Analysis of a Thermal Conductivity Measurement Technique Formulated as an Inverse Heat Conduction Problem

[redacted]

Abstract. Thermal analysis and solution of heat problems most often utilizes known thermal conductivity material data which is typically experimentally determined from heat flux measurements through the application of Fourier's law. The challenge posed by this approach is the need for known thermal conductivity reference materials which may be inhomogeneous and have large associated uncertainties in industrial physics applications. In this paper we investigate the feasibility of developing a thermal conductivity measurement system that utilizes known radiometric input sources and temperature output measurements which may have smaller relative uncertainties by formulating the system as an inverse heat conduction problem utilizing recently reported research results from the fields of geophysics and mathematical optimization.

1. Introduction

Thermal physics analysis and solution of heat problems often utilizes known thermal conductivity material data which is typically experimentally determined from heat flux measurements through the application of Fourier's law $q'' = -k\nabla T$, where $q''/[\mathrm{W\,m^{-2}}]$ is the heat flux, $k/[\mathrm{W\,m^{-1}\,K^{-1}}]$ is the thermal conductivity, and $T/[\mathrm{K}]$ is the absolute temperature following the nomenclature in [10]. The use of Fourier's law presents a straight forward mechanism to define and infer the thermal conductivity through the ratio of the heat flux measured using standard techniques as discussed in [37], and the temperature gradient for a specified direction of heat flow where the unknown thermal conductivity may be expressed in terms of known reference quantities such as thermal conductivity, wall thickness and wall temperature amongst other experimental measurements for homogeneous isotropic materials as illustrated in figure 1.

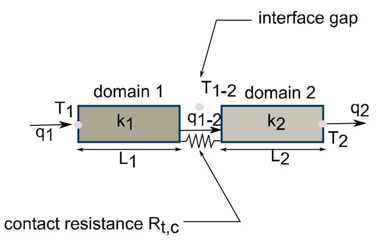

Figure 1. Composite wall system modelled as a 1D thermal circuit. In this model the unknown thermal conductivity k_2 is expressed as $k_2 = \frac{L_2}{A}\left(\frac{T_1 - T_2}{q} - \frac{L_1}{k_1 A} - R_{t,c}\right)^{-1}$ and the uncertainty may be estimated by standard techniques such as the GUM and GS1 as discussed in [11, 12, 13]

Unfortunately materials such as aluminium/steel thermal properties may be inhomogeneous and/or non-isotropic either from physical effects in the smelting process or manufacturing effects from the fabrication of structures requiring knowledge of thermal conductivity such as reflectors/concentrators in for example solar plants [7] where in addition the thermal conductivity may vary with temperature [36, 30] as illustrated in figure 2 for a selection of materials.

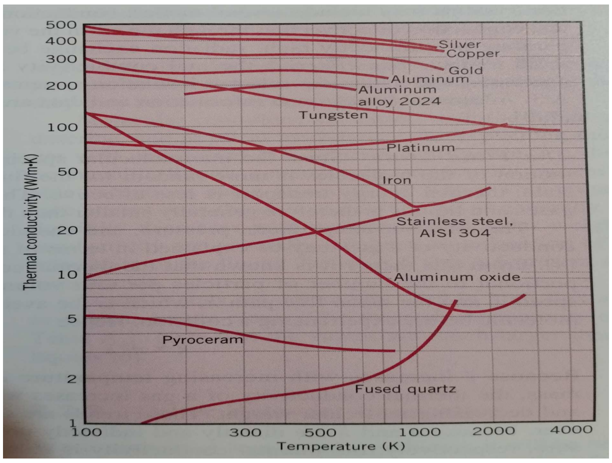

Figure 2. Illustration of thermal conductivity temperature dependence for selection of industrial/engineering materails (Graphic source: [10, page 47])

As a result it is desirable in applied industrial research contexts to infer thermal conductivity information directly by an inverse problem formulation using direct temperature measurements which are more practical and experimentally convenient, either when reference thermal conductivity materials are unavailable for prior testing, impractical due to prevailing operating conditions, or when in situ process or condition monitoring measurements are necessary.

