INVERSE ESTIMATION OF THERMAL CONDUCTIVITY PARAMETERS IN NONLINEAR STEADY HEAT CONDUCTION PROBLEMS

(Anggaran Songsang Parameter Konduktiviti Terma dalam Masalah Pengalihan Haba Tetap tak Linear)

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ABSTRACT

The precise determination of the thermal conductivity is crucial for material characterization in engineering applications. However, the accurate identification of temperature-dependent thermal conductivity poses a significant challenge. This article proposed an adjoint-based inverse method to identify the thermal conductivity in the context of nonlinear steady heat conduction scenarios. The simulated temperature associated with the nonlinear steady heat conduction problem was quantified by employing the finite element method. The inverse retrieval of the thermal conductivity parameters was performed utilizing the adjoint method. Numerical examples were presented and analyzed to demonstrate the effectiveness of the proposed approach to identify the thermal conductivity parameters. For both numerical examples, three parameters of thermal conductivity were recovered utilizing temperature distribution with around 30 iterations and remarkably low objective function values. These results demonstrated the validity of the proposed method even in cases when the initial guess was far away from the target parameter value. The findings demonstrated the potential of the adjoint method in effectively determining the thermophysical parameters by solving the inverse heat conduction problems.

Keywords: FEM; temperature-dependent thermal conductivity; adjoint method; inverse problem *ABSTRAK*

Penentuan yang tepat bagi konduktiviti terma adalah sangat penting untuk pencirian bahan dalam aplikasi kejuruteraan. Namun, mengenal pasti konduktiviti terma yang bergantung kepada suhu merupakan satu cabaran besar. Artikel ini mencadangkan kaedah songsang berasaskan adjoint untuk mengenal pasti konduktiviti terma dalam senario pengaliran haba mantap nonlinier. Suhu simulatif yang berkaitan dengan masalah tersebut diukur menggunakan kaedah elemen terhingga. Pengambilan terbalik parameter konduktiviti terma dilakukan dengan ketepatan dan kepresisian yang tinggi melalui kaedah adjoint, yang terkenal dengan ketepatan dan penumpuan yang cepat. Contoh numerik dibentangkan dan dianalisis untuk menunjukkan keberkesanan pendekatan yang dicadangkan dalam pengenalan parameter konduktiviti terma. Hasil kajian ini membuktikan kesahihan kaedah yang dicadangkan walaupun tekaan awal jauh dari nilai parameter sasaran. Penemuan ini menunjukkan potensi kaedah adjoint dalam menentukan parameter termofizik dengan berkesan melalui penyelesaian masalah pengaliran haba songsang.

Kata kunci: konduktiviti terma bergantung kepada suhu, kaedah adjoint, masalah songsang

1. Introduction

Understanding the relationship between temperature and thermal conductivity is essential in heat conduction problems. In engineering applications, like thermal management in electronics, subsurface heat transport in geophysical processes, and temperature-dependent thermal conductivity are crucial (Brookfield *et al.* 2009; Ekpu *et al.* 2011; Hoq *et al.* 2016; Moore & Shi 2014). However, direct measurement of nonlinear thermal conductivity requires expensive

experiments utilizing cutting-edge equipment (Alifanov 2012; Huang & Chin, 2000). Therefore, the cost-effective inverse heat transfer problem (IHTP) has received significant attention since its invention in the 1960s to identify thermophysical parameters. In recent years, the inverse approach has been utilized to identify the material properties, including thermal conductivity, which can be spatial-dependent, constant or temperature-dependent (Artyukhin 1981), heat transfer coefficient (Mohebbi & Sellier 2016a; Zhang & Delichatsios 2009), specific heat, heat flux (Liu 2012; Mohebbi & Sellier 2016b), and boundary conditions (Ramos et al. 2022). The forward problem in IHTPs is typically solved by the singular boundary method (SBM), finite element method (FEM), finite difference method (FDM), and finite volume method (FVM). FEM is highly applicable in almost all branches of scientific study; even cubic B-spline FEM has been applied to solve second order Volterra-integro differential equation (Ali & Senu 2025). The bi-quadratic triangular Galerkin's finite element method (QGFEM) is also employed to solve two-dimensional heat conduction problems (Hoq et al. 2020; Hoq et al. 2016; Sulaeman et al. 2018). The thermophysical properties of the material under study are then determined by utilizing the temperature distribution obtained from the forward problem. Among the inverse methods, the Levenberg-Marquardt method (LMM) determines the thermal conductivity coefficient for anisotropic media (Chen et al. 2016). The Bayesian approach and Markov Chain Monte Carlo (MCMC) technique can recover the heat transfer coefficient and thermal conductivity (Gnanasekaran & Balaji 2011). Additionally, the conjugate gradient technique (CGM) is able to estimate the temperature-dependent and spatially varying thermal conductivity in the contexts of functionally graded materials (Mohebbi et al. 2021). In addition to these studies, a hybrid method that combines a modified genetic algorithm and LMM has been utilized to simultaneously estimate the temperature-dependent thermal conductivity and heat capacity.

