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A three-dimensional inverse forced convection problem in estimating surface heat flux by conjugate gradient method

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Abstract

A three-dimensional (3D) transient inverse forced convection problem is solved in the present study using the Conjugate Gradient Method (CGM) and the general purpose commercial code CFX4.2-based inverse algorithm to estimate the unknown boundary heat flux in a three-dimensional irregular duct flow problem. The advantage of calling CFX4.2 as a subroutine in the present inverse calculation lies in that many difficult but practical 3D inverse convection problem can be solved under this construction. Results obtained by using the conjugate gradient method to solve this 3D inverse forced convection problems are justified based on the numerical experiments. It is concluded that accurate boundary fluxes can be estimated by the conjugate gradient method except for the inlet surface and final time. The reason and improvement of this singularity are addressed. Finally, the effects of the height of duct, velocity of the inlet fluid and measurement errors on the inverse solutions are discussed.

Keywords: Inverse problem; Forced convection; Conjugate gradient method; Heat flux estimation

1. Introduction

The direct heat convection problems are concerned with the determination of flow velocity field and fluid temperature at interior points of a region when the initial and boundary conditions, thermophysical properties and heat generation are specified. In contrast, the inverse heat convection problem involves the determination of the surface conditions (i.e. the surface temperatures and heat fluxes) from the knowledge of the temperature measurements taken on the fluid surface.

The inverse heat conduction problems can be seen quite often in the literature or books [1–5] but not for the inverse heat convection problem. Huang and Ozisik [6] used conjugate gradient method to estimate the surface heat fluxes in a fully developed velocity inverse convection problem. Li et al. [7] and Prud'homme and Nguyen [8] have solved the natural convection problems. The above inverse problems are all two-dimensional and in regular (rectangular) domain. However, the three-dimensional inverse convection problems with irregular domain is never seen in the literature.

There are many commercial codes available for solving fluid dynamic and heat transfer problems, such as CFX4.2, UNIC, PHOENICS, etc. Those codes can be used to calculate many practical but difficult direct thermal problems. If one can device an inverse algorithm, which has the ability to com-

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Nomenclature

C_p	heat capacity
f	body force
h	heat transfer coefficient
J	functional defined by Eq. (6)
J'	gradient of functional defined by Eq. (15a)
k	thermal conductivity
M	number of measurement data
p	direction of descent defined by Eq. (7b)
P	pressure
q	unknown surface heat flux
T	calculated temperature
ΔT	solution of sensitivity problem
u, v, w	velocity in x-, y- and z-directions, respectively
$\mathbf{V}$	velocity vector
Y	measured temperature

Greek symbols

β	search step size defined by Eq. (10)
γ	conjugate coefficient defined by Eq. (7c)
Ω	computational domain
λ	solution for adjoint problem
ω	random number
ε	convergence criteria
σ	standard deviation of the measurement errors
ρ	density
ν	kinematic viscosity of fluid
μ	viscosity
Φ	viscous heating term
$\delta()$	the Dirac delta function

Superscript

$\hat{}$	estimated values

municate with those commercial codes by means of data transportation, a generalized 3D inverse heat transfer problem can thus be established. Huang and Wang [9] have applied the above idea to a 3D inverse heat conduction problem in estimating the surface heat fluxes in any irregular domain and obtained good estimations.

The objective of the present study is to utilize the CFX4.2 code as the subroutine in solving the 3D inverse forced convection problems by Conjugate Gradient Method (CGM). CFX 4.2 is available from AEA technology [10] and the method of control volume is used to solve the thermal problems.

The CGM is also called an iterative regularization method, which means the regularization procedure is performed during the iterative processes and thus the determination of optimal regularization conditions is not needed. The present work addresses the developments of the conjugate gradient algorithms for estimating unknown boundary heat fluxes in a 3D forced convection problem. The conjugate gradient method derives from the perturbation principles and transforms the inverse problem to the solution of three problems, namely, the direct, sensitivity and the adjoint problem. These three problems are solved by CFX4.2 and the calculated values are used in CGM for inverse calculations. The bridge between CFX4.2 and CGM is the INPUT/OUTPUT file. Those files should be arranged such that CFX and CGM can recognize their format. Moreover, the Fortran compiler Visual Fortran 6.0 [11] is used to compile the main program since it's subroutine SYSTEM has the ability to switch the computational environment from main program to CFX.

Finally, the inverse solutions for two transient heat convection problems with irregular duct geometry and different boundary conditions will be illustrated to show the validity of using the CGM in the present 3D inverse convection problem.

2. The direct problem

To illustrate the methodology for developing expressions for use in determining unknown surface heat flux in an irregular duct flow problem by CGM and CFX4.2, we consider the following a three-dimensional inverse forced convection problem. 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 $\mathbf{V}$ and temperature T_1 on inlet surface S_1. The boundary condition on S_2 is of the third kind with heat transfer coefficient h and ambient temperature T_∞. The boundary conditions on the remaining surfaces S_3, S_4 and S_5 are all assumed insulated, while surface S_6 (upper surface) is subjected to an unknown heat flux $q(S_6, t)$, which is a function of surface positions and time. Fig. 1(a) shows the geometry and the coordinates for the three-dimensional physical problem considered here. We should note that the wall thickness is neglected and therefore the thermal conduction is also neglected in the present study.

