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Estimating the heat source and the heat transfer coefficient simultaneously in a living tissue by conjugate gradient method

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Keywords- *Hyperthermia; Inverse Problem; Heat Source; Heat Flux; Conjugate Gradient Method*

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I. INTRODUCTION

One way for treating tumor region is increasing its temperature to a specific quantity, while the temperature in neighboring healthy parts remains in the safe range [1]. This method is named hyperthermia and it can be used with some other types of cancer therapy methods, such as chemotherapy and radiotherapy. The temperature distribution in the tissue should be controlled to achieve a safe and effective treatment. Instead of using experimental devices, the inverse methodology can be employed to obtain boundary conditions or material's thermal properties for the desired temperature distribution. In this method the temperature of medium is regarded as additional information and therefore, unknown quantities are obtained.

Several investigations are carried out optimizing controllable parameters to achieve the desired temperature distribution along the living tissue. Dhar et al. [2] obtained time dependent heating power in a multilayered tissue to attain desirable temperature distribution across the tumor. Ren et al. [3], used boundary element method to obtain the heat source in biological bodies. Kuznetsov [4] fixed the total volumetric heat generation due to spatial heat source in the Pennes equation over the treatment procedure in order to formulate an optimal problem to maximize the tumor temperature. He showed that the maximization of temperature and of the thermal dose is not necessarily equivalent.

Another issue that concerns inverse bio-heat transfer problem is obtaining thermal properties of the living tissue. Liu et al, [5] studied the inverse non-Fourier bio-heat transfer problem by dual phase lag model. In this model, phase lag times are estimated with the experimental data. Yang et al. [6] considered the non-Fourier effect of finite heat propagation and estimated the unknown time-dependent surface heat flux of a living skin tissue by conjugate gradient method. Aghayan et al. [7] estimated the overall heat transfer coefficient of the cooling system of RF capacitive hyperthermia treatment by using conjugate gradient method. The effects of measurement errors and sensor positions are also investigated.

Pennes equation [8] is a simple bio-heat transfer equation which is used widely for modeling the heat transfer in the living tissue. In this equation, the heat exchange between blood and tissue is considered as a heat sink. Deng et al. [9] solved this problem analytically by the Green function method. The condition of using this equation is investigated by several researchers. Horng et al. [10] indicated that the Pennes equation is appropriate to model the heat exchange from vessels with diameters less than 0.5mm. Kou et al. [11] applied one equation porous model (OEPM) and solved it with the Green function method. This model is organized based on combination of the energy conservation equations of tissue and blood into one single energy equation and the porous medium concept. Yuan [12] proposed two equation porous models (TEPM) and compared results with one equation porous model. The comparison indicated that OEPM is appropriate for simulating the temperature and the thermal dose distribution accurately until the diameter of the blood vessels distributed in the tissue is less than 30 μm.

Applying inverse method to simultaneously obtain thermal properties of tissue is reported rarely in the literature. Huang et al. [13] used the conjugate gradient method to determine the optical diffusion and the absorption coefficients of tissue simultaneously. Huang et al. [14] considered the effect of measurement errors and applied Levenberg-Marquardt method to estimate the effective thermal conductivity and the volumetric heat capacity of a living tissue simultaneously.

Administering the surface temperature by skin cooling is the most appropriate way for controlling the temperature in the tissue. However, this method is only efficient for controlling the temperature of limited parts which are positioned near the skin. Another way of controlling the tissue temperature is adjusting the external heat source properly. Since the external heat source and the heat transfer coefficient at the skin surface are two major controllable parameters in hyperthermia, the perfect solution is to estimate them simultaneously for the desired temperature distribution. In this paper conjugate gradient method with adjoint problem is applied as the inverse method, and these two parameters are estimated.

II. MATHEMATICAL MODELING

A schematic of tissue model is shown in Fig. 1. The temperature of superficial tissue is increased by the external heat source. It is assumed that no significant blood vessel (any vessel with a diameter larger than 30μm [12]) is passed from the tissue. Thermo physical properties of tissue are constant, and the modeled tissue is composed of only one layer with mean properties. Perfusion is assumed to be uniform through time and space. The formulation of direct, sensitivity, and adjoint problems are needed to solve problem by conjugate gradient method. These equations are obtained as follows.

