A STUDY ON THERMAL INITIAL PROPERTIES FOR INVERSE TECHNIQUE

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ABSTRACT

The Levenberg–Marguardt algorithm is used to study on convergence for inverse heat conduction in the unsteady state. In this model, the finite volume method is used to obtain an estimated temperature, which is necessary for minimizing inverse error. Six simulations were performed to investigate the sensitivity to initial thermo-physical properties such as thermal conductivity (k) and heat capacity $(\rho C_p \equiv C)$ by changing three different damping ratios of the Levenberg–Marquardt algorithm. Our results show that an appropriate selection of thermal-physical properties and damping ratio helps numerical stability and convergence and reduces convergence time.

Keywords: inverse heat conduction; Levenberg–Marguardt algorithm; inverse error; convergence time.

ÉTUDE SUR LES PROPRIÉTÉS THERMIQUES INITIALES POUR LA TECHNIQUE INVERSE

RÉSUMÉ

L'algorithme Levenberg–Marquardt est utilisé pour étudier la convergence pour la conductivité thermique inverse en présence d'un état instable. Dans ce modèle, la méthode de volume fini est utilisée pour obtenir une estimation de la température, laquelle est nécessaire pour minimiser une erreur inverse. Six simulations ont été faites pour étudier la sensibilité aux propriétés thermo-physiques, telles que la conductivité thermiques (k) et la capacité d'énergie $(\rho C_p \equiv C)$ en changeant trois différents rapports d'amortissement de l'algorithme Levenberg–Marquardt. Nos résultats indiquent une sélection appropriée des propriétés thermo-physiques et le rapport d'amortissement aide la stabilité numérique et la convergence et réduit le temps de convergence.

Mots-clés : conductivité thermique inverse ; algorithme Levenberg–Marquardt ; erreur inverse ; temps de convergence.

NOMENCLATURE

C_p	heat capacity (J/°C)
d_k	damping parameters
k	thermal conductivity (W/m°C)
q_0	constant heat flux (W/m^2)
T	estimated temperature (°C)
T_m	measured temperature (°C)
Greek symbols	
χ	weighting factor
ρ	density (kg/m^3)

1. INTRODUCTION

In an inverse heat conduction problem (IHCP), the goal is to accurately estimate heat transfer coefficients such as constant thermal conductivity k and heat capacity $\rho C_p \equiv C$. The inverse heat conduction technique was of great importance as an alternative for the potential problem in space shuttle design (e.g., aerodynamic heat estimation of the shuttle surface during reentry), because there were no durable sensors on the highly heated surfaces. For many practical heat transfer problems it is impossible to obtain an exact solution by means of analytical techniques. Instead, numerical methods are used, which allow many such problems to be solved quickly. For a numerical simulation of a system involving temperature, input parameters must be determined to solve a specific problem. Although mechanical properties such as Young's modulus of elasticity and compressive strength can be determined from laboratory-based experiments, direct measurements are not always possible. For this reason, the inverse technique is very useful in dealing with system parameters such as material properties, or thermal properties from indirect measurements. Many methods are available to indirectly determine system parameters; these include the general minimization procedure [1], the weighted least square method [2], the Bayesian decision-theoretic approach [3] and Kalman filtering techniques [4]. However, all the inverse techniques have mathematically ill-posed problems when a matrix is integrated from the indirect measurement data. Many methods have been developed to improve ill-posed problems [5–9]. In addition, estimated solutions are also very sensitive to input data which can cause a significant estimation error in case that the numbers of expected parameters are increased in practical problems.

In this study, the effect of initial thermo-physical properties on computation time was studied for the case of multi-input parameters in a semi-infinite slab subjected to a constant heat flux. Two parameters, thermal conductivity k and heat capacity C, were estimated for given measured temperatures of the plate in an unsteady condition. For an estimated unsteady temperature comparison with measured temperature data for two thermo-physical parameters, the finite volume method was used to calculate temperatures at some points for each time step. The Levenberg–Marguardt algorithm [10] as an iteration solver for IHCPs was employed for the steepest descent convergence. To study the effect of poor estimation of initial properties on estimated time, six case studies were conducted on two different groups by changing the damping parameter of the Levenberg–Marguardt algorithm.

