Combining Integral Transforms and Bayesian Inference in the Simultaneous Identification of Variable Thermal Conductivity and Thermal Capacity in Heterogeneous Media

Carolina P. Naveira-Cotta

Helcio R. B. Orlande

Renato M. Cotta[1]
e-mail: cotta@mecanica.coppe.ufrj.br

LTTC—Laboratory of Transmission and Technology of Heat, Mechanical Engineering Department – Escola Politécnica & COPPE, Universidade Federal do Rio de Janeiro, UFRJ, Cx. Postal 68503—Cidade Universitária, 21945-970 Rio de Janeiro, RJ, Brasil

This work presents the combined use of the integral transform method, for the direct problem solution, and of Bayesian inference, for the inverse problem analysis, in the simultaneous estimation of spatially variable thermal conductivity and thermal capacity for one-dimensional heat conduction within heterogeneous media. The direct problem solution is analytically obtained via integral transforms and the related eigenvalue problem is solved by the generalized integral transform technique (GITT), offering a fast, precise, and robust solution for the transient temperature field. The inverse problem analysis employs a Markov chain Monte Carlo (MCMC) method, through the implementation of the Metropolis-Hastings sampling algorithm. Instead of seeking the functions estimation in the form of local values for the thermal conductivity and capacity, an alternative approach is employed based on the eigenfunction expansion of the thermophysical properties themselves. Then, the unknown parameters become the corresponding series coefficients for the properties eigenfunction expansions. Simulated temperatures obtained via integral transforms are used in the inverse analysis, for a prescribed concentration distribution of the dispersed phase in a heterogeneous media such as particle filled composites. Available correlations for the thermal conductivity and theory of mixtures relations for the thermal capacity are employed to produce the simulated results with high precision in the direct problem solution, while eigenfunction expansions with reduced number of terms are employed in the inverse analysis itself, in order to avoid the inverse crime. Gaussian distributions were used as priors for the parameter estimation procedure. In addition, simulated results with different randomly generated errors were employed in order to test the inverse analysis robustness. [DOI: 10.1115/1.4004010]

Keywords: heat conduction, integral transforms, inverse problem, Bayesian inference, Monte Carlo Markov chain (MCMC), thermophysical properties, heterogeneous media, dispersed systems

Introduction

Heat conduction in heterogeneous media may be treated through effective thermophysical properties with space variability in their functional representation, when the characterization of these physical properties is to be made almost on a case to case basis. Therefore, it becomes an interest to develop a methodology for the identification of physical properties already on the finished material or system. Thus, the problem that is addressed here is that of providing a reliable prediction of the thermal properties functions in heterogeneous media, even without the knowledge of the physical properties of each component in the mixture and their relative concentrations and without employing in advance a specific theoretical model among those proposed in the literature. Such inverse problem analysis shall then allow for the verification of the adequacy of the existing models or even for their appropriate modification, or alternatively, the formulation of novel predictive expressions. The literature on inverse problems in heat conduction is quite vast, as reviewed in Refs. [1–4]. For this reason, we have focused our attention here on few previous works that have also addressed the estimation of spatially variable thermal properties [5–13].

Regarding the solution of the direct heat conduction problem for a heterogeneous medium in transient state, the procedure employed in this work has been recently advanced [14,15], based on the classical integral transform technique (CITT) [16]. Since we deal with a linear heat conduction problem with space variable coefficients, integral transformation results into a decoupled transformed ordinary differential system, which is capable of being analytically solved. Nevertheless, the solution of the corresponding auxiliary eigenvalue problem for the classical integral transform technique demands the use of computational methodologies, such as the generalized integral transform technique (GITT) [16–19]. In this work, we make use of the GITT, which has been successfully applied to the solution of eigenvalue problems with variable coefficients and irregular domains [20,21]. Another possibility here exploited is to express the variable coefficients themselves as eigenfunction expansions [14]. This procedure is particularly useful for the fully analytical evaluation of the coefficients of the algebraic system in

[1]Corresponding author.