The mathematical formulation of this linear heat convection problem is given by:

Continuity equation

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

Momentum equation

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

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

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

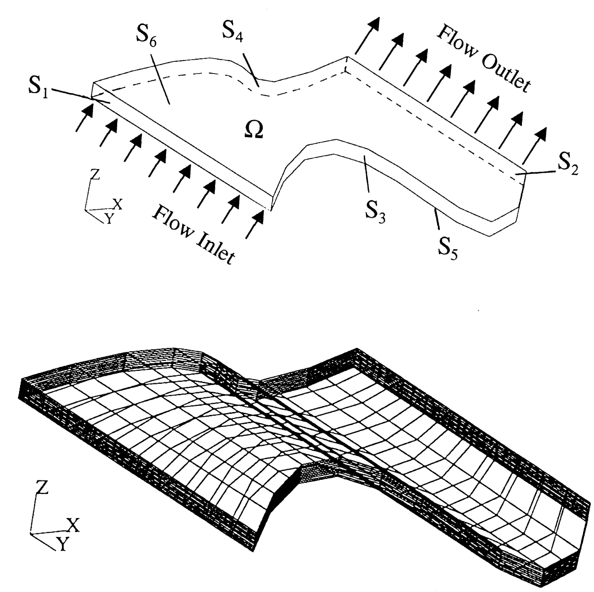

Fig. 1. The geometry and coordinates (a) and the grid system (b) for the test case 1.

Here f is the body force, ρ is the density, P is the pressure and ν is the kinematic viscosity of fluid. The above properties are all assumed constant.

Energy equation

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

Subjected to the following boundary conditions

$$T=T_1 \quad \text{on } S_1,\ t>0 \tag{3b}$$

$$-k\frac{\partial T}{\partial n}=h(T-T_\infty) \quad \text{on } S_2,\ t>0 \tag{3c}$$

$$\frac{\partial T}{\partial n}=0 \quad \text{on } S_3 \text{ to } S_5,\ t>0 \tag{3d}$$

$$k\frac{\partial T}{\partial n}=q(S_6,t)=\,? \quad \text{on } S_6,\ t>0 \tag{3e}$$

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

Here C_p is the heat capacity, k is the thermal conductivity, μ is the viscosity, and Φ is the viscous heating term, 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 letting the following notations,

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

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

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

$$\rho C_\text{p}\frac{\text{D}T}{\text{D}t}=k\nabla^2(T)+\mu\Phi \quad \text{in } \Omega,\ t>0 \tag{5c}$$

The solution for the above 3D 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. The direct problem considered here is concerned with the determination of the flow velocity field and fluid temperature when all the boundary conditions at all boundaries are known.

3. The inverse problem

For the inverse problem, the boundary heat flux on S_6 is regarded as being unknown, but everything else in Eqs. (1)–(3) is known. In addition, temperature readings taken at some appropriate locations and time on S_5 are considered available.

Let the temperature reading taken on S_5 be denoted by $Y(S_5, t) \equiv Y(x_m, y_m, z_m, t) \equiv Y_m(t)$, $m = 1$ to M, where M represents the number of measured temperature extracting points. We note that the measured temperature $Y_m(t)$ contain measurement errors. Then the inverse problem can be stated as follows: by utilizing the above-mentioned measured temperature data, $Y_m(t)$ estimate the unknown boundary heat flux $q(S_6, t)$.

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

$$J\left[q(S_6, t)\right] = \int_{t=0}^{t_f} \sum_{m=1}^{M} \left[T(x_m, y_m, z_m, t) - Y(x_m, y_m, z_m, t)\right]^2 \mathrm{d}t$$

$$= \int_{t=0}^{t_f} \sum_{m=1}^{M} \left[T_m(t) - Y_m(t)\right]^2 \mathrm{d}t \tag{6}$$

here, $T_m(t)$ are the estimated or computed temperatures at the measured temperature extracting locations (x_m, y_m, z_m) at time t. These quantities are determined from the solution of the direct problem given previously by using an estimated $\hat{q}(S_6, t)$ for the exact $q(S_6, t)$. Here the hat "ˆ" denotes the estimated quantities and t_f is the final time.

4. Conjugate gradient method for minimization

The following iterative process based on the conjugate gradient method [12] is now used for the estimation of unknown heat flux $q(S_6, t)$ by minimizing the functional $J[q(S_6, t)]$

$$\hat{q}^{n+1}(S_6, t) = \hat{q}^{n}(S_6, t) - \beta^n P^n(S_6, t) \quad \text{for} \quad n = 0, 1, 2, \ldots \tag{7a}$$

where β^n is the search step size from iteration n to iteration $n+1$, and $P^n(S_6, t)$ is the direction of descent (i.e. search direction) given by

$$P^n(S_6, t) = J'^n(S_6, t) + \gamma^n P^{n-1}(S_6, t) \tag{7b}$$

which is a conjugation of the gradient direction $J'^n(S_6, t)$ at iteration n and the direction of descent $P^{n-1}(S_6, t)$ at iteration $n-1$. The conjugate coefficient is determined from

$$\gamma^n = \frac{\int_{t=0}^{t_f} \int_{S_6} (J'^n)^2 \, \mathrm{d}S_6 \, \mathrm{d}t}{\int_{t=0}^{t_f} \int_{S_6} (J'^{n-1})^2 \, \mathrm{d}S_6 \, \mathrm{d}t} \quad \text{with } \gamma^0 = 0 \tag{7c}$$

We note that when $\gamma^n = 0$ for any n, in Eq. (7b), the direction of descent $P^n(S_6, t)$ becomes the gradient direction, i.e. the "Steepest descent" method is obtained. The convergence of the above iterative procedure in minimizing the functional J is guaranteed in [13].

To perform the iterations according to Eq. (7a), we need to compute the step size β^n and the gradient of the functional $J'^n(S_6, t)$. In order to develop expressions for the determination of these two quantities, a "sensitivity problem" and an "adjoint problem" are constructed as described below.

4.1. Sensitivity problem and search step size

The direct problem considered here is a forced convection problem and the properties of fluid are all assumed constant. For this reason when perturbing the unknown heat flux, the continuity and momentum equations remain unchanged. This implies that we do not have to recalculate the velocity field in the sensitivity problem.

