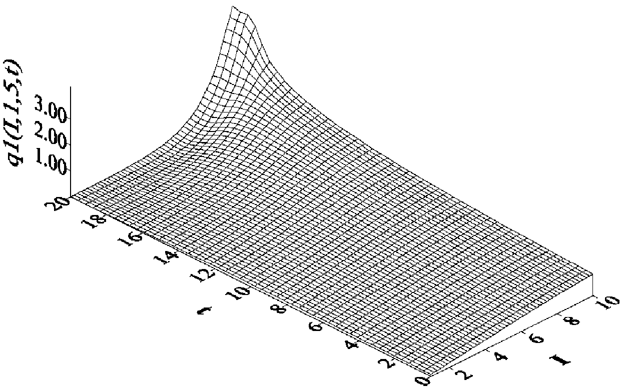

Fig. 5a Estimated boundary heating flux $q_1(I, 1, 5, t)$ with $t_f = 20$ and $\alpha_i = 0.0$ in test case 1.

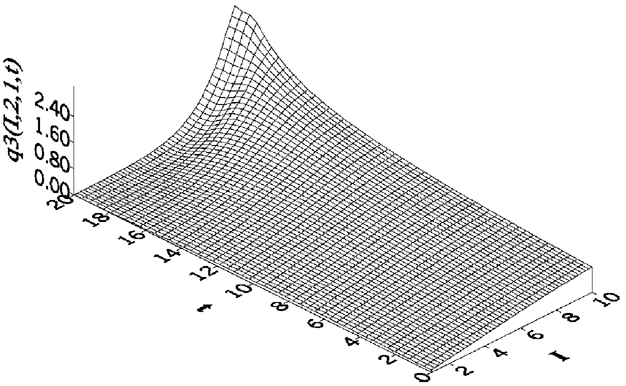

Fig. 5b Estimated boundary heating flux $q_3(I, 2, 1, t)$ with $t_f = 20$ and $\alpha_i = 0.0$ in test case 1.

According to the observations of our numerical results, the heating function on each surface becomes almost a constant wall heat flux during heating process, and it is very easy to be controlled. Moreover, the oscillatory behavior is improved significantly near $I = 10$ and final time. However, the accuracy of the estimated final temperature becomes poor because the average error for the desired and estimated temperature at $t_f = 12$ s is ERR = 21.25%.

Finally we would like to test the effectiveness of the flow velocity of fluid to the heating functions. We consider a numerical experiment that the calculating conditions are the same as the original conditions for short time heating (i.e., $t_f = 12$ s) except that $u = 0.2$ m/s is used. By setting $\varepsilon = 25$, after only three iterations the average error for the desired and estimated temperature at $t_f = 12$ s is now increased from ERR = 6.69% to ERR = 9.26%. This implies that it is more difficult to perform the optimal heating when the velocity of fluid is increased. The reason for this is because the temperature fields will change more drastically as the flow velocity increases; therefore, it is more difficult to control the temperature fields as the fluid flows faster.

B. Numerical Test Case 2

To show the potential of the present algorithm for use in a general three-dimensional optimal heating problem, we consider an irregular duct domain in the second test case. The geometry of this case is shown in Fig. 6a. The inlet and outlet flows are perpendicular to the vertical inlet S_9 and outlet S_{10}, respectively; the aspect ratio for both inlet and outlet surfaces is 0.5. The boundary conditions and grid system are similar to test case 1, and the grid system for the present study is shown in Fig. 6b.

The desired temperature distributions at final time $t_f = 12$ s are now assumed on two desired surfaces and are given as

$$Y(4, J, K, t_f) = 6.6^\circ\text{C} \qquad 1 \leqq J \leqq 10, \quad 1 \leqq K \leqq 10 \tag{24a}$$

$$Y(10, J, K, t_f) = 9^\circ\text{C} \qquad 1 \leqq J \leqq 10, \quad 1 \leqq K \leqq 10 \tag{24b}$$

where J and K represent the grid index in domain Ω.