Contributed by the Heat Transfer Division of ASME for publication in the JOURNAL OF HEAT TRANSFER. Manuscript received December 21, 2009; final manuscript received April 11, 2011; published online August 31, 2011. Assoc. Editor: Ofodike A. Ezekoye.

the transformed eigenvalue problem. Therefore, all manipulations can be expressed in terms of simpler eigenfunctions, allowing for analytical integrations and additional derivations to be performed exactly in symbolic computation platforms [22].

Among the various available solution techniques of inverse problems [1–4], this work uses Bayesian inference for the simultaneous estimation of spatially variable thermal capacity and conductivity, in one-dimensional transient heat conduction problems of heterogeneous media, by employing the Markov chain Monte Carlo method (MCMC) [23–30]. The Metropolis-Hastings algorithm is used for the sampling procedure [31,32], which is implemented in the MATHEMATICA platform [22]. This sampling procedure is in general the most expensive computational task for solving an inverse problem by the Markov chain Monte Carlo method, since the direct problem is calculated for each state of the chain. In this context, the use of a fast, accurate, and robust computational implementation of the direct solution is extremely important. Thus, the integral transformation approach discussed above becomes very attractive for the combined use with the Bayesian estimation procedure, since all steps in the method are determined analytically at once by symbolic computation and the single numerical repetitive task is the solution of an algebraic matrix eigenvalue problem [14]. This same combination of approaches has been recently and quite successfully applied to the estimation of space variable thermal conductivity in two-phase dispersed systems, once the a priori information on the dispersed phase concentration is available [15].

Instead of seeking the function estimation in the form of local values for the thermal properties, an alternative approach is employed here, which is based on the eigenfunction expansion of the unknown properties. Then, the unknown parameters become the corresponding series coefficients. Simulated temperatures obtained via integral transforms are used in the present inverse analysis. From the prescription of the concentration distribution of the dispersed phase, available correlations for the thermal conductivity and theory of mixtures relations for the thermal capacity are employed to produce the simulated data with high precision in the direct problem solution, while eigenfunction expansions with reduced number of terms are employed in the inverse analysis itself, in order to avoid the so called inverse crime. Gaussian distributions were used as priors for the parameter estimation procedure, with different uncertainties for comparison purposes. In addition, simulated results with different randomly generated errors were employed in order to test the inverse analysis robustness.

Problem Formulation and Direct Problem Solution

We consider a one-dimensional special case of the general formulation on transient heat conduction presented and solved in Ref. [14], for the temperature field $T(x,t)$, in the region $x\in[0,L]$. The formulation includes the space variable thermal conductivity and heat capacity, as shown in problem (1) below. The heat conduction equation with the corresponding initial and boundary conditions are given by

$$\rho(x)c_p(x)\frac{\partial T_m(x,t)}{\partial t}=\frac{\partial}{\partial x}\left(k(x)\frac{\partial T_m(x,t)}{\partial x}\right)-\frac{h_{eff}(x)}{L_z}(T_m(x,t)-T_\infty)+\frac{q(x,t)}{L_z},0<x<L;t>0 \quad (1a)$$

$$T_m(x,0)=T_\infty \quad (1b)$$

$$\left.\frac{\partial T_m(x,t)}{\partial x}\right|_{x=0}=0,\quad t>0 \quad (1c)$$

$$\left.\frac{\partial T_m(x,t)}{\partial x}\right|_{x=L}=0,\quad t>0 \quad (1d)$$

Problem (1) covers a typical one-dimensional transient thermal conductivity experimental setup for a thermally thin plate, including prescribed heat flux at one face and convective heat losses at the opposite face, according to Fig. 1, and it is based on a lumped formulation across the sample thickness. The coefficients $\rho(x)c_p(x)$ and $k(x)$, are thus responsible for the information related to the heterogeneity of the medium. The space variation of the temperature is then promoted by the variation of the applied heat flux and eventually also of the effective heat transfer coefficient. The exposed plate surface is required so as to allow for temperature measurements acquisition via infrared thermography [27].