The energy equation for the sensitivity problem is obtained from the original direct problem defined by Eq. (3) in the following manner: It is assumed that when $q(S_6, t)$ undergoes a variation Δq, T is perturbed by ΔT. Then replacing in the direct problem q by $q + \Delta q$ and T by $T + \Delta T$, subtracting from the resulting expressions the direct problem and neglecting the second-order terms, the following sensitivity problem for the sensitivity function ΔT are obtained.

$$\rho C_p \frac{\mathrm{D}\Delta T}{\mathrm{D}t} = k\nabla^2(\Delta T) \quad \text{in } \Omega, \, t > 0 \tag{8a}$$

$$\Delta T = 0 \quad \text{on } S_1, \, t > 0 \tag{8b}$$

$$-k\frac{\partial \Delta T}{\partial n} = h\Delta T \quad \text{on } S_2, \, t > 0 \tag{8c}$$

$$\frac{\partial \Delta T}{\partial n} = 0 \quad \text{on } S_3 \text{ to } S_5,\ t > 0 \tag{8d}$$

$$k\frac{\partial \Delta T}{\partial n} = \Delta q(S_6, t) \quad \text{on } S_6,\ t > 0 \tag{8e}$$

$$\Delta T = 0 \quad \text{in } \Omega,\ t = 0 \tag{8f}$$

The CFX 4.2 is used to solve this sensitivity problem.

The functional $J(\hat{q}^{n+1})$ for iteration $n+1$ is obtained by rewriting Eq. (6) as

$$J(\hat{q}^{n+1}) = \int_{t=0}^{t_f} \sum_{m=1}^{M} \left[T_m(\hat{q}^n - \beta^n P^n) - Y_m\right]^2 \mathrm{d}t \tag{9a}$$

where we replaced $\hat{q}^{n+1}$ by the expression given by Eq. (7a). If temperature $T_m(\hat{q}^n - \beta^n P^n)$ is linearized by a Taylor expansion, Eq. (9a) takes the form

$$J(\hat{q}^{n+1}) = \int_{t=0}^{t_f} \sum_{m=1}^{M} \left[T_m(\hat{q}^n) - \beta^n \Delta T_m(P^n) - Y_m\right]^2 \mathrm{d}t \tag{9b}$$

where $T_m(\hat{q}^n)$ is the solution of the direct problem by using estimate $\hat{q}^n$ for exact q at (x_m, y_m, z_m) and time t. The sensitivity functions $\Delta T_m(P^n)$ are taken as the solutions of problem (8) at the measured temperature extracting positions (x_m, y_m, z_m) and time t by letting $\Delta q = P^n$. The search step size β^n is determined by minimizing the functional given by Eq. (9b) with respect to β^n. The following expression results:

$$\beta^n = \frac{\displaystyle\int_{t=0}^{t_f} \sum_{m=1}^{M} \left[T_m(t) - Y_m(t)\right]\Delta T_m(t)\, \mathrm{d}t}{\displaystyle\int_{t=0}^{t_f} \sum_{m=1}^{M} \left[\Delta T_m(t)^2\right] \mathrm{d}t} \tag{10}$$

4.2. Adjoint problem and gradient equation

The continuity and momentum equations for the adjoint problem are the same as in the direct problem for the reason stated before. To obtain the energy equation for the adjoint problem, Eq. (3a) is multiplied by the Lagrange multiplier (or adjoint function) $\lambda(x, y, z, t)$ and the resulting expression is integrated over the correspondent space and time domains. Then the result is added to the right-hand side of Eq. (6) to yield the following expression for the functional $J[q(S_6, t)]$:

$$J\big[q(S_6, t)\big] = \int_{t=0}^{t_f} \int_{S_5} [T - Y]^2 \delta(x - x_m)\delta(y - y_m) \times \delta(z - z_m)\, \mathrm{d}S_5\, \mathrm{d}t + \int_{t=0}^{t_f} \int_{\Omega} \lambda \left\{ k\nabla^2 T - \rho C_p \frac{\mathrm{D}T}{\mathrm{D}t} \right\} \mathrm{d}\Omega\, \mathrm{d}t \tag{11}$$

The variation ΔJ is obtained by perturbing q by Δq and T by ΔT in Eq. (11), subtracting from the resulting expression the original Eq. (11) and neglecting the second-order terms. We thus find

$$\Delta J = \int_{t=0}^{t_f} \int_{S_5} 2(T - Y)\Delta T \delta(x - x_m)\delta(y - y_m)\delta(z - z_m) \times \mathrm{d}S_5\, \mathrm{d}t + \int_{t=0}^{t_f} \int_{\Omega} \lambda \left[k\nabla^2(\Delta T) - \rho C_p \frac{\mathrm{D}\Delta T}{\mathrm{D}t} \right] \mathrm{d}\Omega\, \mathrm{d}t \tag{12}$$

where $\delta(\cdot)$ is the Dirac delta function and (x_m, y_m, z_m), $m = 1$ to M, refer to the measured temperature extracting positions. In Eq. (12), the domain integral term containing Laplace operator is reformulated based on the Green's second identity, the domain integral term containing substantial derivative is reformulated based on the Reynold's second transport theorem; the boundary conditions of the sensitivity problem given by Eqs. (8b)–(8e) are utilized.

The vanishing of the integrands containing ΔT leads to the following adjoint problem for the determination of $\lambda(x, y, z, t)$:

$$\rho C_p \frac{\mathrm{D}\lambda}{\mathrm{D}t} + k\nabla^2(\lambda) = 0 \quad \text{in } \Omega,\ t > 0 \tag{13a}$$

$$\lambda = 0 \quad \text{on } S_1,\ t > 0 \tag{13b}$$

$$-k\frac{\partial \lambda}{\partial n} = \lambda\big(h + \rho C_p \mathbf{V} \cdot \mathbf{n}\big) \quad \text{on } S_2,\ t > 0 \tag{13c}$$

$$\frac{\partial \lambda}{\partial n} = 0 \quad \text{on } S_3 \text{ and } S_4,\ t > 0 \tag{13d}$$

$$k\frac{\partial \lambda}{\partial n} = 2(T - Y)\delta(x - x_m)\delta(y - y_m)\delta(z - z_m) \quad \text{on } S_5,\ t > 0 \tag{13e}$$

$$\frac{\partial \lambda}{\partial n} = 0 \quad \text{on } S_6,\ t > 0 \tag{13f}$$

$$\lambda = 0 \quad \text{in } \Omega,\ t = t_f \tag{13g}$$

Here **V** and **n** are the velocity and normal unit vectors, respectively. The adjoint problem is different from the standard initial value problems in that the final time conditions at time $t = t_f$ is 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 the CFX4.2 can be used to solve the above adjoint problem.