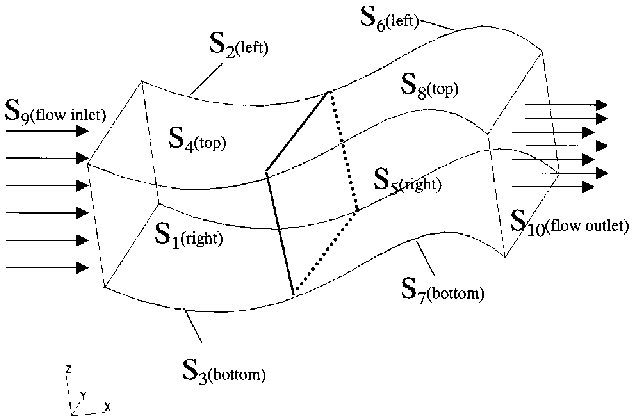

Fig. 6a Geometry and coordinates for test case 2.

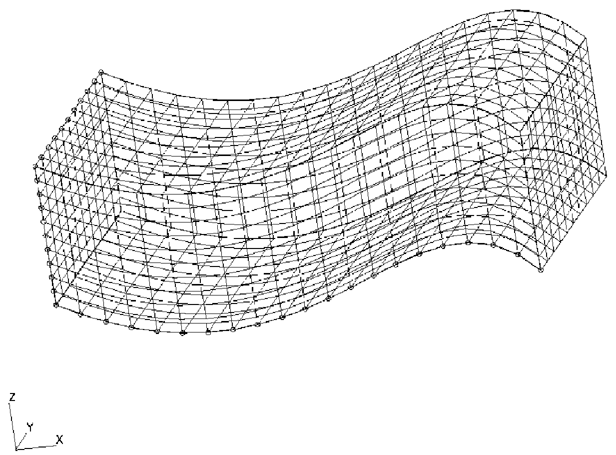

Fig. 6b Grid system for test case 2.

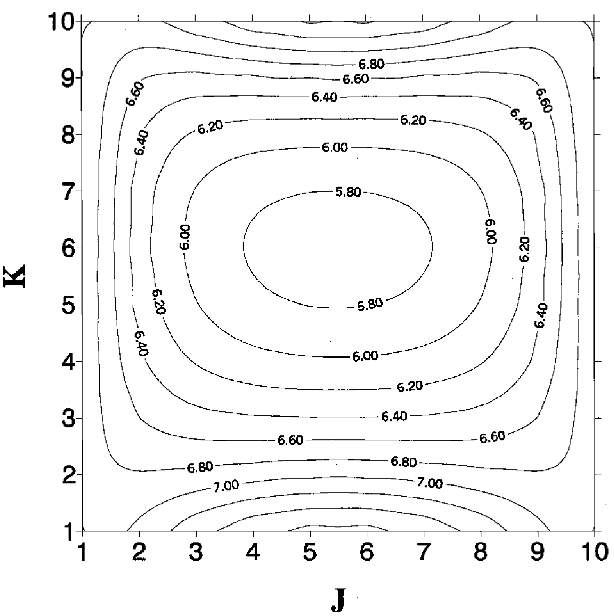

Fig. 7a Estimated temperatures $T(4, J, K, 12)$ for $Y(4, J, K, 12) = 6.6$ and $\alpha_i = 0.0$ in test case 2.