The formal exact solution of problem (1) is then obtained with the classical integral transform method [16] and is written as:

$$T(x,t)=T_\infty+\sum_{i=1}^{\infty}\tilde{\psi}_i(x)\int_0^t\bar{g}_i(t)e^{-\mu_i^2(t-t)}dt' \quad (2)$$

where the eigenvalues μ_i and eigenfunctions $\psi_i(x)$ are obtained from the eigenvalue problem that contains the information about the heterogeneous medium, in the form:

$$\frac{d}{dx}\left[k(x)\frac{d\psi_i(x)}{dx}\right]+(\mu_i^2w(x)-d(x))\psi_i(x)=0,\ x\in[0,L] \quad (3a)$$

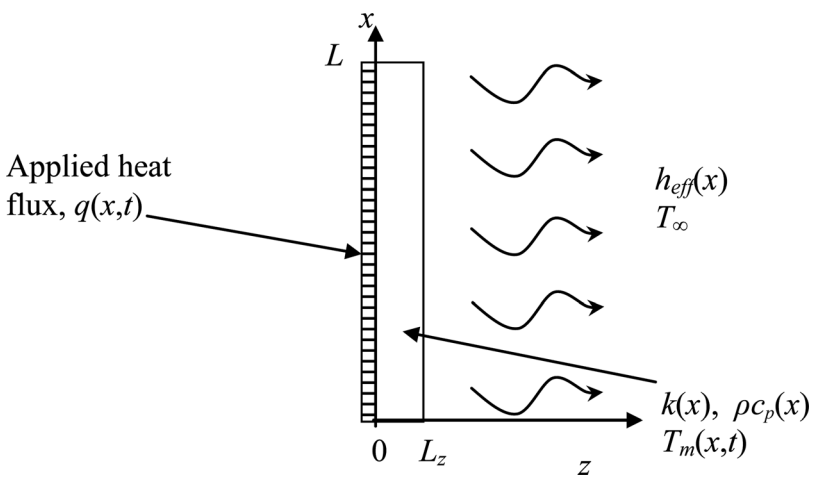


Fig. 1 Schematic representation of experimental setup for thermophysical properties determination, employed in the direct/inverse problem solutions

with boundary conditions

$$\frac{d\psi_i(x)}{dx} = 0, \quad x = 0, \tag{3b}$$

$$\frac{d\psi_i(x)}{dx} = 0, \quad x = L \tag{3c}$$

Also, the other quantities that appear in the exact solution (2) are computed after solving problem (3), such as

$$\tilde{\psi}_i(x) = \frac{\psi_i(x)}{\sqrt{N_i}}, \text{ normalized eigenfunctions} \tag{4a}$$

$$N_i = \int_0^L w(x)\psi_i^2(x)dx, \text{ normalization integrals} \tag{4b}$$

$$\bar{g}_i(t) = \int_0^L P(x,t)\tilde{\psi}_i(x)dx, \text{ transformed source terms} \tag{4c}$$

where

$$w(x) = \rho(x)c_p(x); \tag{4d}$$

$$d(x) = \frac{h_{eff}(x)}{L_z}; \tag{4e}$$

$$P(x,t) = \frac{q(x,t)}{L_z} + d(x)T\infty \tag{4f}$$

It is quite desirable from the point of view of the inverse analysis to employ a flexible computational approach to handle the eigenvalue problem with arbitrarily variable coefficients, problem (3). Thus, the GITT is here employed in the solution of the Sturm-Liouville problem (3) via the proposition of a simpler auxiliary eigenvalue problem, and expanding the unknown eigenfunctions in terms of the chosen basis, and this solution procedure is detailed in Refs. [14,15].