In general accurate heat sources such as calibrated lasers or electrical resistance heating elements, and temperature measurement devices such as thermocouples or resistance thermometers, are simple and straightforward to procure and utilize. As a result in this paper we opt to analyze a system in which the thermal conductivity may be inferred through an Inverse Heat Conduction Problem (IHCP) modelling approach utilizing just radiometric/electrical heating sources and temperature measurements which are easily accessible and which avoids the need for specific reference thermal conductivity material components, and specialist heat flux instruments and blackbody equipment [23].

2. Literature Review

Within the statistical literature simulation problems may typically be classified as either direct/forward or indirect/inverse where in general terms the former are cases in which PDE parameters are known and one utilizes this information to solve for the PDE solution, whilst in the latter one utilizes the PDE solution to infer the underlying PDE parameters.

In the context of thermal physics a direct/forward problem would correspond to using known thermophysical properties such as thermal conductivity and/or specific heat capacity as inputs with suitable boundary conditions for a boundary $\Gamma = \partial\Omega$ to solve the heat diffusion equation $\nabla \cdot (k\nabla T) + \dot{q} = \rho c_p \frac{\partial T}{\partial t}$ for some problem domain Ω whilst an indirect/inverse problem would in a certain sense "work backwards" to use the PDE temperature field solution to infer the corresponding thermophysical parameters as discussed in [27]. Traditionally inverse problem studies have been common in the geophysical sciences to determine rock densities, gravitional field strengths, and in oil and gas exploration as discussed in [26, 25, 24] with newer insights into Monte Carlo based inverse parameter uncertainties reported in [4], and which has generally been formulated and solved using the Monte Carlo and Levenberg-Marquardt techniques as outlined in [32, 4].

For IHCP studies methods of solution have mainly to date traditionally consisted of the Levenberg-Marquardt and conjugate gradient techniques for mixtures of problems in laboratory thermophysical testing and space vehicle atmospheric reentry design and research studies after the development of techniques such as Tikhonov regularization which were able to modify and reformulate the original ill-posed/unstable inverse problems as approximate well-posed problems.

More recently investigations in inverse theory problems across different fields has involved applications of newly developed techniques such as the variational iteration method or (VIM) [6], the method of fundamental solutions or MFS [8, 9, 14, 15, 16, 18, 21, 22, 35], the lattice Boltzmann method or LBM [17], heuristic approaches drawing from a mixture of techniques [20, 5], and meshfree approaches [34]. Finite difference methods for IHCP studies are further discussed in [29, 28] who explore how the Tikhonov regularization method may be used to regularize the ill-conditioned linear system of equations for a non-steady two dimensional heat conduction problem, and a iteration approach to determine the regularization parameter was explored in [33]. A measurement methodology for infrared thermography of inverse models that used a maximum entropy principle was reported in [19] for a die forging application in order to deduce the unknown boundary condition of a heat flux using a finite difference discritization.

3. Mathematical Development

Based on the literature review we opt for simplicity since the underlying problem is nonlinear to use a Levenberg-Marquardt optimization in our formulation to avoid a Tikhonov regularization. Utilizing the heat diffusion equation $\nabla \cdot (k\nabla T) + \dot{q} = \rho c_p \frac{\partial T}{\partial t}$ which reduces to a generalized two dimensional Poisson equation $\frac{\partial}{\partial x}(k\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(k\frac{\partial T}{\partial y}) = -\dot{q}$ in the special case for steady-state conditions for a planar domain for the particular geometry of the experimental system illustrated in figure 2 where the domain Ω is a circular region of diameter D where the boundary Γ is held at a constant temperature T_f, where $T/[\mathrm{K}]$ is the temperature, $k/[\mathrm{W\,m^{-1}\,K^{-1}}]$ the thermal conductivity of the sample, and $\dot{q}$ is an energy sink/source term which is positive if energy is generated within the medium and negative if energy is being consumed.