Although a good number of studies have been done focusing on inverse identification of thermal conductivity parameters, few studies addressed the simultaneous identification of multiple thermal condcutivity parameters for nonlinear steady heat conduction problem. Thus, this study focused on the simultaneous identification of three thermal conductivity parameters of non-linear steady heat conduciton problems. The proposed procedure took the advantage of FEM as supplied by the software package FeniCS (Alnæs et al. 2015; Farrell et al. 2013) to obtain the temperature distribution. The FEM method is powerful in solving heat conduction problems as it is flexible for complex geometry, boundary conditions, and material properties for non-linear problems. Nevertheless, FEM has some shortcomings due to the high computational cost, complex processing, and mesh quality; specifically, for lager mesh and 3D domain, computational cost increases (Erhunmwun & Ikponmwosa 2017; Jagota et al. 2013). In this study, the adjoint method was employed to inverse identify the functional form of thermal conductivity for nonlinear steady heat conduction problems. The quasi-Newton approach, called limited-memory BFGS approximation (Liu & Nocedal 1989) updated the thermal conductivity parameters without requiring the computation of the Hessian matrix, thereby reducing the computational cost. To the author's best knowledge, this article is the first to apply the adjoint method to estimate temperature-dependent thermal conductivity. While the focus of this work was on regular geometry, the proposed method has the potential to be applied to irregular geometry as well.

The remainder of this article is organized as follows: the Method section develops the mathematical formulation of the steady and nonlinear 2D heat conduction problem. Subsequently, the adjoint method in the context of the inverse problem is presented. The Results section demonstrates the feasibility of estimating temperature-dependent thermal conductivity. Finally, the summary and the concluding remarks are given in the Conclusion section.

2. Methods

This section briefly discusses the mathematical background of the forward and inverse problems for the identification of temperature-dependent thermal conductivity.

2.1. Forward problem

The mathematical model under consideration is expressed in Eq. (1):

$$\nabla \left[k(T) \nabla T \right] = 0, x \in [0, l], y \in [0, l], \Omega = (0, l) \times (0, l)$$
(1)

where, T(x,y) represents temperature, k(T) is the quadratic function representing temperature-dependent thermal conductivity. The heat flux, denoted by q, is on the left boundary, Γ_1 is determined by Eq. (2).

$$\int_0^l k(T) \frac{dy}{dx} \bigg|_{x=0} dy = -q \tag{2}$$

To solve the nonlinear steady heat conduction problem, the FEM (Bathe 2007) is employed and the corresponding weak formulation of Eq. (1) is expressed in Eq. (3).

$$\int_{\Omega} k \nabla T \cdot \nabla (\delta T) d\Omega = \int_{\Gamma_1} (\delta T) \overline{q} d\Gamma \tag{3}$$

Where, δT denotes the virtual temperature field and \overline{q} represents the heat flux on the boundary Γ_1 . The thermal conductivity is temperature-dependent and defined in Eq. (4).

$$k(T) = a + bT + cT^2 \tag{4}$$

2.2. Inverse problem

The initial conditions, boundary conditions, and material properties are known to obtain the temperature field in the forward problem. Conversely, in the inverse problem, the thermal conductivity parameters are unknown, while the other related conditions are assumed to be known. Therefore, the temperature field has been employed to retrieve the unknown thermal conductivity parameters. The inverse identification is performed by minimizing the objective function defined by Eq. (5).

$$J(T) = \frac{1}{2} \int_{\Omega} (T - T^*)^2 d\Omega \tag{5}$$

T and T^* are the computed and measured temperatures, respectively. The goal is to compute the thermal conductivity parameters a, b, and c by minimizing the objective function in Eq. (5). In order to efficiently minimize the objective function, it is essential to calculate the gradient of the objective functional Eq. (5) with respect to the thermal conductivity parameters. To achieve

this, we have chosen to employ a quasi-Newton approach. Specifically, we utilized a limited-memory BFGS approximation of the Hessian implemented in the FEniCS platform.