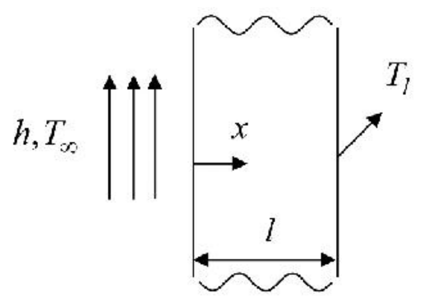

Fig. 1. Schematic of a one-dimensional tissue model

A. The Direct Problem

One dimensional Pennes equation is applied. The mathematical formulation of governing equation, boundary conditions, and initial condition of the direct problem can be expressed as:

$$\rho_t c_t \frac{\partial T}{\partial t} = k_t \frac{\partial^2 T}{\partial x^2} + \rho_b c_b \omega_b \left(T_b - T\right) + Q_m + Q(t) \tag{1}$$

$$-k_t \frac{\partial T(0,t)}{\partial x} = h\left(T_\infty - T(0,t)\right) \tag{2}$$

$$T(l,t) = 37^{0C} \tag{3}$$

$$T(x,0) = 37^{0C} \tag{4}$$

where $Q(t)$ is the heat source, the subscripts t, b, and ∞ refer to the tissue, blood, and the cooling fluid, respectively. T, ρ, c, and k are temperature, density, specific heat, and thermal conductivity, respectively. The metabolic heat generation is demonstrated by Q_m and the final time of measurement is denoted by t_f.

B. The Inverse Problem

In the inverse problem, all the parameters in the direct problem are considered to be known, except the heat source and the heat transfer coefficient. Temperature distribution which is obtained from the direct problem is considered as additional information. The difference between the temperature data from the direct problem and the temperature data which is obtained by solving the inverse problem should be minimized. In this case, the following functional should minimize:

$$J\left[Q(t), h(t)\right] = \sum_{m=1}^{M} \int_{t=0}^{t_f} \left[Z_m(t) - T_m(t)\right]^2 dt \tag{5}$$

where $Z_m(t)$ and $T_m(t)$ are refer to measured temperature and computed temperature at the sensor locations, respectively.

2.2.1 The Sensitivity Problem

The sensitivity problem can be obtained by perturbing the heat source $Q(t)$ by $\Delta Q(t)$ and the temperature $T(x,t)$ by ΔT_1. The subscripts (1) refer to perturbing the temperature when the heat source is changed. These perturbed quantities should be replaced in the direct problem. Then, by subtracting the original direct problem from this resulting relation, the sensitivity problem is obtained. By neglecting second order terms, the sensitivity equation, the boundary conditions and the initial condition are obtained as follows:

$$\rho_t c_t \frac{\partial \Delta T_1}{\partial t} = k_t \frac{\partial^2 \Delta T_1}{\partial x^2} - \rho_b c_b \omega_b \Delta T_1 + \Delta Q(t) \tag{6}$$

$$k_t \frac{\partial \Delta T_1(0,t)}{\partial x} = h \Delta T_1(0,\mathrm{t}) \tag{7}$$

$$\Delta T_1(l,t) = 0 \tag{8}$$

$$\Delta T_1(x,0) = 0 \tag{9}$$

Similar to this process, the sensitivity problem for the heat transfer coefficient can be obtained. The sensitivity equation, the boundary conditions and the initial condition for the sensitivity problem for the $h(t)$ are as follows:

$$\rho_t c_t \frac{\partial \Delta T_2}{\partial t} = k_t \frac{\partial^2 \Delta T_2}{\partial x^2} - \rho_b c_b \omega_b \Delta T_2 \tag{10}$$

$$-k_t \frac{\partial \Delta T_2(0,t)}{\partial x} = -h \Delta T_2(0,\mathrm{t}) + \Delta h(T_\infty - T(0,t)) \tag{11}$$

$$\Delta T_2(l,t) = 0 \tag{12}$$
$$\Delta T_2(x,0) = 0 \tag{13}$$

where the subscript (2) refer to the condition in which the temperature variation is caused by the changes in the heat transfer coefficient.