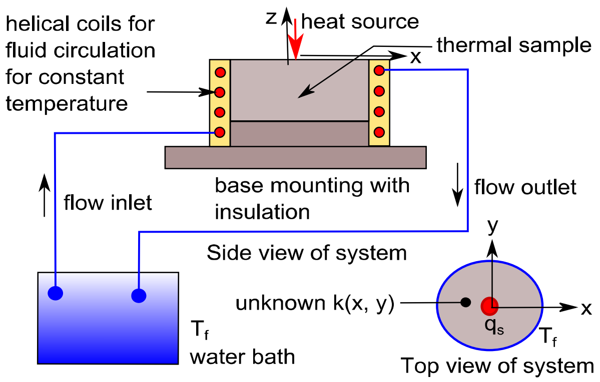

Figure 3. Experimental inverse heat conduction problem (IHCP) system to test for thermal conductivity

Adopting a radial basis function discretization following the discussions in [2, 3, 34] we approximate the thermal conductivity as $k = \sum_{i=1}^{N_k} \alpha_i \varphi_k(||\boldsymbol{x} - \boldsymbol{x}_i||$, and the temperature field as $T = \sum_{j=1}^{N_T} \beta_j \varphi_T(||\boldsymbol{x} - \boldsymbol{x}_j||$. For the temperature field let N_T be the total number of points composed of N_I interior points and N_B boundary points such that $N_T = N_I + N_B$. In this approach it is not necessarily the case that $N_k = N_T$ however this will simplify subsequent calculations. The terms α_i ($i = 1, \ldots, N$) and β_j ($j = 1, \ldots, N$) are coefficients that are used to build up the $k(\boldsymbol{x})$ and $T(\boldsymbol{x})$ fields for $\boldsymbol{x} \in \Omega$ in terms of the RBF's φ_k and φ_T respectively. Utilizing Gaussian RBF's for simplicity to illustrate the approach adopted of form $\varphi_k = e^{-\varepsilon_k^2 r^2}$ and $\varphi_T = e^{-\varepsilon_T^2 r^2}$ where $r = \sqrt{(x - x_i)^2 + (y - y_i)^2}$ and where ε_k and ε_T are suitable shape parameters for the thermal conductivity and temperature fields respectively, and substituting into the generalized two dimensional Poisson equation we then have using the short hand $r_i = r$ for points in the interior that $0 = \frac{\partial k}{\partial x}\frac{\partial T}{\partial x} + k\frac{\partial^2 T}{\partial x^2} + \frac{\partial k}{\partial y}\frac{\partial T}{\partial y} + k\frac{\partial^2 T}{\partial y^2} + \dot{q}$ where $k = \sum_{i=1}^{N_k}[\alpha_i e^{-\varepsilon_k^2 r_i^2}]$, $\frac{\partial k}{\partial x} = \sum_{i=1}^{N_k}[-2\varepsilon_k^2(x - x_i)\alpha_i e^{-\varepsilon_k^2 r_i^2}]$, $\frac{\partial^2 k}{\partial x^2} = \sum_{i=1}^{N_k}[-2\varepsilon_k^2 \alpha_i\{1 - 2\varepsilon_k^2(x - x_i)^2\}e^{-\varepsilon_k^2 r_i^2}]$, and similar expressions for the corresponding temperature field.

Let T_k be the experimental measured temperature and θ_k the estimated temperature for some choice of assumed parameter $\boldsymbol{P}$, where in our particular problem the parameter is used to specify the thermal conductivity. Constructing an objective function $S(\boldsymbol{P}) = \sum_{k=1}^{N}[T_k - \theta_k(\boldsymbol{P})]^2$ it follows that we solve the IHCP by determining the choice of parameter such that $S(\boldsymbol{P})$ is minimized. The objective function may be written in matrix form by specifying the measured and estimated temperatures as a column vectors $\boldsymbol{T}^\mathsf{T} = [T_1, \ldots, T_N]$ and $\boldsymbol{\theta}^\mathsf{T} = [\theta_1, \ldots, \theta_N]$ and then constructing the objective function as $S(\boldsymbol{P}) = [\boldsymbol{T} - \boldsymbol{\theta}(\boldsymbol{P})]^T[\boldsymbol{T} - \boldsymbol{\theta}(\boldsymbol{P})]$. A solution will occur when $\nabla S(\boldsymbol{P}) = 0$ which after algebraic manipulations reduces to the following equations