It is also of interest to express the variable coefficients themselves as eigenfunction expansions [14,15]. This is particularly advantageous in the solution of problem (3). All the related integrals can then be expressed in terms of eigenfunctions, allowing for straightforward analytical evaluations [14,15]. For instance, the coefficient $w(x)$ can be expanded in terms of eigenfunctions, together with a filtering solution to enhance convergence, in the following form:

$$w(x) = w_f(x) + \sum_{k=1}^{\infty} \tilde{\Gamma}_k(x)\bar{w}_k, \qquad \text{inverse} \tag{5a}$$

$$\bar{w}_k = \int_0^L \hat{w}(x)[w(x) - w_f(x)]\tilde{\Gamma}_k(x)dx, \qquad \text{transform} \tag{5b}$$

where $\hat{w}(x)$ is the weighting function for the chosen normalized eigenfunction $\tilde{\Gamma}_k(x)$. This eigenfunction basis is chosen with first order boundary conditions, while the filtering function would be a simple analytic function that satisfies the boundary values for the original coefficients. This procedure shall also be of interest in the function estimation task, when the transformed thermal properties coefficients will be the parameters to be estimated.

Inverse Problem Solution Via Bayesian Inference

Consider the vector of parameters appearing in the physical model formulation as

$$\mathbf{P}^T \equiv [P_1, P_2, \ldots, P_{Np}] \tag{6}$$

where N_p is the number of parameters. For the solution of the inverse problem of estimating $\mathbf{P}$, we assume available the measured temperature data given by

$$(\mathbf{Y} - \mathbf{T})^T = \left(\vec{Y}_1 - \vec{T}_1, \vec{Y}_2 - \vec{T}_2, ..., \vec{Y}_{N_t} - \vec{T}_{N_t}\right) \tag{7}$$

where $\vec{Y}_i$ contains the measured temperatures for each of the N_x sensors at time t_i, $i = 1, \ldots, N_t$, that is,

$$(\vec{Y}_i - \vec{T}_i) = (Y_{i1} - T_{i1}, Y_{i2} - T_{i2}, ..., Y_{iN_x} - T_{iN_x}) \quad \text{for } i = 1, \ldots, N_t \tag{8}$$

so that we have $N_m = N_x N_t$ measurements in total. Bayes' theorem can then be stated as [23–25]

$$p_{\text{posterior}}(\mathbf{P}) = p(\mathbf{P}|\mathbf{Y}) = \frac{p(\mathbf{P})p(\mathbf{Y}|\mathbf{P})}{p(\mathbf{Y})} \tag{9}$$

where $p_{\text{posterior}}(\mathbf{P})$ is the posterior probability density, that is, the conditional probability of the parameters $\mathbf{P}$ given the measurements $\mathbf{Y}$; $p(\mathbf{P})$ is the prior density, that is, a statistical model for the information about the unknown parameters prior to the measurements; $p(\mathbf{Y}|\mathbf{P})$ is the likelihood function, which gives the relative probability density (loosely speaking, relative probability) of different measurement outcomes $\mathbf{Y}$ with a fixed $\mathbf{P}$; and $p(\mathbf{Y})$ is the marginal probability density of the measurements, which plays the role of a normalizing constant.

In this work, we assume that the measurement errors are Gaussian random variables, with known (modeled) means and covariances and that the measurement errors are additive and independent of the unknowns. With these hypotheses, the likelihood function can be expressed as [23–25]

$$p(\mathbf{Y}|\mathbf{P}) = (2\pi)^{-M/2}|\mathbf{W}|^{-1/2}\exp\left\{-\frac{1}{2}[\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T\mathbf{W}^{-1}[\mathbf{Y} - \mathbf{T}(\mathbf{P})]\right\} \tag{10}$$

where $\mathbf{W}$ is the covariance matrix of the measurement errors.

When it is not possible to analytically obtain the corresponding marginal distributions, one needs to use a method based on simulation [23–25]. The inference based on simulation techniques uses samples to extract information about the posterior distribution, $p(\mathbf{P}|\mathbf{Y})$. As a sample is always a partial substitute of the information contained in a density, simulation-based methods are inherently approximate. Several sampling strategies are proposed in the literature, including the MCMC, adopted in this work that converges to a stationary distribution, which is the distribution of interest in the problem.