2.3. Derivation of the adjoint equation

Consider the heat equation as follows:

$$C(T,k) = 0 (6)$$

Differentiating the objective function regarding the thermal conductivity parameters β (say) leads to the expression Eq. (7).

$$\frac{dJ}{d\beta} = \frac{\partial J}{\partial T} \frac{dT}{d\beta} \tag{7}$$

In the equation Eq. (7), $\partial J/\partial \beta$ is straight-forward. Conversely, $\partial J/\partial T$ requires the differentiation of the heat equation. Consequently, Eq. (6) is differentiated with respect to the thermal conductivity parameter β .

$$-\frac{\partial C}{\partial T}\frac{dT}{d\beta} = \frac{\partial C}{\partial \beta} \tag{8}$$

The relation in Eq. (8) demonstrates the tangent linear system corresponding to the objective functional Eq. (5). Assuming the tangent linear system is invertible, then Eq. (8) turns,

$$\frac{dT}{d\beta} = -\left(\frac{\partial C}{\partial T}\right)^{-1} \frac{\partial C}{\partial \beta} \tag{9}$$

Using Eq. (9) in Eq. (7), we get,

$$\frac{dJ}{d\beta} = -\frac{\partial J}{\partial T} \left(\frac{\partial C}{\partial T}\right)^{-1} \frac{\partial C}{\partial \beta} \tag{10}$$

Defining adjoint variable, λ as,

$$\lambda \left(\frac{\partial C}{\partial T}\right)^T = \left(\frac{\partial J}{\partial T}\right)^T \tag{11}$$

Eq. (11) is the adjoint equation corresponding to the forward problem Eq. (1) and the objective functional Eq. (5). Solving the adjoint Eq. (11) and substituting it into Eq. (7), we obtain the derivative of the objective functional as follows:

$$\frac{dJ}{d\beta} = \lambda^* \frac{\partial C}{\partial \beta} \tag{12}$$

2.4. Convergent criteria

In the inverse problems, the iteration process is terminated when the objective function meets the criteria: $|grad(J)| \le \varepsilon$, where ε represents a positive number of sufficiently small magnitude.

2.5. Computational procedure

The computational technique employed in this study involves the following steps:

Step 1.	In the forward problem, the FEM is employed to obtain the temperature distribution, incorporating the temperature-dependent thermal conductivity.		
	incorporating the temperature-dependent thermal conductivity.		
Step 2.	Initialize the adjoint method: initiate with an initial value for the thermal conductivity		
	parameters.		
Step 3.	Compute the objective function and its gradient utilizing the adjoint model.		
	Evaluate the convergence condition. If the condition is met, terminate the iteration; otherwise, update the optimization parameters, go to Step 2, and repeat the optimization procedure.		
Step 5.	The iteration stops either when the gradient of the objective functional falls below a predefined tolerance or when the maximum allowable number of iterations has been reached.		

The flowchart of the computational procedure is shown in Figure 1.

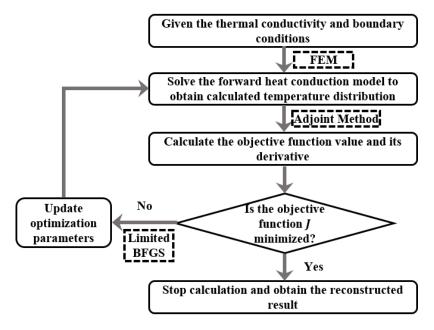


Figure 1: Flowchart of the proposed inversion method.

3. Results and Discussion

In the subsequent sections, the previously presented adjoint approach addressed the inverse solution of the nonlinear steady heat conduction problem. We examined the two numerical examples to evaluate the efficiency and accuracy of the presented inverse framework.

3.1. *Case I*

The first example under consideration was a 2D object, as shown in Figure 2(a). The physical dimensions of the object were 0.1×0.1 (dimensionless). The domain was discretized as FE mesh into a 34×34 bilinear element. The left boundary was assigned to $T_L = 1\%$, and the right boundary remained consistent with its initial value. The heat flux applied to the left boundary was determined by Eq. (3). The expression $T = T_L - (T_L - T_R)x/L$ determined the temperature at the top and bottom boundaries.