2. IHCP FOR THERMAL CONDUCTIVITY AND HEAT CAPACITY

Figure 1 shows a semi-infinite slab subjected to a constant heat flux q_0 [W/m^2]. The slab has unknown thermal conductivity $k(x)$ and heat capacity $\rho C_p(x)$ for the inverse problem. If both thermal conductivity and heat capacity are only a function of the direction normal to the surface of the sample plate, we can consider the two properties as a function of x. For this case, the thermal conductivity equations are described

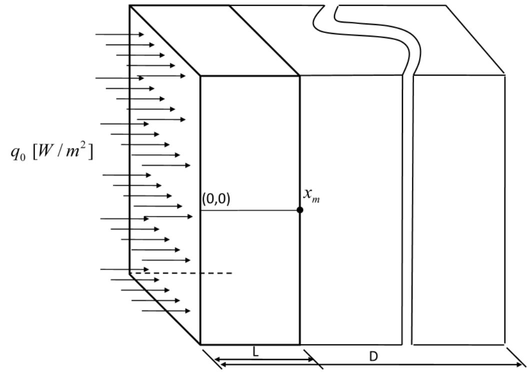

Fig. 1. Geometry for IHCP. $L = 0.05$ m for $L \ll D$.

as follows:

$$\begin{aligned} \rho C(x)\frac{\partial T(x,t)}{\partial t} &= \frac{\partial}{\partial x}\left[k(x)\frac{\partial T}{\partial x}\right] \quad (0 < X < L, t > 0) \\ k(0)\frac{\partial T(0,t)}{\partial x} &= q_0 \quad (x = 0, t > 0) \\ q(x,t) &= 0 \quad (t = 0) \end{aligned} \tag{1}$$

If temperatures along the plate are measured at multiple locations $x_i (i = 0, 1, 2, \ldots, N)$ at times ^{t_i}, the basic concept of the inverse problem is to minimize Eq. (2) for all estimated parameters. Thus,

$$E = \sum_i [T_{m,i} - T_s(I_j)]^2, \quad j = 1, 2, 3, 4, \ldots, M \tag{2}$$

where $T_{m,i}$ is the measured temperature, and $T_i(I_j)$ is the estimated temperature from Eq. (1) by guessing the unknown parameters. For minimization, if Eq. (2) is differentiated with respect to unknown parameters I_j, the formulation of the inverse problem is described as $\partial E/\partial I = 2J^T(T_s - T_m) = 0$. Here,

$$T_s = [T_{s,1} \;\; T_{s,2} \;\; \bullet \;\; T_{s,N}], T_m = [T_{m,1} \;\; T_{m,2} \;\; \bullet \;\; T_{m,N}], I = [I_1 \;\; I_2 \;\; \bullet \;\; I_m] \tag{3}$$

$$J = \frac{\partial T_s}{\partial T^T} = \begin{bmatrix} \frac{\partial T_{s,1}}{\partial I_1} & \frac{\partial T_{s,1}}{\partial I_2} & \cdots & \frac{\partial T_{s,1}}{\partial I_M} \\ \frac{\partial T_{s,2}}{\partial T_1} & \frac{\partial T_{s,2}}{\partial I_2} & \cdots & \frac{\partial T_{s,2}}{\partial I_M} \\ \vdots & & & \\ \frac{\partial T_{s,N}}{\partial I_1} & \frac{\partial T_{s,N}}{\partial I_2} & \cdots & \frac{\partial T_{s,N}}{\partial I_M} \end{bmatrix}, \quad N \geq M. \tag{4}$$

The Levenberg–Marquardt algorithm [10] is expressed as

$$I_j^{k+1} = I_j^k + (J^T J + d_k \vec{I})^{-1} J^T (T_s - T_m), \quad k = 1, 2, 3, \ldots, \tag{5}$$

where d_k are damping parameters.

2.1. Finite Volume Method

The T_s can be obtained numerically or mathematically for unknown parameters ρC_p and k in Eq. (2). In practice, it is not always possible to obtain a solution for a specific case. For this reason, a variety of problems require a numerical simulation to estimate T_s in Eq. (2).

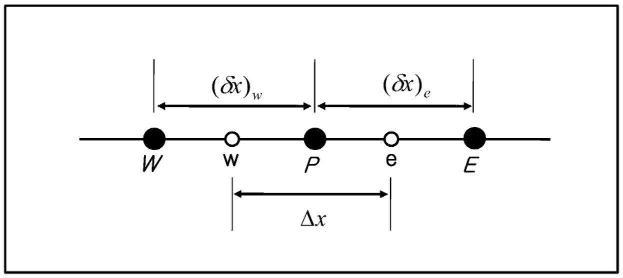

Fig. 2. Grid points for finite volume method in 1-D coordinates.