Finally, the following integral term is left

$$\Delta J = \int_{t=0}^{t_f} \int_{S_6} \lambda \Delta q(S_6, t)\, dS_6\, dt \tag{14a}$$

From definition [12], the functional increment can be presented as

$$\Delta J = \int_{t=0}^{t_f} \int_{S_6} J'[q(S_6, t)] \Delta q(S_6, t)\, dS_6\, dt \tag{14b}$$

A comparison of Eqs. (14a) and (14b) leads to the following expression for the gradient of functional $J'[q(S_6, t)]$ of the functional $J[q(S_6, t)]$:

$$J'[q(S_6, t)] = \lambda(x, y, z)|_{\text{on } S_6} \tag{15a}$$

We note that the gradient J' on inlet surface S_1 and at final time $t = t_f$ are always equal to zero since $\lambda(S_1, t_f) = 0$ and $\lambda(\Omega, t_f) = 0$. If the initial guess values of q^0 cannot be predicted correctly before the inverse calculation, the estimated values of heat flux q will deviate from exact values near the inlet surface and final time conditions. This is the case in the present study! Now the artificial gradients at the interface of S_1 and S_6 and final time are defined as follows

$$J'(S_6, t) = -\lambda(S_6 + \Delta x, t)|_{\text{on } S_1 \cap S_6} \tag{15b}$$

$$J'(S_6, t_f) = \lambda(S_6, t_f - \Delta t) \tag{15c}$$

where Δx and Δt denote the space and time increment used in CFX4.2.

By using the artificial gradient equations (15b) and (15c) in the gradient equation (15a), the singularity on inlet surface S_1 and at final time $t = t_f$ can be avoided in the present study and a reliable inverse solution can be obtained.

4.3. Stopping criterion

If the problem contains no measurement errors, the traditional check condition is specified as

$$J[\hat{q}^{n+1}(S_6, t)] < \varepsilon \tag{16a}$$

where ε is a small-specified number. However, the observed temperature data may contain measurement errors. Therefore, we do not expect the functional equation (6) to be equal to zero at the final iteration step. Following the experiences of the authors [6,9], we use the discrepancy principle as the stopping criterion, i.e. we assume that the temperature residuals may be approximated by

$$T_m(t) - Y_m(t) \approx \sigma \tag{16b}$$

where σ is the standard deviation of the measurements, which is assumed to be a constant. Substituting Eq. (16b) into Eq. (6), the following expression is obtained for stopping criteria ε:

$$\varepsilon = M\sigma^2 t_f \tag{16c}$$

Then, the stopping criterion is given by Eq. (16a) with ε determined from Eq. (16c).

5. Computational procedure

The computational procedure for the solution of this inverse problem using conjugate gradient method may be summarized as follows:

Suppose $\hat{q}^n(S_6, t)$ is available at iteration n.

Step 1. Solve the direct problem given by Eqs. (1)–(3) for $T(x, y, z, t)$.

Step 2. Examine the stopping criterion given by Eq. (16a) with ε given by Eq. (16c). Continue if not satisfied.

Step 3. Solve the adjoint problem given by Eq. (13) for $\lambda(x, y, z, t)$.

Step 4. Compute the gradient of the functional J' from Eq. (15).

Step 5. Compute the conjugate coefficient γ^n and direction of descent P^n from Eqs. (7c) and (7b), respectively.

Step 6. Set $\Delta q = P^n$, and solve the sensitivity problem given by Eq. (8) for $\Delta T(x, y, z, t)$.

Step 7. Compute the search step size β^n from equation (10).

Step 8. Compute the new estimation for $\hat{q}^{n+1}$ from Eq. (7a) and return to Step 1.

6. Results and discussion

The objective of this work is to show the validity of the CGM in estimating the boundary heat flux $q(S_6, t)$ in the inverse forced convection problems with no prior information on the functional form of the unknown quantities.

To illustrate the accuracy of the conjugate gradient method in predicting boundary heat flux $q(S_6, t)$ in an arbitrary duct domain Ω with 3D inverse analysis from the knowledge of transient temperature recordings, two specific examples having different form of heat fluxes and duct domains are considered here.

In order to compare the results for situations involving random measurement errors, we assume normally distributed uncorrelated errors with zero mean and constant standard deviation. The simulated inexact measurement data **Y** can be expressed as

$$\mathbf{Y} = \mathbf{Y}_{\text{exact}} + \omega\sigma \tag{17}$$

where $\mathbf{Y}_{\text{exact}}$ the solution of the direct heat convection problem with an exact boundary heat flux $q(S_6, t)$; σ is the standard deviation of the measurements; and ω is a random variable that is generated by subroutine DRNNOR of the IMSL [14] and will be within -2.576 to 2.576 for a 99% confidence bound.

One of the advantages of using the conjugate gradient method to solve the inverse problems is that the initial guesses of the unknown quantities can be chosen arbitrarily. In all the test cases considered here, the initial guesses of $\hat{q}(S_6, t)$ is taken as $\hat{q}(S_6, t)_{\text{initial}} = 0.0$.

6.1. Numerical test case 1

The geometry for the test case 1 is shown in Fig. 1(a), which represents an arbitrarily irregular domain having thin uniform thickness in z direction. If this thickness is more, the estimated fluxes may be damped (This matter will be discussed later).