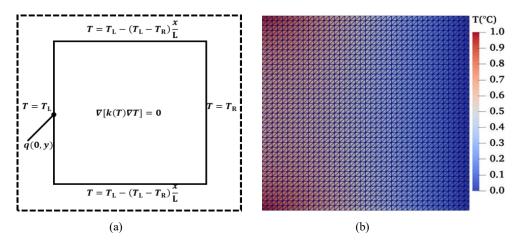


Figure 2: (a) boundary condition (b) temperature distribution obtained from the forward problem

Figure 2(a) presents the boundary and additional conditions of the model. Equation Eq. (5) describes the thermal conductivity, with the parameters a, b, and c having values of 1.75, 0.75, and 0.075, respectively. The temperature distribution obtained from the forward problem employing FEM is presented in Figure 2(b). In the inverse approach, the thermal conductivity parameters a, b, and c were recovered utilizing the temperature distribution data, while all other conditions remained constant. To start the inverse optimization, the initial estimation of the variables a, b, and c was set to 0.1, far from the three target parameters.

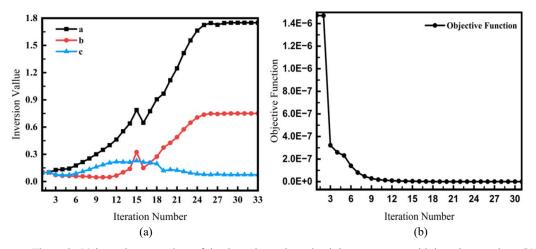


Figure 3: (a) inversion procedure of the three thermal conductivity parameters with iteration numbers (b) convergence process of the objective function

The convergence trend shown in Figure 3(a) illustrates the inverse identification of three parameters, 1.75, 0.75, and 0.075, corresponding to a, b, and c, respectively. The iterative process of the objective function in the inverse approach is shown in Figure 3(b), demonstrating its convergence with the iteration number. Figure 3(a) demonstrates the convergence of multiparameters to their actual value attained with a total of 33 iterations. The objective function value decreased sharply with iteration numbers and converged quickly. Furthermore, the final objective function reached a remarkably low value of 2.08×10^{-18} , indicating the successful attainment of the multi-parameters to their respective targets.

We also tested the effectiveness of the adjoint-based inverse method with varying initial guesses of 0.01 and 0.001. In both cases, we observed that the parameters a, b, and c were identified successfully with a bit increased iteration. Figure 4 shows that for initial guess 0.01, it took 39 iterations to be converged, whereas for initial guess 0.001, it took 41 iterations to be converged.

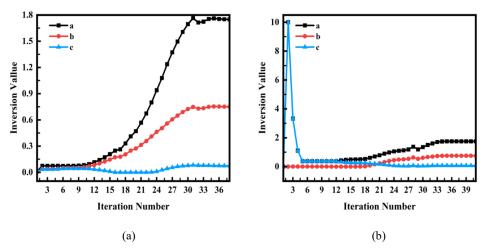


Figure 4: (a) Inversion procedure of the three thermal conductivity parameters with initial guess 0.01 (b) Inversion procedure of the three thermal conductivity parameters with initial guess 0.001

3.2. *Case II*

The second numerical example was the thermal conductivity parameters inversion of a two-dimensional model, as demonstrated in Figure 5(a). The physical domain was discretized into 30×30 rectangles, each divided into a pair of triangles. The left boundary was assigned to $T_L = 1$ °C; the right boundary maintained 0°C. Eq. (3) determined the heat flux at the left boundary while the remaining boundaries were thermally insulated. The temperature-dependent thermal conductivity was represented in Eq. (5), where the parameters were a = 1.2, b = 0.8, and c = 0.04

Regarding the inverse approach, the thermal conductivity parameters a = 1.2, b = 0.8, and c = 0.04 were unknown and required determination, while all other conditions remained unchanged. The temperature distribution obtained from the forward model, as displayed in Figure 5(b), required additional data for the inverse identification. The initial guesses assigned to the parameters a, b, and c were 0.1. The convergence history, shown in Figure 6(a), illustrates the progression of three recovered parameters, 1.2, 0.8, and 0.04, labelled as a, b, and c. It is evident from Figure 6(a) that convergence was achieved following a total of 31 iterations. Besides that, Figure 6(b) represents the convergence process of the objective function. The objective function converged quickly and attained a remarkably low final value of 4.33×10^{-19} .

The low objective function value and quick convergence of the three parameters indicated the efficiency and robustness of the adjoint-based inverse framework. In this numerical example, we also tested the effectiveness of the proposed adjoint-based inverse method with varying initial guesses of 0.01 and 0.001. Figure 7 attests that the three parameters a, b, and c converged with 33 iterations for the initial guess of 0.01, whereas 39 iterations were needed for the initial guess of 0.001. This proved the robustness of the proposed inverse method.