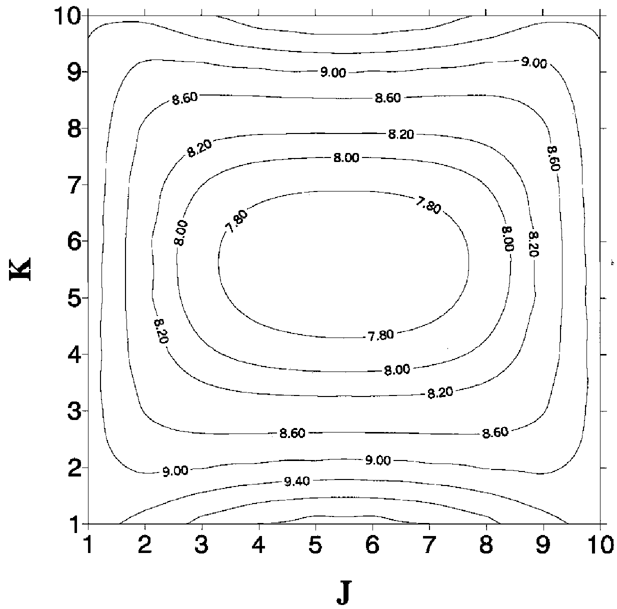

Fig. 7b Estimated temperatures $T(10, J, K, 12)$ for $Y(10, J, K, 12) = 9.0$ and $\alpha_i = 0.0$ in test case 2.

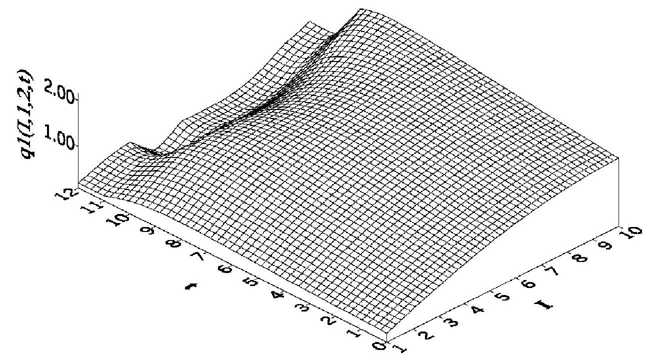

Fig. 8a Estimated boundary heating flux $q_1(I, 1, 2, t)$ with $t_f = 12$ and $\alpha_i = 0.0$ in test case 2.

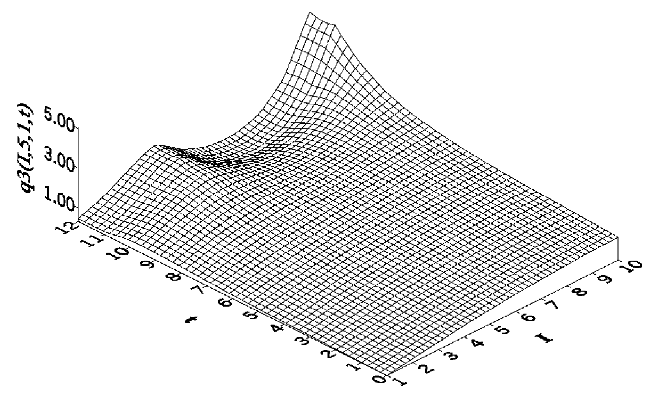

Fig. 8b Estimated boundary heating flux $q_3(I, 5, 1, t)$ with $t_f = 12$ and $\alpha_i = 0.0$ in test case 2.

The optimal control problem is examined by using $t_f = 12$ s and $\alpha_i = 0.0$; therefore, a total of 4800 unknown discreted heating fluxes are to be estimated at the same time in the heat process. If the stopping criterion ε is set as $\varepsilon = 25$, after four iterations the solutions for optimal heating functions $q_i(S_i, t)$ can be obtained.

Figures 7a and 7b show the contour plots for the estimated final temperature distributions $T(I, J, K, 12)$, on $I = 4$ and 10, respectively. Figures 8a and 8b show the estimated heating functions $q_1(I, 1, 2, t)$ and $q_3(I, 5, 1, t)$, respectively. It is obvious from Fig. 8 that the estimated heating functions exhibit oscillatory behavior near $I = 4$ to 10 and final time. The average error for the desired and estimated temperature at $t_f = 12$ s is calculated as ERR $= 6.9\%$.

From the preceding two numerical test cases we concluded that the conjugate gradient method can be applied successfully in this three-dimensional optimal heating problem for predicting the optimal boundary heating functions $q_i(S_i, t)$ on S_i.