The parameters that used in the present study are taken as $\mathbf{V} = u = 0.1$, $k = 1$, $\rho = 1$, $C_p = 1$, $\mu = 1$, $h = 1$, $T_\infty = 1$ and $T_0 = 0$. The boundary conditions on S_3, S_4 and S_5 (bottom surface) are all insulated, the boundary conditions on S_1 and S_2 are subjected to first and third kind conditions, respectively, while a unknown heat flux $q(S_6, t)$ is prescribed on S_6 (upper surface). The grids along x, y and z directions are all taken as 10. Time interval is chosen as 15 i.e. $t_f = 15$, and a time step $\Delta t = 1$ is used. Therefore, a total of 1500 unknown discretized heat fluxes are to be determined in the present study. The number of measured temperature-extracting positions M is taken as 100. The grid system for test case 1 is shown in Fig. 1(b).

We now present below the numerical experiments in determining $q(S_6, t)$ by the inverse analysis using the CGM.

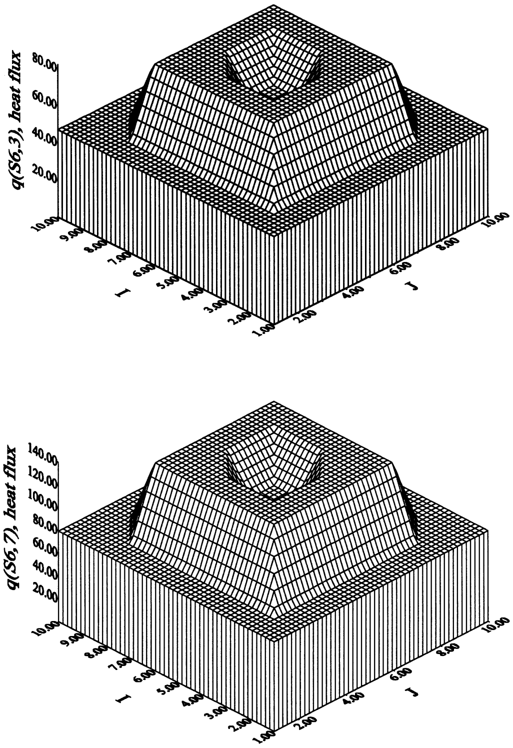

Fig. 2. The exact 3D plot of heat flux $q(S_6, t)$ for test case 1 at $t = 3$ and 7.

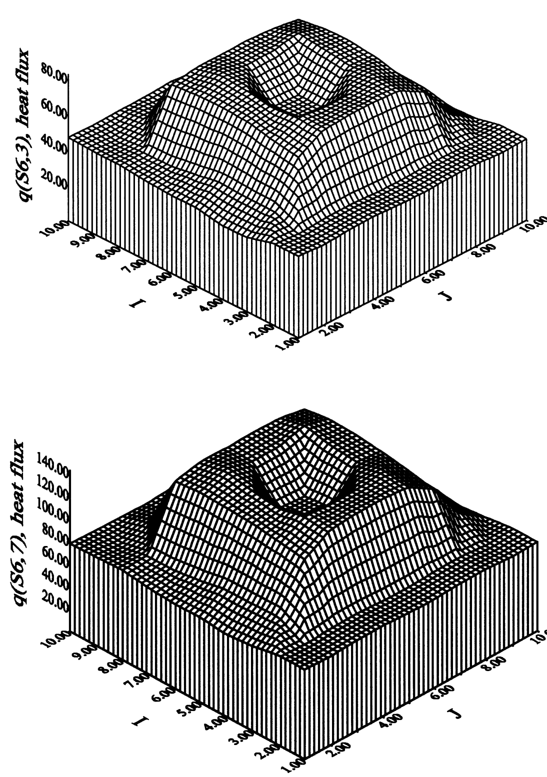

Fig. 3. The estimated 3D plot for heat flux $q(S_6, t)$ at $t = 3$ and 7 by using $\sigma = 0.0$ and $u = 0.1$.

The unknown transient boundary heat flux $q(S_6, t)$ (or $q(I, J, t)$) on S_6 is assumed as

$$
\begin{aligned}
&q_1(I, J, t) = 80 \times \sin\left(\frac{t}{t_f}\pi\right), && \begin{matrix}1 \le I \le 10\\ 1 \le J \le 10\end{matrix} && 15 \ge t \ge 0\\
&q_2(I, J, t) = 60 \times \sin\left(\frac{t}{t_f}\pi\right), && \begin{matrix}3 \le I \le 8\\ 3 \le J \le 8\end{matrix} && 15 \ge t \ge 0\\
&q_3(I, J, t) = -30 \times \sin\left(\frac{t}{t_f}\pi\right), && \begin{matrix}5 \le I \le 6\\ 5 \le J \le 6\end{matrix} && 15 \ge t \ge 0\\
&q(I, J, t) = (q_1 + q_2 + q_3), && \text{in } \Omega && 15 \ge t \ge 0
\end{aligned}
\tag{18}
$$

where I and J represent the grid index on surface S_6. It is obvious from Eq. (18) that $q(S_6, t_f) = 0$ due to sinusoidal function. Since $\hat{q}(S_6, t)_{\text{initial}} = 0.0$, we concluded that the singularity at final time t_f will not happen in this case and accurate inverse solutions can be obtained. The exact 3D plot for $q(S_6, t)$ at $t = 3$ and 7 is shown in Fig. 2.

The inverse analysis is first performed by assuming exact measurements, $\sigma = 0.0$. The estimated 3D plot for $q(S_6, t)$ after 60 iterations at $t = 3$ and 7 is shown in Fig. 3. It can be seen from Fig. 3 that the estimations are accurate except for the locations of discontinuity. The average error for this case is calculated as 3.75% where the average error for the estimated heat flux is defined as

Average error

$$
\% = \left[\sum_{I=1}^{10}\sum_{J=1}^{10}\sum_{t=1}^{t_f}\left|\frac{q(I, J, t) - \hat{q}(I, J, t)}{q(I, J, t)}\right|\right] \div (10 \times 10 \times t_f) \times 100\% \tag{19}
$$

here I and J represent the index of discreted unknown heat fluxes on S_6 and t denotes the index of discrete time, while $q(I, J, t)$ and $\hat{q}(I, J, t)$ denote the exact and estimated values of boundary heat flux.