The most commonly used Monte Carlo method with Markov chain algorithms are the Metropolis-Hastings, here employed, and the Gibbs sampler [24,25]. The Markov chain according to the generic label of Metropolis-Hastings, comes from the articles of Metropolis et al. [31] and Hastings [32], later on complemented by the works of Barker [33] and Peskun [34]. The Metropolis-Hastings algorithm uses the same idea of the rejection methods, i.e., a value is generated from an auxiliary distribution and accepted with a given probability. This correction mechanism ensures the convergence of the chain for the equilibrium distribution. That is, the algorithm includes an additional step, where the transition mechanism depends on a proposal for a transition and a stage of assessing the equilibrium density, but this is represented by the global transition via the probability of acceptance.

The unknown quantities in the heat conduction problem addressed here are the heat capacity, $w(x)$, the thermal conductivity of the medium, $k(x)$, and the effective heat transfer coefficient, $h_{\text{eff}}(x)$. However, the approach adopted in solving the direct problem was to expand the coefficients functions in terms of eigenfunctions, so that the unknown quantities are in fact the

coefficients of the eigenfunction expansions and the two values of each property at the boundaries, employed in the solution procedure as a filter. Before addressing the estimation of the unknown parameters, the behavior of the determinant of the information matrix $\mathbf{J}^T\mathbf{J}$ [3] is analyzed in order to inspect the influence of the number of parameters to be estimated in the solution of the inverse problem.

Results and Discussion

The inverse problem solution here illustrated involves the analysis of an abrupt variation of particles concentration in a two phase dispersed system. In order to examine the accuracy and robustness of the proposed inverse analysis, we have made use of simulated measured temperature data along the length of the domain, in the transient regime, such as obtained through infrared thermography [27]. Such measurements were obtained from the solution of the direct (forward) problem by specifying the functions and values for the filler concentration distribution and thermophysical properties. The simulated data were disturbed by a Gaussian error with a zero mean and constant and known variance, in order to simulate actual measured temperature data. For the results of the inverse analysis to be presented below, we have employed the parameter values shown in Table 1 for the generation of the simulated measured data, as extracted from [35,36] for a polyethylene matrix filled with alumina particles.

The space variable distribution for the abrupt variation of the concentration of the filler into the matrix is governed by the parameter γ in the function below:

$$\phi(x) = \phi_{x=0} + (\phi_{x=L} - \phi_{x=0})\delta(x) \tag{11a}$$

$$\delta(x) = \frac{1}{1 + e^{-\gamma(x-x_c)}} \tag{11b}$$

with x_c being the transition position between the regions of lower and higher concentrations of the filler.

The direct problem solution was obtained from the generalized integral transform technique as previously discussed. A thorough convergence analysis was performed to select the number of terms in the temperature expansion, as well as the number of terms in the coefficients expansion.

From the availability of the filler concentration distribution along the domain, Eq. (11*a*), the heat capacity along the space coordinate is directly determined from the theory of mixtures. Thus, the coefficient $w(x)$ is considered as known in the direct problem analysis to produce simulated experimental data, given as

$$w(x) = 1 + \left(\frac{\rho_d c_{p_d}}{\rho_m c_{p_m}} - 1\right)\phi(x) \tag{12}$$

where the subscript d stands for the dispersed phase (filler) properties while m stands for the matrix phase properties. For the thermal conductivity calculation, the volumetric content of the filler is not sufficiently informative to yield a good prediction of this physical property [32,33], especially for high concentrations. Many theoretical and empirical models have been proposed to predict the effective thermal conductivity of two-phase dispersed systems, and comprehensive review articles have discussed the applicability of many of these models.

Lewis and Nielsen [37] proposed a model that attempts to include the effect of the shape of the particles and the orientation or type of packing for a two-phase system. The resulting expression is given as

$$k_c = k_m\left[\frac{1 + AB\phi}{1 - B\phi\psi}\right], \tag{13a}$$

$$\text{where } B = \frac{(k_d/k_m) - 1}{(k_d/k_m) + A} \text{ and} \tag{13b}$$

$$\psi = 1 + \left(\frac{1 - \phi_m}{\phi_m^2}\right)\phi \tag{13c}$$

The values of A and ϕ_m are suggested in Ref. [34] for a number of different geometric shapes and orientations, such as $A = 1.50$ for spheres and $\phi_m = 0.637$ for random packing.