2.2.2 The adjoint Problem

The adjoint problem is obtained by multiplying the direct problem by the Lagrange multipliers $\lambda(x,t)$ and integrating over the corresponding time and space domain. This expression should be added to right-hand side of Eq. (5). So, the following expression is obtained for the functional:

$$\begin{aligned} J_1[Q(t)] &= \sum_{m=1}^{M}\int_{t=0}^{t_f}\left[T_m(t)-Z_m(t)\right]^2 dt + \\ &\int_{t=0}^{t_f}\int_{x=0}^{L}\lambda(x,t)\left[k_t\frac{\partial^2 T}{\partial x^2}+\rho_b c_b \omega_b\left(T_b-T\right)+Q_m+Q(t)-\rho_t c_t\frac{\partial T}{\partial t}\right]dxdt \end{aligned} \tag{14}$$

The variation of the above relation is obtained by perturbing $T(x,t)$ by $\Delta T_1(x,t)$. Then the original expression (Eq. 14) subtracted from the resulting relation, and second order terms are neglected, thus the following relation is obtained:

$$\begin{aligned} \Delta J_1 &= 2\int_{t=0}^{t_f}\int_{x=0}^{l}\left[T_m(t)-Z_m(t)\right]\Delta T(x,t)\delta(x-x_m)dxdt + \\ &\int_{t=0}^{t_f}\int_{x=0}^{L}\lambda(x,t)\left[k_t\frac{\partial^2 \Delta T}{\partial x^2}-\rho_b c_b \omega_b \Delta T+\Delta Q-\rho_t c_t\frac{\partial \Delta T}{\partial t}\right]dxdt \end{aligned} \tag{15}$$

The second term in the right hand side of Eq. (15) is integrated by parts. After some mathematical operation and utilizing the initial and boundary conditions of the sensitivity problem the adjoint problem is obtained as follows:

$$\begin{aligned} -\rho_t c_t\frac{\partial \lambda}{\partial t} &= 2\left[T_m(\tau)-Z_m(\tau)\right]\delta(x-x_m) \\ &+k_t\frac{\partial^2 \lambda}{\partial x^2}-\rho_b c_b \omega_b \lambda \end{aligned} \tag{16}$$

$$k_t\frac{\partial \lambda(0,t)}{\partial t} = h\lambda(0,t) \tag{17}$$
$$\lambda(l,t) = 0 \tag{18}$$
$$\lambda(x,t_f) = 0 \tag{19}$$

The following integral term is remains:

$$\Delta J_1\left[Q(t)\right] = \int_{t=0}^{t_f}\int_{x=0}^{L}\lambda(x,t)\Delta Q(t)dxdt \tag{20}$$

2.2.3 The Gradient Equation

By assuming that the unknown function $Q(t)$ belongs to the square integrable functions in the domain $0<t<t_f$, we can write:

$$\Delta J_1\left[Q(t)\right] = \int_{t=0}^{t_f} J'_1\left[Q(t)\right]\Delta Q(t)dt \tag{21}$$

where $J'_1\left[Q(t)\right]$ is the gradient of functional $J\left[Q(t)\right]$. By comparing Eq.(20) and (21) the relation for the gradient of functional $J\left[Q(t)\right]$ is obtained as follows:

$$J'_1\left[Q(t)\right] = \int_{t=0}^{t_f}\lambda(x,t)dx \tag{22}$$

Similarly, the effect of the variation of the functional (14) by change in the heat transfer coefficient can be obtained by perturbing $T(x,t)$ by $\Delta T_2(x,t)$ and $h(t)$ by $\Delta h(t)$. After similar mathematical operation, the adjoint problem is found identical to the one for $Q(t)$. The gradient equation for this case is obtained from the following relation:

$$J'_2\left[h(t)\right] = -\lambda(0,t)\left(T(0,t)-T_\infty\right) \tag{23}$$

2.2.4 Conjugate Gradient Method for Minimization

The iterative procedure of the conjugate gradient method for evaluating $Q(t)$ and $h(t)$ at the $(k+1)^{th}$ step is as follows:

$$Q^{k+1}(t) = Q^k(t) - \beta_1^k P_1^k(t) \tag{24}$$
$$h^{k+1}(t) = h^k(t) - \beta_2^k P_2^k(t) \tag{25}$$

in these equations β^k is the search step size and P^k is the direction of descent. The directions of descent are obtained from the following relations:

$$P_1^k = J'^k_1 + \gamma_1^k P_1^{k-1} \tag{26}$$
$$P_2^k = J'^k_2 + \gamma_2^k P_2^{k-1} \tag{27}$$

in the above equation, γ^k is the conjugate coefficient at k^{th} step. The conjugate coefficients is obtained as follows:

$$\gamma_1^k = \frac{\int_{x=0}^{L} \{J'^k_1[Q(t)]\}^2 dx}{\int_{x=0}^{L} \{J'^{k-1}_1[Q(t)]\}^2 dx}, \ \ with \ \gamma_1^0 = 0. \tag{28}$$

$$\gamma_2^k = \frac{\int_{x=0}^{L} \{J'^k_2[h(t)]\}^2 dx}{\int_{x=0}^{L} \{J'^{k-1}_2[h(t)]\}^2 dx}, \ \ with \ \gamma_2^0 = 0. \tag{29}$$

Finally, the search step sizes are obtained as following relations:

$$\beta_1^k = \frac{\sum_{m=1}^{M}\int_{t=0}^{t_f}\left[T_m(t)-Z_m(t)\right]\Delta T_m\left(P_1^k\right)dt}{\sum_{m=1}^{M}\int_{t=0}^{t_f}[\Delta T_m\left(P_1^k\right)]^2\, dt} \tag{30}$$

$$\beta_2^k = \frac{\sum_{m=1}^{M}\int_{t=0}^{t_f}\left[T_m(t)-Z_m(t)\right]\Delta T_m\left(P_2^k\right)dt}{\sum_{m=1}^{M}\int_{t=0}^{t_f}[\Delta T_m\left(P_2^k\right)]^2\, dt} \tag{31}$$

in these equation $\Delta T_m\left(P_1^k\right)$ and $\Delta T_m\left(P_2^k\right)$ are obtained by solving the sensitivity problems. In the first sensitivity problem $\Delta Q(t)$ is substituted by P_1^k , and in the second one $\Delta h(t)$ is substituted by P_2^k .

2.2.5 Stopping Criterion

The stopping criterion for this method for the case that contains no measurement error is specified as follows:

$$J(Q^{k+1}, h^{k+1}) < \varepsilon \tag{32}$$

where ε is a small specified number, that can be used as the stopping criterion. Measurement errors in the temperature data is also considered in the solution. By assuming $Z_m(t) - T_m(t) = \sigma$ as the standard deviation of the measurement error, the stopping criteria ε can be obtained from the discrepancy principle:

$$\varepsilon = M\sigma^2 t_f . \tag{33}$$

III. RESULTS AND DISCUSSION

Achieving desired temperature distribution at the tumor region cannot be simply obtained, since it is being affected by several parameters. Inaccessibility of boundary conditions in the tissue except the skin condition and disability of current equipments to generate the demanded heat source are the most important problems to achieve safe and efficient therapy. Both the external heat source and the heat transfer coefficient of cooling fluid are considered as objectives of this study.

One dimensional Pennes equation with cooling condition at skin is regarded as the governing equation. The reasonable length is $l = 0.03$m as demonstrated in other studies [9]. The final time is chosen as 60s. The thermo-physical properties of the tissue are demonstrated in table 1.

TABLE I. THERMO PHYSICAL PROPERTIES OF TISSUE

Properties	Value
c_t, c_b	4200 J/kg.K
ρ_t, ρ_b	1000 kg/m^3
k_t	0.5 W/m.K
Q_m	3380 W/m^3
ω_b	0.0005 ml/s/ml
T_b	37°C

Finite volume approach with the fully implicit method is used to solve direct, sensitivity, and adjoint problems. In order to solve discretized equations, TDMA method is implemented. The code is verified and the grid size and time step are found as $3*10^{-4}$m and 1s, respectively. The direct problem is validated by Deng's analytical solution [9]. First, the direct problem is solved with known heat source and heat transfer coefficient and as a result the temperature distribution is obtained. Hence, the pseudo measurement is ready to be imported into the inverse procedure. In this problem sensors are located on the grid location.

The applicability of conjugate gradient method is assessed by two numerical test cases.

A. *Numerical test case 1*

In the first case, the triangular profiles are considered for the time-dependent heat source and the heat transfer coefficient.

Fig. 2. compares exact values of the heat source with estimated results and Fig. 3. compares the exact values of the heat transfer coefficient with estimated ones which are obtained by the inverse method.