Next, let's discuss the influence of varying the inlet velocity on the inverse solutions. The inverse calculations for $u = 0.2$ is then performed and 3D plot for the estimated heat flux at $t = 3$ and 7 is shown in Fig. 4. It is obvious that the estimated heat flux is not that accurate as was for $u = 0.1$. The reason for this is because when the inlet velocity is increased, the information for $q(S_6, t)$ on the measurement surface S_5 is

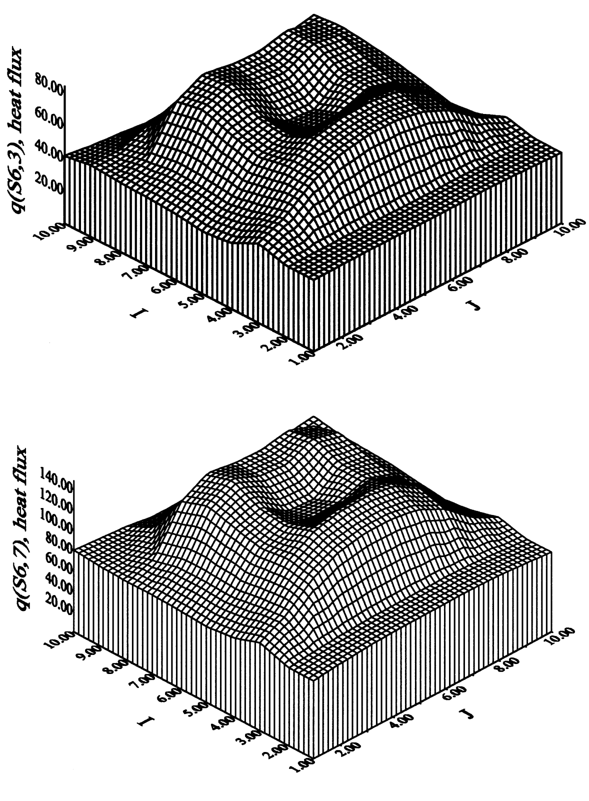

Fig. 4. The estimated 3D plot for heat flux $q(S_6, t)$ at $t = 3$ and 7 by using $\sigma = 0.0$ and $u = 0.2$.

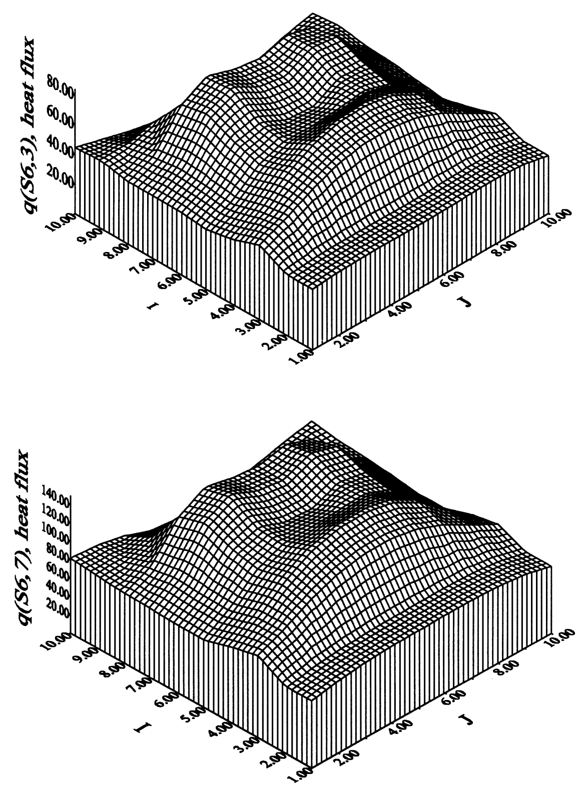

Fig. 5. The estimated 3D plot for heat flux $q(S_6, t)$ at $t = 3$ and 7 by using $\sigma = 0.0$, $u = 0.1$ and tripled thickness in z-direction.

damped due to the fact that more energy is carried away by the fluid. The average error for this case is calculated as 8.86%.

What will happen when the thickness in z-direction is increased? To test this situation we perform another numerical experiment by assuming that the thickness in z-direction is tripled (letting $u = 0.1$). The estimation for $q(S_6, t)$ must be worse than as shown in Fig. 3 since the information for $q(S_6, t)$ on the measurement surface S_5 is damped due to the fact that the thickness is increased. The 3D plot for the estimated heat flux at $t = 3$ and 7 is shown in Fig. 5 and the average error for this case is calculated as 12.15%.

Finally, let's discuss the influence of the measurement errors on the inverse solutions for $u = 0.1$ and thin thickness in z-direction (original thickness). First, the measurement error for the temperatures measured by sensors is taken as $\sigma = 8.0$ (about 1.5% of the average measured temperature), then error is increased to $\sigma = 16.0$ (about 3.0% of the average measured temperature). The estimated 3D plot for $q(S_6, t)$ at $t = 3$ and 7 is shown in Figs. 6 and 7, respectively, where the average error in Fig. 6 is 7.22% and in Fig. 7 9.54%. The stopping criteria ε is calculated from Eq. (16c) and the number of iterations are 33 and 23 for