$$\begin{aligned}
-2\mathbf{J}^\mathsf{T}(\boldsymbol{P})[\boldsymbol{T} - \boldsymbol{\theta}(\boldsymbol{P})] &= \mathbf{0} \\
\mathbf{J} &= \begin{bmatrix}
\frac{\partial\theta_1}{\partial P_1} & \frac{\partial\theta_1}{\partial P_2} & \frac{\partial\theta_1}{\partial P_3} & \cdots & \frac{\partial\theta_1}{\partial P_M} \\
\frac{\partial\theta_2}{\partial P_1} & \frac{\partial\theta_2}{\partial P_2} & \frac{\partial\theta_2}{\partial P_3} & \cdots & \frac{\partial\theta_2}{\partial P_M} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\frac{\partial\theta_N}{\partial P_1} & \frac{\partial\theta_N}{\partial P_2} & \frac{\partial\theta_N}{\partial P_3} & \cdots & \frac{\partial\theta_N}{\partial P_M}
\end{bmatrix}
\end{aligned}$$

where as previously mentioned N is the total number of measured/estimated temperatures, M is specified as the total number of parameters such that $\boldsymbol{P}^\mathsf{T} = [P_1, \ldots, P_M]$, and $\mathbf{J}(\boldsymbol{P}) = [\frac{\partial\boldsymbol{\theta}^\mathsf{T}(\boldsymbol{P})}{\partial\boldsymbol{P}}]^\mathsf{T}$ is the corresponding Jacobian matrix of the objective function system. For linear problems the unknown parameter to be determined may be calculated as $\boldsymbol{P} = (\mathbf{J}^\mathsf{T}\mathbf{J})^{-1}\mathbf{J}^\mathsf{T}\boldsymbol{T}$ however for a nonlinear inverse problem it may be observed that the Jacobian matrix, also known as the sensitivity matrix, has a functional dependence on the parameter $\boldsymbol{P}$ and as a result must be solved iteratively using a local linearization. In order for a suitable iteration procedure to converge it is necessary that $|\mathbf{J}^\mathsf{T}\mathbf{J}| \neq 0$ otherwise the IHCP is ill-conditioned. Whilst Tikhonov regularization is possible to solve a resultant ill-conditioned linear system $\boldsymbol{\Lambda\theta} = \boldsymbol{B}$ of form $\boldsymbol{\theta}_\alpha = [\boldsymbol{\Lambda}^\mathsf{T}\boldsymbol{\Lambda} + \alpha(\mathbf{R}^{(s)})^\mathsf{T}]^{-1}\boldsymbol{\Lambda}^\mathsf{T}\boldsymbol{B}$ where $\mathbf{R}^{(s)}$ for $s = 0, 1, 2$ is a Tikhonov regularization matrix following the overview presented in [28] where α is the regularization parameter.

Different approaches are possible for estimating α and whilst there is no definitive method the L-curve method appears common within the mathematical literature but is difficult to implement. To avoid these difficulties we opt to use the Levenberg-Marquardt method which is also amenable for potentially ill-conditioned systems and which has the advantage of being well established with existing implementations [31] that are relatively straightforward to implement and which incorporate newer mathematical optimization techniques such as the homotopy approach [1].

Based on our RBF discritization set $N_k = N_T$ to simplify the algebra when constructing the corresponding Jacobian matrix and note that our approach then specifies the parameters as $\boldsymbol{P}^\mathsf{T} = [\alpha_1, \ldots, \alpha_M]$ and the estimated temperature field as $\boldsymbol{\theta}(\boldsymbol{P})$ as the solution of the generalized Poisson equation as previously indicated. The algorithm to implement the IHCP formulated thermal conductivity measurement technique may now be conveniently summarized as follows:

(i) specify the spatial coordinates (x_i, y_i) for the points in the interior Ω and for the points (x_b, y_b) on the boundary Γ
(ii) assign the associated measured interior temperatures as T_i along with associated heat source/sink terms $\dot{q}_i$ taking note of the known boundary temperatures $T_f(x_b, y_b)$
(iii) construct the Jacobian matrix $\mathbf{J}$ either symbolically/numerically using the assumed values from the RBF parameterization
(iv) solve the nonlinear inverse problem using the Levenberg-Marquardt method for the given measured temperature data and assumed parameter values and iterate until convergence to the required accuracy level is achieved
(v) the associated parameter uncertainties $u(\alpha_i)$ $(i = 1, \ldots, M)$ in the RBF formulation of the thermal conductivity field may be constructed from Monte Carlo simulations and statistical post-processing of the results using simulation inputs obtained by sampling from the measured temperature values and their associated reported uncertainties
(vi) the parameter uncertainties may then be used as inputs in a GUM/GS1 uncertainty quantification calculation for the thermal conductivity uncertainty at any particular spatial coordinate within the domain