For the heat conduction equation with an unsteady term, the discretization equation [11] is derived by integrating Eq. (1) over the control volume shown in Fig. 2. For simplicity, the terms ρC_p and k are assumed to be constants. Thus, we have

$$\rho C_p \int_w^e \int_t^{t+\Delta t} \frac{\partial T(x,t)}{\partial t} dt dt = \int_t^{t+\Delta t} \int_w^e \frac{\partial}{\partial x}\left[k\frac{\partial T}{\partial x}\right] dx dt. \tag{6}$$

We can obtain Eq. (8) in terms of the grid point temperature, as shown in Fig. 2:

$$\begin{aligned} a_P T_P &= a_E[\chi T_E + (1-\chi)T_E^0] + a_W[\chi T_W + (1-\chi)T_W^0] + [a_P^0 - (1-\chi)a_E + (1-\chi)a_W]T_P^0 \\ a_E &= \frac{k_e}{(\delta\chi)_e}, \quad a_W = \frac{k_w}{(\delta\chi)_w}, \quad a_P^0 = \rho C_P \frac{\Delta\chi}{\Delta t} \\ a_P &= \chi a_E + \chi a_W + \chi a_P^0, \end{aligned} \tag{7}$$

where χ is a weighting factor between 0 and 1 [11].

A constant flux condition was applied to the left of the slab and a zero flux value was set at $t = 0$. The heat conduction equation was solved using the one-dimensional (1-D) finite volume method. The resulting algebraic equations were solved along a grid line by the tridiagonal matrix algorithm (TDMA). A line-by-line iteration technique was employed until converged results were obtained throughout the computational domain in our simulation. The convergence criterion was specified as 10^{-5} for the heat conduction equation.

2.2. Analytical Solution

$$\begin{aligned} \frac{\partial Q(x,t)}{\partial t} &= \alpha \frac{\partial^2 Q(x,t)}{\partial x^2} \quad (0 < x < \infty, t > 0) \\ Q(x,t) &= 0 \quad (x = 0, t > 0) \\ Q(x,0) &= -f_0 \quad (t = 0). \end{aligned} \tag{8}$$

For a given constant flux boundary condition, Eq. (2) can be converted into Eq. (8) by taking a new dependent variable, $Q(x,t) = q(x,t) - f_0$. Then, the solution was determined in terms of $q(x,t), k, \alpha, x$ and t [12], where $\alpha = k/\rho C_p$.

$$T(x,t) = \frac{2f_0}{k}\left[\left(\frac{\alpha t}{x}\right)^{1/2} e^{-x^2/4\alpha t} - \frac{x}{2}\,\mathrm{erfc}(x/\sqrt{4\alpha t})\right], \tag{9}$$

where the function erfc means the complimentary error function:

$$\mathrm{erfc} = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2}\, dt \tag{10}$$

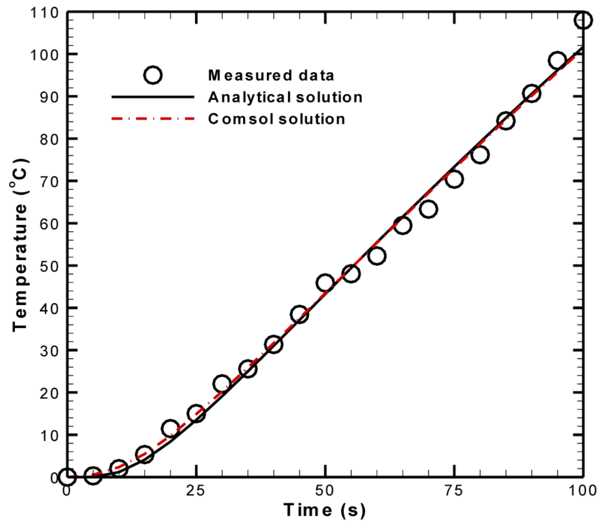

Fig. 3. Comparison of measured, analytical, comsol temperature.