Zero value is considered as an initial guess, for both the heat source and the heat transfer coefficient. The average relative errors for the time-dependent heat source and the heat transfer coefficient are computed in order to study the validity of the inverse method. These relative errors are defined as following relations:

$$\text{ERR1\%} = \sum_{j=1}^{60}\left|\frac{Q(j)-\bar{Q}(j)}{Q(j)}\right| / 60 \times 100\% \tag{36}$$

$$\text{ERR}\,2\% = \sum_{j=1}^{60} \left| \frac{h(j) - \bar{h}(j)}{h(j)} \right| / \, 60 \times 100\% \tag{37}$$

where $\bar{Q}(j)$ and $\bar{h}(j)$ are represented as estimated values of the time-dependent heat source and the heat transfer coefficient respectively and j represents the index of time step.

In this test case, for exact measurements, i.e. $\sigma = 0.0$, the average errors for $Q(t)$ and $h(t)$ are computed as $ERR1 = 1.78\%$ and $ERR2 = 2.037\%$,respectively.

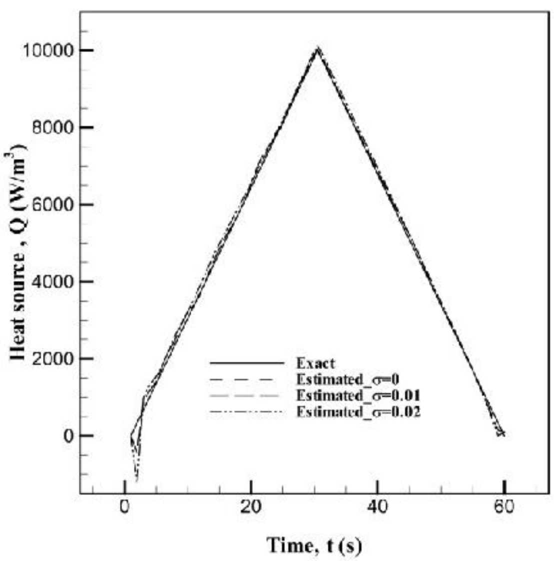

Fig. 2. Estimated heat source for different measurement errors (case 1)

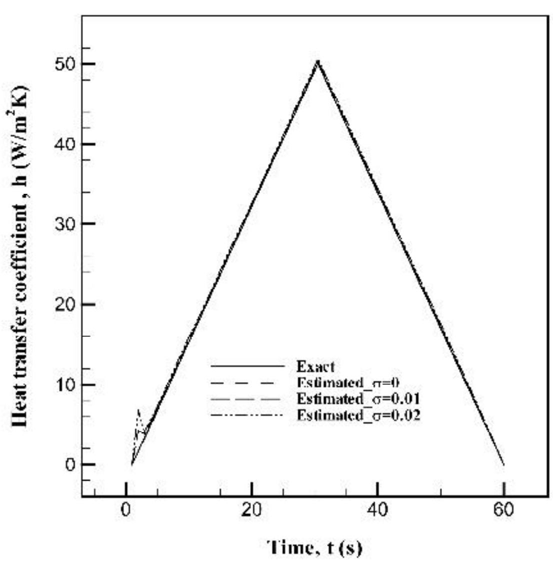

Fig. 3. Estimated heat transfer coefficient for different measurement errors (case 1)

The effect of the measurement errors on the inverse solution is also studied by calculating the average relative errors. In the case of $\sigma = 0.01$, the average errors for $Q(t)$ and $h(t)$ are computed as $ERR1 = 7.56\%$ and $ERR2 = 4.08\%$, respectively. Finally, for $\sigma = 0.02$, the average errors for $Q(t)$ and $h(t)$ are found as $ERR1 = 14.04\%$ and $ERR2 = 8.09\%$, respectively. The relative average errors for both functions have a reasonable increase following the trend of measurement errors. (use equation module for the all relations)

3.1 Numerical test case 2

The accuracy of simultaneous estimation of the heat source and the heat transfer coefficient with conjugate gradient method is also examined by the step profile. is considered for the time-dependent heat source and the heat transfer coefficient.

The maximum value for $Q(t)$ in the numerical test case 2 is considered equal to the one in the numerical test case 1, and the same rule is carried out for $h(t)$ .Fig. 4. and Fig. 5. compare the solution of the inverse and the direct problems for the second test case.