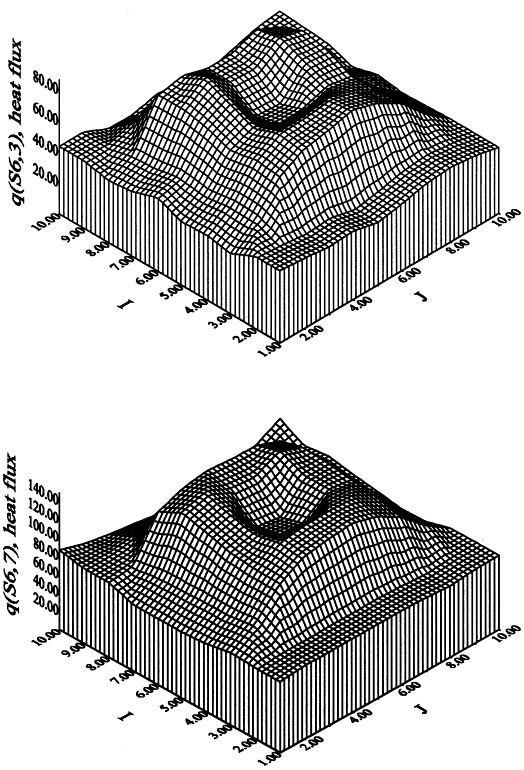

Fig. 6. The estimated 3D plot for heat flux $q(S_6, t)$ at $t = 3$ and 7 by using $\sigma = 8.0$ and $u = 0.1$.

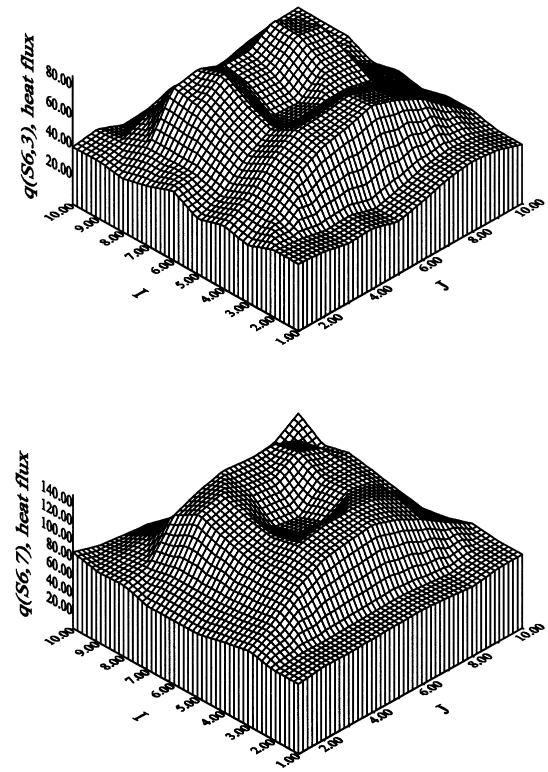

Fig. 7. The estimated 3D plot for heat flux $q(S_6, t)$ at $t = 3$ and 7 by using $\sigma = 16.0$ and $u = 0.1$.

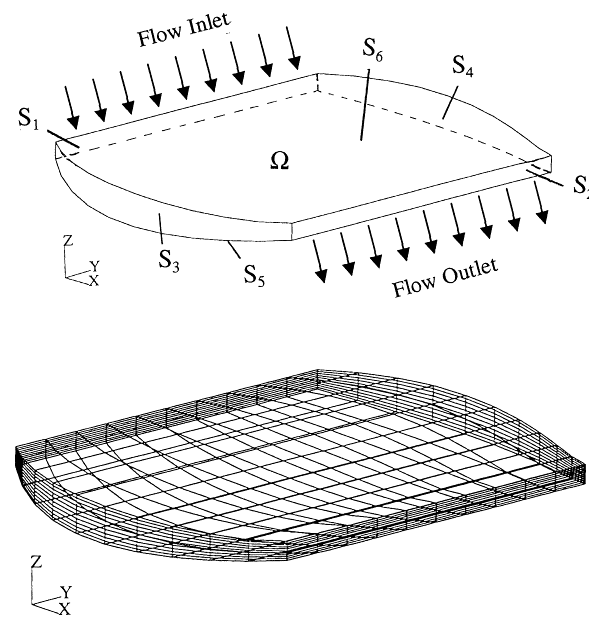

Fig. 8. The geometry and coordinates (a) and the grid system (b) for the test case 2.

the above two test cases. This implies that reliable inverse solutions can still be obtained when measurement errors are considered.

6.2. Numerical test case 2

The geometry for test case 2 is now considered as a non-uniform thickness in z-direction and is shown in Fig. 8(a), while the grid system is shown in Fig. 8(b). The parameter used in this test case are the same as were used in test case 1. The unknown boundary heat flux $q(S_6, t)$ is assumed as

$$
\begin{aligned}
&q(I, J, t) = 4 \times \sin\left(\frac{t}{15}\pi\right) \times \left[20 - (8 - I)^2 - (3 - J)^2\right] + 20, && 5 \le I \le 10,\ 1 \le J \le 5 && 15 \ge t \ge 0 \\
&q(I, J, t) = 7.5 \times \sin\left(\frac{t}{22}\pi\right) \times \left[17 - (2 - I)^2 - (7 - J)^2\right] + 22, && 1 \le I < 5,\ 5 < J \le 10 && 15 \ge t \ge 0 \\
&q(I, J, t) = 20, && \text{else} && 15 \ge t \ge 0
\end{aligned}
\tag{20}
$$

The exact 3D plot for $q(S_6, t)$ at $t = 3$ and 7 is shown in Fig. 9. One should note that in test case 2 we still use $\hat{q}(S_6, t)_{\text{initial}} = 0.0$, but now $q(S_6, t_f) \neq 0$, therefore, we concluded that the singularity at final time t_f will happen in this case and the modified gradient at final time in Eq. (15c) must be used to overcome this singularity. However, the inverse solutions near final time under this consideration are still not accurate, therefore, the estimated heat flux at the last few time steps are going to be discarded to ensure good estimations are obtained.