3. RESULTS AND DISCUSSION

To validate the IHCP model for identifying the unknown constant thermal conductivity k, W/(m°C) and heat capacity $\rho C_p \equiv C$, kJ/(m^3 °C), of a solid, the semi-infinite slab shown in Fig. 1 is considered [13]. A plate of thickness [L] is assumed to be infinite in the x-direction. The plate has an initially uniform temperature, and is suddenly subjected to a constant heat flux ($q_0 = 150$ W/m^2) at the surface $x = 0$. Temperatures were obtained at the surface ($L = 0.05$ m) with time. In Table 1, the temperatures taken at the surface are shown for time $t = 0$ to $t = 100$ s. The inverse technique model was employed by using the least squares approach with the Levenberg–Marquardt algorithm in Eq. (6), and iterations continued until the convergence criterion of 10^{-5} was satisfied. In this study, the finite volume method was used to calculate T_s in Eq. (3) in order to minimize the error. From the IHCP estimation of the thermo-physical properties, the thermal conductivity and heat capacity were identified as $k = 0.03135$ W/(m°C) and $\rho C_p = 1184.051$ kJ/(m^3 °C), respectively. To verify the simulation result, the temperatures with time were compared to the analytical solutions from Eq. (10) using the identified the thermal conductivity and heat capacity obtained from the simulation results. In addition, the result of the commercial software (Comsol Multiphysics 3.5a) is compared for the validation. Figure 3 shows that the measured temperatures are in good agreement with the analytical solutions and comsol solution using the identified the thermal conductivity and heat capacity ($k = 0.03135$ W/(m°C) and $\rho C_P = 1184.051$ kJ/(m^3 °C)). Figure 4 represents the geometry of numerical simulation. We conclude that the IHCP model can identify the thermal conductivity and heat capacity. In practice, since an IHCP is very sensitive to the estimated input value, six case studies were conducted in order to evaluate the sensitivity to initial values of computation time and conversion for three different damping ratios. Groups with good and bad initial guesses for the thermo-physical properties were investigated using the IHCP model, as shown in Table 2.

For group 2, we used a value of 0.017 W/m°C for thermal conductivity and 6,000 kJ/m^3 °C for heat capacity. Figures 5 and 6 show the convergence times for each case. Group 1 is faster than the group 2 with respect to convergence time. This means that a better initial guess provides faster convergence time. In particular, when a small damping ratio is used, the computational speed increases in each group. This is exactly the same that the Levenberg–Marquardt algorithm reduces to the Newton method, which gives fast result. However, in group 2, case 6 (damping ratio = 0) did not converge, while in group 1, case 3 was the fastest. This is the reason that a non-zero damping factor helps a local or global convergence especially

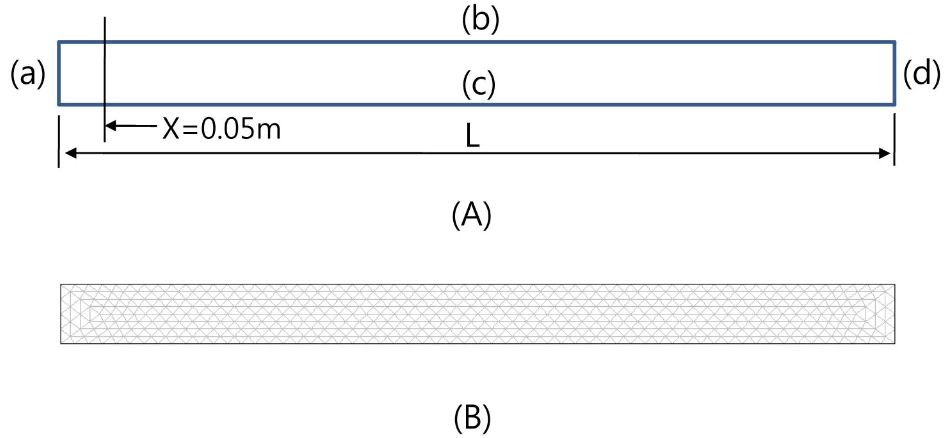

Fig. 4. Geometry of numerical simulation. The boundary conditions are (a) $-n\cdot(-k\nabla T)=q_0=150$ [W/m^2], (b) $-n\cdot(-k\nabla T)=0$, (c) $-n\cdot(-k\nabla T)=0$ and (d) $n\cdot(-k\nabla T)=0$ for (A). $L=3$ m is longer than a measurement point X and X is a measurement point with time. The number of elements is 2049 for (B).