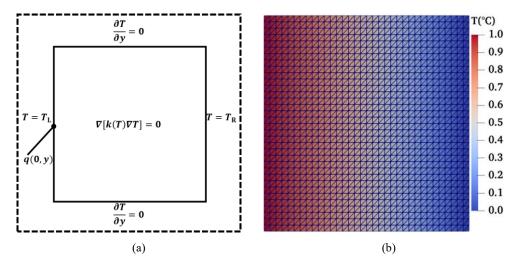


Figure 5: (a) boundary condition (b) temperature distribution obtained from the forward problem

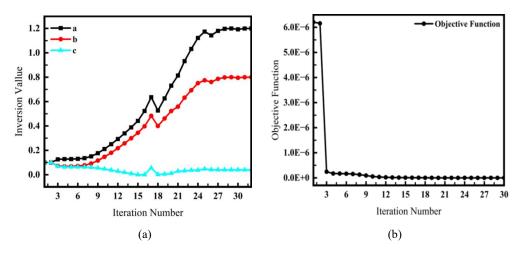


Figure 6: (a) Inversion procedure of the multiple thermal conductivity parameters with iteration numbers (b)

Convergence process of the objective function

The above two numerical examples demonstrated that the proposed adjoint-based inverse approach had the potential to inverse identify the thermal conductivity parameter quickly with improved accuracy than the modified conjugate gradient methods reported previously (Cui et al. 2014; Yang et al. 2019) as it did not require the computation of the Hessian matrix. In the case of irregular geometry, the numerical stability of the inverse method decreases with

increasing complex geometry due to complicated mesh; small changes in parameters make the sensitivity analysis challenging (Duda 2015).

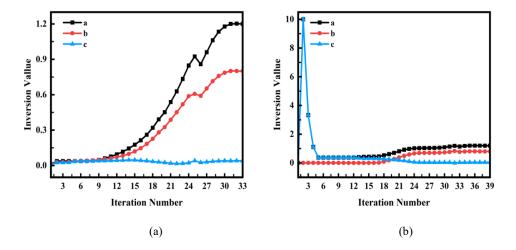


Figure 7: (a) inversion procedure of the three thermal conductivity parameters with initial guess 0.01 (b) inversion procedure of the three thermal conductivity parameters with initial guess 0.001

4. Error Analysis

The relative error was performed between the thermal conductivity parameters obtained through the adjoint method with the target value aiming to assess the accuracy of the outcomes, as given by Eq. (14).

$$e = \sqrt{\frac{\sum_{i=1}^{N} (A_i - A_i^*)^2}{\sum_{i=1}^{N} (A_i)^2}} \times 100\%$$
(14)

where, A_i denote target parameters, A_i^* represents the recovered parameter of temperature-dependent thermal conductivity, and N signifies the total number of nodes in the domain.

Table 1: Relative error between target and estimated thermal conductivity parameters.

Parameters	First example	Second Example
а	$1.77 \times 10^{-5} \%$	$2.72 \times 10^{-6} \%$
b	$1.69 \times 10^{-5} \%$	$4.49 \times 10^{-6} \%$
c	$6.03 \times 10^{-5} \%$	1.85×10^{-5} %

Table 1 depicts the relative error, underscoring the effectiveness of the proposed approach in recovering multiple parameters with high accuracy. The precision of the adjoint technique was readily apparent from the relative error values calculated for all parameters in the two cases. Remarkably, both examples stood out with a relative error in the order of around 10⁻⁵. These findings collectively underscored the robustness and accuracy inherent in the proposed method.

5. Conclusion

This study presents an inverse approach for the simultaneous identification of multiple thermal conductivity parameters in the context of 2D nonlinear steady heat conduction problems. Temperature distribution was obtained utilizing FEM by solving the forward problem. The adjoint method was utilized in inverse analysis to effectively minimize the objective function and accurately retrieve the desired parameters. The numerical findings demonstrated that the proposed adjoint method can simultaneously invert the three parameters of thermal conductivity by utilizing measured temperature distribution with only around 30 iterations and remarkably low objective function value of the order 10⁻¹⁹. Additionally, the relative error for all three parameters of both examples stood out in the order around 10⁻⁵. In summary, the proposed inverse framework has better efficiency, higher precision, and robustness. The outcome of this can contribute to the fields of material science, manufacturing, electronic and semiconductor industries, as steady-state nonlinear thermal analysis plays a pivotal role in the final stage of system design and evaluations. Our subsequent objective is to experimentally validate the proposed adjoint approach to address inverse heat conduction problems and to extend for complex geometry.

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