4. Discussion

In this paper we have investigated how to use an IHCP formulation as a means to determine thermal conductivity values for materials from experimental temperature measurements and numerical simulations. Potential benefits of the method that have been investigated are that there is no need for specialist laboratory reference thermal conductivity material standards, the method can be applied in industrial/plant environments with standard equipment/instruments with minimal physical complexity, and that the numerical algorithm to implement the method may be utilized to accurately relate and estimate the thermal conductivity uncertainties in terms of the input experimental data.

[1] R. L. Burden and J. D. Faires. *Numerical Analysis*. Brooks/Cole, 7th edition, 2001.
[2] G. E. Fasshauer. *Meshfree Approximation Methods with MATLAB*. World Scientific Publishing, 2007.
[3] G. E. Fasshauer and J. G. Zhang. On choosing optimal shape parameters for RBF approximation. *Numerical Algorithms*, 45:345–368, 2007.
[4] J. L. Fernandez-Martinez, Z. Fernandez-Muniz, J. L. G. Pallero, and L. M. Pedruelo-Gonzalez. From Bayes to Tarantola: New insights to understand uncertainty in inverse problems. *Journal of Applied Geophysics*, 98:62–72, 2013.
[5] A. Frackowiak, N. D. Botkin, M. Cialkowski, and K. H. Hoffman. A fitting algorithm for solving inverse problems of heat conduction. *International Journal of Heat and Mass Transfer*, 53:2123–2127, 2010.
[6] F. Geng and Y. Lin. Application of the variational iteration method to inverse heat source problems. *Computers and Mathematics with Applications*, 58:2098–2102, 2009.
[7] H. Hasuike, Y. Yoshizawa, A. Suzuki, and Y. Tamaura. Study on design of molten salt solar receivers for beam-down solar concentrator. *Solar Energy*, 80:1255–1262, 2006.
[8] Y. C. Hon and T. Wei. A fundamental solution method for inverse heat conduction problem. *Engineering Analysis with Boundary Elements*, 28(5):489–495, 2004.
[9] Y. C. Hon and T. Wei. The method of fundamental solution for solving multidimensional inverse heat conduction problems. *CMES Comput Model Eng Sci*, 7(2):119–132, 2005.
[10] F. P. Incropera and D. P. DeWitt. *Fundamentals of Heat and Mass Transfer*. John Wiley & Sons, 4th edition, 1996.
[11] JCGM/WG1. Evaluation of measurement data – guide to the expression of uncertainty in measurement (JCGM 100:2008). Technical report, BIPM/IEC/IFCC/ILAC/ISO/IUPAC/IUPAP/OIML, September 2008.
[12] JCGM/WG1. Evaluation of measurement data – supplement 1 to the "guide to the expression of uncertainty in measurement" – propagation of distributions using a Monte Carlo method (JCGM 101:2008). Technical report, BIPM/IEC/IFCC/ILAC/ISO/IUPAC/IUPAP/OIML, September 2008.

[13] JCGM/WG1. Evaluation of measurement data – supplement 2 to the "guide to the expression of uncertainty in measurement" – extension to any number of output quantities (JCGM 102:2011). Technical report, BIPM/IEC/IFCC/ILAC/ISO/IUPAC/IUPAP/OIML, October 2011.

[14] B. Jin and L. Marin. The method of fundamental solutions for inverse source problems associated with the steady-state heat conduction. *International Journal for Numerical Methods in Engineering*, 69:1570–1589, 2007.

[15] B. Tomas Johansson, D. Lesnic, and T. Reeve. A method for fundamental solutions for two-dimensional heat conduction. *International Journal of Computer Mathematics*, 88(8):1697–1713, 2011.

[16] B. Tomas Johansson, D. Lesnic, and T. Reeve. A method for fundamental solutions for the radial symmetric inverse heat conduction problem. *International Communications in Heat and Mass Transfer*, 39:887–895, 2012.