The parameter estimation problem of interest in this work involves the coefficients of the eigenfunction expansion of $w(x)$ and $k(x)$, as well as the two values of these coefficients at the boundaries that are used in the linear filter function of the expansion process. The unknown parameters also involve the effective heat transfer coefficient, which is considered to be constant in the present inverse analysis. Thus, the parameters and the number of parameters to be estimated are given by

$$\mathbf{P} = [w_{x=0}, w_{x=L}, \bar{w}_1, \bar{w}_2, \bar{w}_3, ..., \bar{w}_{N_w}, k_{x=0}, k_{x=L}, \bar{k}_1, \bar{k}_2, \bar{k}_3, ..., \bar{k}_{N_k}, d],$$
$$\text{with } N_P = N_w + N_k + 5 \tag{14}$$

where

$$w(x) = w_f(x) + \sum_{k=1}^{N_w} \tilde{\Gamma}_k(x)\bar{w}_k \tag{15a}$$

$$k(x) = k_f(x) + \sum_{k=1}^{N_k} \tilde{\Gamma}_k(x)\bar{k}_k \tag{15b}$$

The prescribed heat flux is also considered to be governed by an abrupt behavior in the space coordinate, such as in Eqs. (11), but using $\gamma = 100$ practically reproducing a step function, and $x_c = 0.5$, for half of the plate length. The two extreme values for the heat flux were taken as $q_0 = 0$, as in Table 1, and $q_L = q_w$. Although q_w was not estimated in the present analysis, due to linear dependency with the remaining parameters, the equation was all divided by the assumed value of q_w, which allows one to recover the estimated parameters, after the inverse analysis, by multiplying the available value of q_w with its associated uncertainty.

Table 1 Parameters values used to generate the simulated measurement data [36]

Length	$L = 0.04$ m
Percent filler concentration at x = 0	$\phi_0 = 0$
Percent filler concentration at x = L_x	$\phi_L = 45$
Matrix properties (HDPE)	$\rho_m = 968$ kg/m^3 $c_{pm} = 2300$ J/kgC $k_m = 0.545$ W/mC
Filler properties (alumina)	$\rho_d = 3970$ kg/m^3 $c_{pd} = 760$ J/kgC $k_d = 36$ W/mC
Effective thermal conductivity model	Lewis and Nielsen ($A = 1.5$; $\phi_m = 0.637$)
Parameters in filler concentration function	$\gamma = 25$ $x_c = 0.2$
Effective heat transfer coefficient	$h_{\text{eff}} = 16.7$ W/m^{2}C
Parameters in applied heat flux function	$\gamma = 100$ $x_c = 0.5$ $q_0 = 0$ W/m^2 $q_L = 598$ W/m^2
Ambient and initial temperature	$T_\infty = 23$ C
Plate thickness	$L_z = 0.003$ m

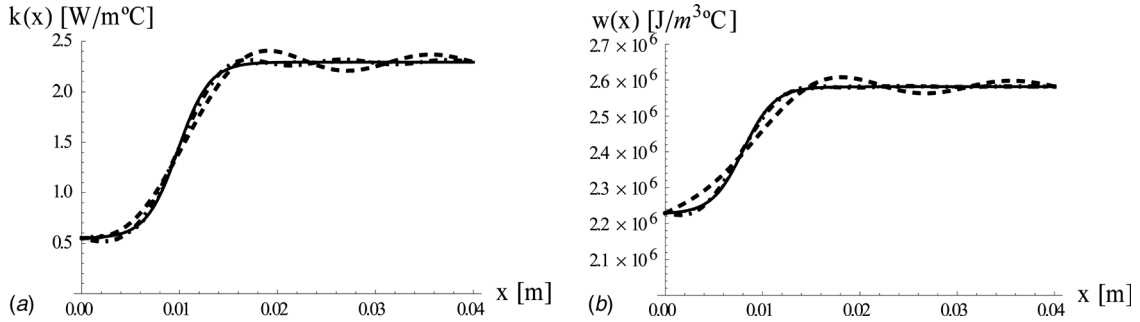


Fig. 2 Convergence behavior of the thermal conductivity and heat capacity expansions [original function-solid line, expansions-dashed (four terms), dot-dashed (seven terms), dotted (ten terms) lines]: (*a*) $k(x)$ $N_k = 4$, 7, and 10 and (*b*) $w(x)$ $N_w = 4$, 7, and 10