IX. Conclusions

The conjugate gradient method with adjoint equation was successfully applied for the solution of a general three-dimensional forced-convection optimal heating problem in determining the optimal boundary heating functions. Three test cases involving different geometry, different final desired temperature distributions, different heating time, and different weighting coefficients were considered. The results show that the conjugate gradient method does not require a priori information for the functional form of the unknown heating functions, and the optimal solutions can be obtained within few number of iterations.

Acknowledgment

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References

[1]Butkovskii, A. G., and Lerner, A. Y., "The Optimal Control Systems with Distributed Parameters," *Automatic Remote Control*, Vol. 21, 1960, pp. 472–477.

[2]Cavin, R. K., III, and Tandon, S. C., "Distributed Parameter System Optimal Control Design via Finite Element Discretization," *Automatica*, Vol. 13, No. 7, 1977, pp. 611–614.

[3]Meric, R. A., "Finite Element Analysis of Optimal Heating of a Slab with Temperature Dependent Thermal Conductivity," *International Journal of Heat and Mass Transfer*, Vol. 22, 1979, pp. 1347–1353.

[4]Meric, R. A., "Finite Element and Conjugate Gradient Methods for a Nonlinear Optimal Heat Transfer Control Problem," *International Journal for Numerical Methods in Engineering*, Vol. 14, No. 6, 1979, pp. 1851–1863.

[5]Ray, W. H., "Some Recent Applications of Distributed Parameter Systems Theory—A Survey," *Automatica*, Vol. 14, No. 3, 1978, pp. 281–287.

[6]Chen, C. J., and Ozisik, M. N., "Optimal Heating of a Slab with a Plane Heat Source of Timewise Varying Strength," *Numerical Heat Transfer, Part A*, Vol. 21, No. 4, 1992, pp. 351–361.

[7]Chen, C. J., and Ozisik, M. N., "Optimal Heating of a Slab with Two Plan Heat Sources of Timewise Varying Strength," *Journal of The Franklin Institute*, Vol. 329, No. 2, 1992, pp. 195–206.

[8]Chen, C. J., and Ozisik, M. N., "Optimal Convective Heating of a Hollow Cylinder with Temperature Dependent Thermal Conductivity," *Applied Scientific Research*, Vol. 52, No. 1, 1994, pp. 67–79.

[9]Huang, C. H., Hsu, G. C., and Jang, J. Y., "A Nonlinear Inverse Problem for the Prediction of Local Thermal Contact Conductance in Plate Finned-Tube Heat Exchangers," *Heat and Mass Transfer*, Vol. 37, Nos. 4–5, 2001, pp. 351–359.

[10]Huang, C. H., "An Inverse Nonlinear Force Vibration Problem of Estimating the External Forces in a Damped System with Time-Dependent System Parameters," *Journal of Sound and Vibration*, Vol. 242, No. 5, 2001, pp. 749–765.

[11]Huang, C. H., Chiang, C. C., and Chen, H. M., "A Shape Identification Problem in Estimating the Geometry of Multiple Cavities," *Journal of Thermophysics and Heat Transfer*, Vol. 12, No. 2, 1998, pp. 270–277.

[12]Huang, C. H., "A Non-Linear Optimal Control Problem in Determining the Strength of the Optimal Boundary Heat Fluxes," *Numerical Heat Transfer, Part B*, Vol. 40, No. 5, 2001, pp. 411–429.

[13]Huang, C. H., and Li, C. Y., "A Three-Dimensional Optimal Control Problem in Determining the Boundary Control Heat Fluxes," *Heat and Mass Transfer* (accepted for publication).

[14]*CFX-4.2 User's Manual*, AEA Technology, Oxfordshire, England, U.K., 1997.

[15]Alifanov, O. M., "Solution of an Inverse Problem of Heat Conduction by Iteration Methods," *Journal of Engineering Physics*, Vol. 26, No. 4, 1974, pp. 471–476.