In test case 2, the estimated $\hat{q}(S_6, t)$ is chosen up to $t = 12$ and the remaining three time steps are neglected. The inverse problem with CGM is first calculated by using exact measurements, i.e. $\sigma = 0.0$. After 60 iterations the 3D plot for the estimated boundary heat flux $q(S_6, t)$ at $t = 3$ and 7 is shown in Fig. 10. It is obvious that the estimated $q(S_6, t)$ for the present inverse solutions is not that accurate when comparing with test case 1. The reason for this is because a non-uniform thickness and thicker thickness are considered in the present case. The average errors for CGM is 6.92% in this case.

Next when considering measurement errors $\sigma = 8.0$ (about 4.0% of the average measured temperature),

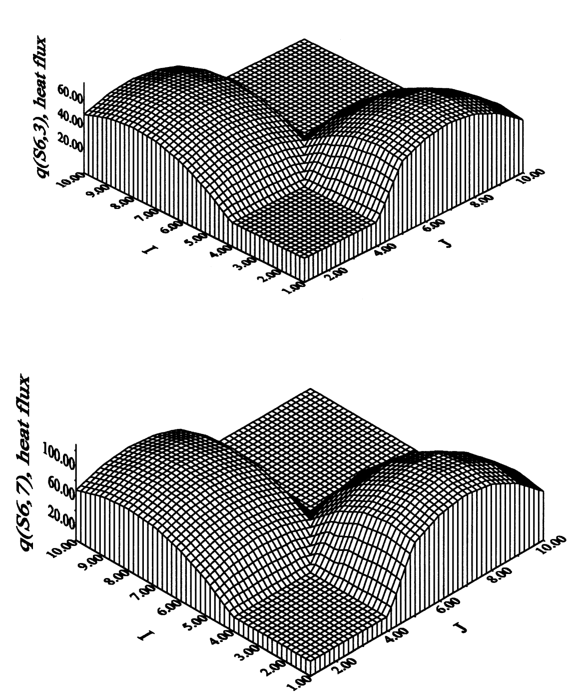

Fig. 9. The exact 3D plot of heat flux $q(S_6, t)$ for test case 2 at $t = 3$ and 7.

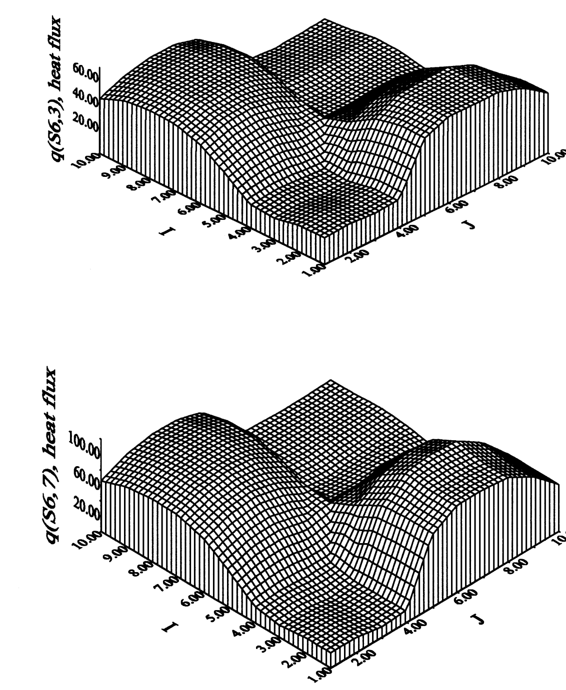

Fig. 10. The estimated 3D plot for heat flux $q(S_6, t)$ at $t = 3$ and 7 by using $\sigma = 0.0$ and $u = 0.1$.

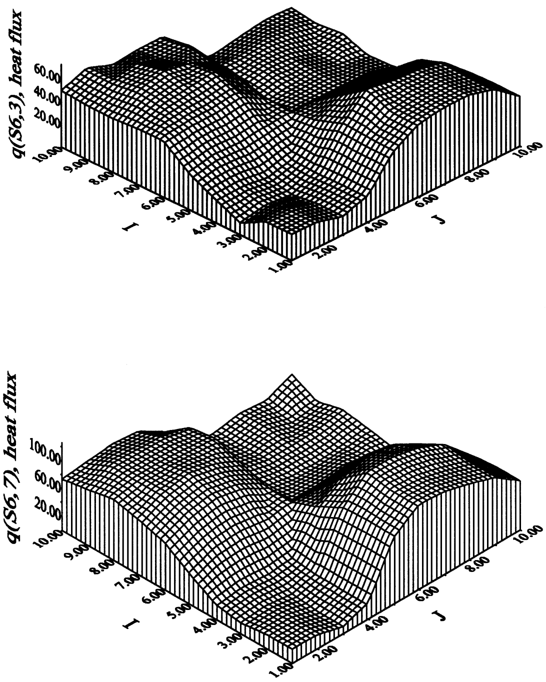

Fig. 11. The estimated 3D plot for heat flux $q(S_6, t)$ at $t = 3$ and 7 by using $\sigma = 8.0$ and $u = 0.1$.

the estimated inverse solutions are shown in Fig. 11. The average errors for CGM is 10.58% for this case.

From the above two test cases we learned that a 3D inverse forced convection problem in estimating unknown boundary heat flux is now completed. Reliable estimations can be obtained when using either exact or error measurements.

7. Conclusions

The Conjugate Gradient Method (CGM) along with the CFX-4.2 was successfully applied for the solution of the three-dimensional inverse forced convection problem to determine the unknown transient boundary heat flux in an irregular duct domain by utilizing simulated temperature readings obtained from sensors. Several test cases involving different shape of duct, duct thickness, inlet velocity, measurement errors and heat fluxes were considered. The results show that the inverse solutions obtained by CGM remain stable and regular as the measurement errors are increased.

From the numerical test cases in the present study, we concluded that the use of CFX-4.2 as the subroutine in the 3D inverse forced convection problem in estimating the unknown boundary heat flux with the conjugate gradient method has been done successfully. By using the same algorithm, many practical but difficult 3D inverse convection problems can also be solved.

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