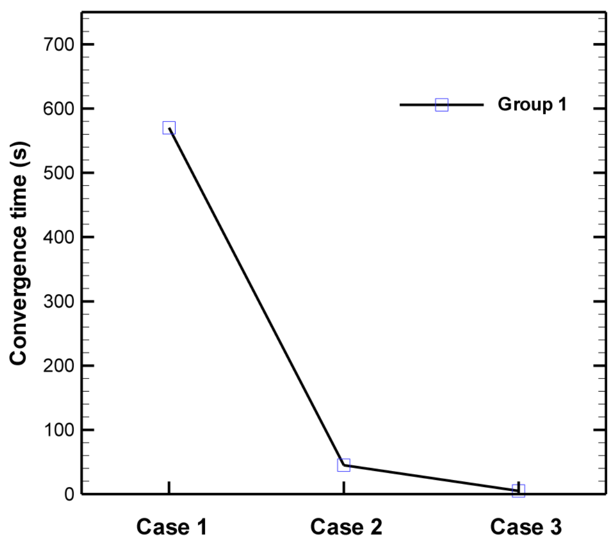

Fig. 5. Convergence times in case of good initial estimates.

at the bad choice of initial properties, but a bigger damping factor generally makes slow convergence. As a result, a damping ratio results in slow convergence, however a non-zero damping ratio helps divergence which comes from the bad choice of initial approximated properties.

A good initial guess produces a fast result when a small damping ratio is used. However, a bad initial guess causes divergence or results in no convergence. For this reason, we must consider an appropriate damping ratio in order to remove system singularity. In addition, we should also consider that a high damping ratio could cause greater convergence time. Thus, some tradeoff will be necessary in terms of computational time and convergence. The Levenberg–Marguardt algorithm provides all the similar values of thermal conductivity and heat capacity, and most of our results were shown to be within an error of 0.001% because the convergence criterion was used as

$$f=\left(\frac{k^n-k^{n-1}}{k^n}\right)<10^{-5}\&\left(\frac{(\rho C_p)^n-(\rho C_p)^{n-1}}{(\rho C_p)^n}\right)<10^{-5}.$$

Table 1. Measurement of temperature vs. time.

Time (s)	Measured T (°C)
0	0
5	0.03
10	1.99
15	5.32
20	11.45
25	15.00
30	22.03
35	25.57
40	31.35
45	38.44
50	45.88
55	48.05
60	52.26
65	59.48
70	63.32
75	70.41
80	76.18
85	84.19
90	90.67
95	98.44
100	107.98

Table 2. Thermo-physical properties for six cases.

Input values	Simulation group 1		
	Case 1	Case 2	Case 3
Damping ratio	0.01	0.001	0
Thermal conductivity (k_o [W/m°C])	0.2	0.2	0.2
Heat capacity (ρC_p [kJ/m^3 °C])	1000	1000	1000
Input values	Simulation group 2		
	Case 4	Case 5	Case 6
Damping ratio	0.01	0.001	0
Thermal conductivity (k_o [W/m°C])	0.017	0.017	0.017
Heat capacity (ρC_p [kJ/m^3 °C])	6000	6000	6000

4. CONCLUSIONS

The Levenberg–Marguardt algorithm and the finite volume method were used to accurately estimate heat transfer coefficients such as constant thermal conductivity k and heat capacity $\rho C_p \equiv C$. Good agreement between the exact and estimated temperature values was obtained. The high damping ratio affects slow convergence, and a non-zero damping ratio helps local or global convergence for a bad initial guess (cases 4 and 5). In this paper, the convergence time increases with increasing the damping ratio, However the non-zero damping factor was favorable with respect to convergence especially at bad choice. It was verified that when the damping ratio goes to zero, the Levenberg–Marguardt algorithm reduces to Newton's method, which results in fast conservation as shown in Figs. 5 and 6. Once convergence occurs, all cases show good results (within 0.01% error) for the thermo-physical properties.

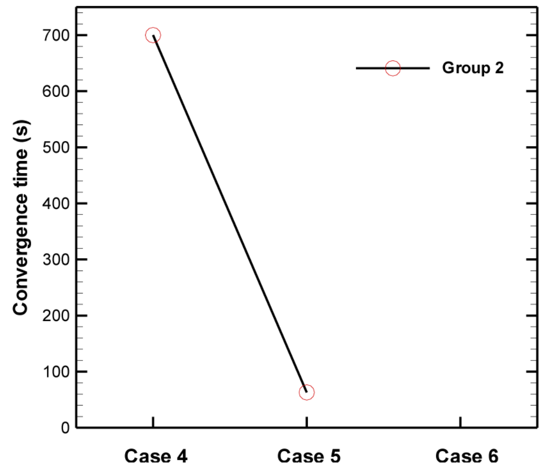

Fig. 6. Convergence times in case of bad initial estimates.

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