In the proposed inverse approach, the truncation orders of the thermal capacity and conductivity expansions, N_w and N_k, thus control the number of parameters to be estimated. The convergence analysis of the $w(x)$ and $k(x)$ expansions, Eqs. (15), is shown in Figs. 2(*a*) and 2(*b*), for three different truncation orders, $N_w = N_k = 4$, 7, and 10, respectively, in dashed, dotted, and dot-dashed lines. The exact function is plotted in solid line. It can be observed that the three increasing truncation orders given in these figures are able to recover the characteristic behavior of the chosen thermal properties functions, following the abrupt change in filler concentration. However, the results for the lowest truncation order, $N_w = N_k = 4$, still show some oscillation around the exact functions, while for $N_w = N_k = 7$ a much closer agreement between the expanded and the exact functions is observed and practically full convergence is achieved with the largest truncation order ($N_w = N_k = 10$).

Based on possible experimental procedures, we have considered two cases for the analysis of the determinant of the information matrix $\mathbf{J}^T\mathbf{J}$: (i) variation of the number of parameters to be estimated with a fixed number of spatial measurements (sensors) and a fixed frequency of measurements; (ii) variation of the number of spatial measurements (sensors) with a fixed frequency of measurements and a fixed number of parameters.

The analyses of the evolution in time of the information matrix determinant, for a total of 12,000 measurements ($N_x = 40$ along the domain and $N_t = 300$ in time), showed that the gradual increase on the number of parameters ($N_P = 13$, 19, and 25, which correspond, respectively, to $N_w = N_k = 4$, 7, and 10, plus the two end values of thermal capacity and conductivity that are filtered from the expansion) markedly decreases the value of the determinant, as illustrated by their values at steady-state, 1.7427×10^{15}, 5.36019, and 5.39711×10^{-23}, respectively, for $N_P = 13$, 19, and 25. Therefore, it has been observed, as expected, that by increasing the number of parameters markedly affects the conditioning of the estimation procedure.

We have also analyzed the information matrix determinant for the fixed case of $N_P = 19$ parameters, but with a variable number of equally spaced measurements along the domain ($N_x = 160$, 40, and 4), where the lowest value of N_x has been considered to inspect the possibility of employing traditional temperature measurement techniques, such as thermocouples, while the higher values represent a thermographic type of temperature measurements. It has been observed that the determinant of the sensitivity matrix significantly decreases by reducing the number of measurements along the domain (1.4734×10^{12}, 5.36019, and 8.10324×10^{-48}, for $N_x = 160$, 40, and 4, respectively). Therefore, based on the information matrix analysis, we have then adopted in the solution of the present inverse problem $N_w = N_k = 4$ or 7 terms in the heat capacity and thermal conductivity expansions ($N_P = 13$ or 19 parameters), $N_x = 40$ spatial measurements, and $N_t = 300$ measurements in time.

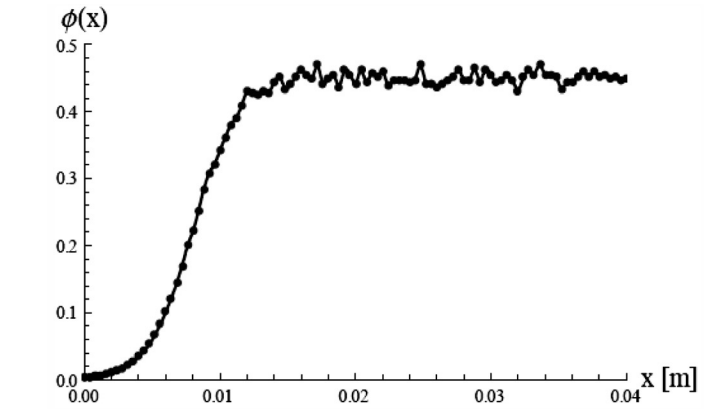
The simulated experimental data were generated with temperature uncertainties of 0.1°C and 0.5°C, obtained from the direct problem solution computed with $N = 50$ terms in the temperature expansion, and $N_k = 14$ terms in both coefficient expansions of $k(x)$ and $w(x)$. The subsequent inverse analysis was performed by using just $N = 15$ terms in the temperature expansion, in order to avoid the so-called inverse crime [23].