Similar to the first case, the inverse problem is solved by zero initial guess value for both the heat source and the heat transfer coefficient. For this test case, the average errors for $Q(t)$ and $h(t)$ are computed as $ERR1 = 4.08\%$ and $ERR2 = 2.21\%$, respectively for exact measurements.

By considering the measurement errors, the average relative errors are obtained. In the case of $\sigma = 0.01$, the average errors for $Q(t)$ and $h(t)$ are found as $ERR1 = 4.14\%$ and $ERR1 = 2.54\%$, respectively.

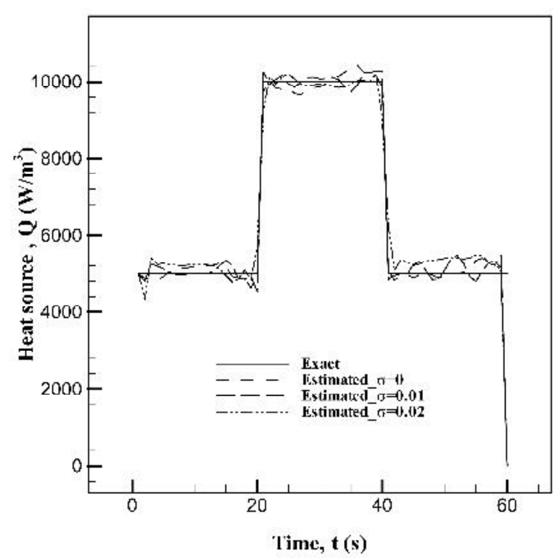

Fig. 4. Estimated heat source for different measurement errors (case 2)

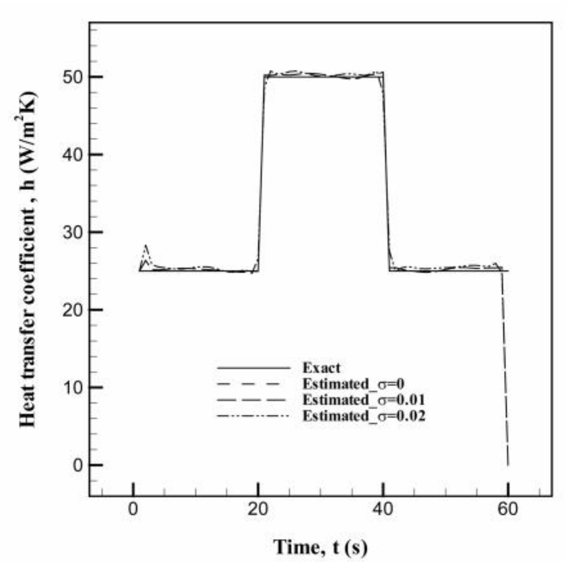

Fig. 5. Estimated heat transfer coefficient for different measurement errors (case 2)

For $\sigma = 0.02$, the average errors for Q(t) and h(t) are calculated as $ERR1 = 6.11\%$ and $ERR2 = 3.69\%$, respectively. Similar to the previous test case, the relative average errors have a reasonable increase following the trend of measurement.

Inaccurate estimation value is easily detectable at the end of time domain in this test case. Paying attention to the adjoint problem and the gradient equation, it can be seen that the gradient equation is null in this point and therefore, the initial guess stays fixed, so it cannot be modified by the procedure. In the first test case, for both the heat source and the heat transfer coefficient, such problem does not exist, because their exact value and initial guess in this point is the same. This problem can be solved easily by considering a larger domain instead of current one.

To observe the effect of initial guess value on the estimated values, $h = 10W/m^2K$ and $Q = 100W$ are applied as initial value for both numerical test cases. The relative errors for all cases including estimation of exact measurements are not altered significantly.

1. CONCLUSIONS

The conjugate gradient method with adjoint problem was applied to determine the time dependent heat source and the heat transfer coefficient simultaneously in a living tissue. One dimensional Pennes equation was utilized for modeling the heat transfer in the tissue. Two numerical test cases were studied. Pseudo-temperature data was used as additional information to solve the inverse problem and the influence of measurement errors was observed. For the test cases considered in this study, this method can simultaneously estimate a heat source and a heat transfer coefficient precisely.

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