[17] H. Kameli and F. Kowsary. Solution of inverse heat conduction problem using the Lattice Boltzmann method. *International Communications in Heat and Mass Transfer*, 39:1410–1415, 2012.

[18] A. Karageorghis, D. Lesnic, and L. Marin. A survey of applications of the MFS to inverse problems. *Inverse Problems in Science and Engineering*, 19(3):309–336, 2011.

[19] P. Lair, J. Dumoulin, and P. Millan. Inverse method for flux characterization using infrared thermography in die forging. *Numerical Heat Transfer, Part A: Applications: An International Journal of Computation and Methodology*, 33:267–277, 1998.

[20] W. Liao, M. Dehghan, and A. Mohebbi. Direct numerical method for an inverse problem of a parabolic partial differential equation. *Journal of Computational and Applied Mathematics*, 232:351–360, 2009.

[21] L. Marin, A. Karageorghis, and D. Lesnic. The MFS for numerical boundary identification in two-dimensional harmonic problems. *Engineering Analysis with Boundary Elements*, 35:342–354, 2011.

[22] M. Mierzwiczak and J. A. Kolodziej. The determination of heat sources in two dimensional inverse steady heat problems by means of the method of fundamental solutions. *Inverse Problems in Science and Engineering*, 19(6):777–792, 2011.

[23] A. Miklavec, I. Pusnik, V. Batagelj, and J. Drnovsek. A large aperture blackbody bath for calibration of thermal imagers. *Measurement Science and Technology*, 24:1–8, 2013.

[24] K. Mosegaard. Quest for consistency, symmetry, and simplicity – the legacy of Albert Tarantola. *Geophysics*, 76(5):W51–W61, 2011.

[25] K. Mosegaard and M. Sambridge. Monte Carlo analysis of inverse problems. *Inverse Problems*, 18:R29–R54, 2002.

[26] K. Mosegaard and A. Tarantola. Monte Carlo sampling of solutions to inverse problems. *Journal of Geophysical Research*, 100(B7):12431–12447, 1995.

[27] M. N. Ozisik and H. R. B. Orlande. *Inverse Heat Transfer – Fundamentals and Applications*. Taylor and Francis, 2000.

[28] R. Pourgholi, A. Esfahani, and M. Abtahi. A numerical solution of a two-dimensional IHCP. *Journal of Applied Mathematics Computation*, 41:61–79, 2013.

[29] R. Pourgholi, M. Rostamian, and M. Emamjome. A numerical method for solving a nonlinear inverse parabolic problem. *Inverse Problems in Science and Engineering*, 18(8):1151–1164, 2010.

[30] R. W. Powell, C. Y. Ho, and P. E. Liley. Thermal conductivity of selected materials. Technical report, National Institute of Standards and Technology (previously NBS), November 1966. http://www.nist.gov/data/nsrds/NSRDS-NBS-8.pdf.

[31] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. *Numerical Recipes – The Art of Scientific Computing*. Cambridge University Press, 3rd edition, 2007.

[32] J. Pujol. The solution of nonlinear inverse problems and the Levenberg-Marquardt method. *Geophysics*, 72(4):W1–W16, 2007.

[33] Z. Qian and X. Feng. Numerical solution of a 2D inverse heat conduction problem. *Inverse Problems in Science and Engineering*, 21(3):467–484, 2013.

[34] K. Rashedi, H. Adibi, J. Amani, and K. Parand. Application of meshfree methods for solving the inverse one-dimensional Stefan problem. *Engineering Analysis with Boundary Elements*, 40:1–21, 2014.

[35] T. Reeve and B. Tomas Johansson. The method of fundamental solutions for a time-dependant two-dimensional cauchy heat conduction problem. *Engineering Analysis with Boundary Elements*, 37:569–578, 2013.

[36] M. R. Rodriguez-Sanchez, A. Soria-Verdugo, J. A. Almendros-Ibanez, A. Acosta-Iborra, and D. Santana. Thermal design guidelines for solar power towers. *Applied Thermal Engineering*, 63:428–438, 2014.

[37] B. K. Tsai, C. E. Gibson, A. V. Murthy, E. A. Early, D. P. DeWitt, and R. D. Saunders. Heat flux sensor calibration. Technical report, National Institute of Standards and Technology, May 2004. NIST Special Publication 250-65 (37 pages).