A relevant aspect in the use of the eigenfunction expansion coefficients as a parameter estimation procedure, is the definition of maximum and minimum values for the coefficients to be estimated, as discussed in Ref. [15], from the corresponding maximum and minimum values of the thermal capacity and conductivity, $w_{\max}, k_{\max}$ and $w_{\min}, k_{\min}$. The adopted step in the search procedure used in the generation of candidates within the minimum-maximum parameters range was 1% of the standard deviation of the Gaussian prior mean of each parameter.

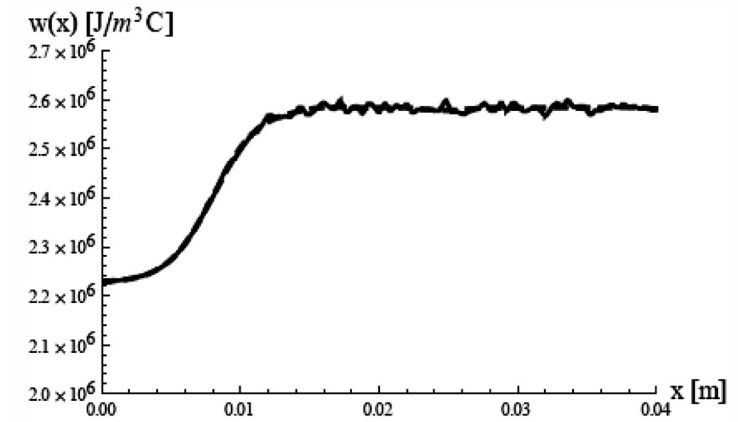
Informative Gaussian distributions were provided as priors for each of the coefficients to be estimated. In building the priors for the thermophysical properties, we have added an uncertainty on the information about the filler concentration distributions, in the form of a 20% standard deviation of the exact value, which was then propagated to the thermal capacity and conductivity prior distributions, as computed from Eqs. (13) and (14) , and illustrated in Figs. 3(*a*)–3(*c*). In these figures, it is plotted, the expansions for the two original coefficients with $N_w = N_k = 7$ in dashed lines and the prior curves including the white noise in solid lines. Table 2 shows the values for the maximum, minimum, the initial search step, and the limiting upper and lower values for the 19 parameters to be estimated.

Three illustrative cases were analyzed aimed at validating and demonstrating the proposed methodology, which are summarized in Table 3. Case 1 has been chosen for validation of the implemented algorithm, by employing $NT = 15$ and $N_w = N_k = 4$ ($NP = 13$ parameters) in both the simulated results and the inverse analysis. The simulated temperature data were produced with a 0.1°C uncertainty, but the uncertainty in the filler concentration prior was not considered. The priors for the thermal capacity and conductivity were allowed to have a standard deviation of 40%, while the effective heat transfer coefficient prior includes a standard deviation of 20%. In case 2, the simulated data were generated with $NT = 50$ and $N_w = N_k = 14$, and the uncertainty on the filler concentration prior information was implemented with standard deviation of 20% of the exact value. All the other parameters were kept equal to case 1, including the number of parameters to be estimated, $NP = 13$, but the uncertainty on the simulated temperature data was markedly increased to 0.5°C. Case 3 is closer to the actual thermophysical properties identification task, where the number of parameters to be estimated was increased to $NP = 19$, with $N_w = N_k = 7$, and the uncertainty on the temperature measurements was kept at 0.5°C. Another difference between the two cases is that the standard deviation of the Gaussian prior for the thermal capacity was lowered to 20% in case 3, which lies on the fact that the uncertainty on the thermal capacity is less affected by changes on the filler concentration.

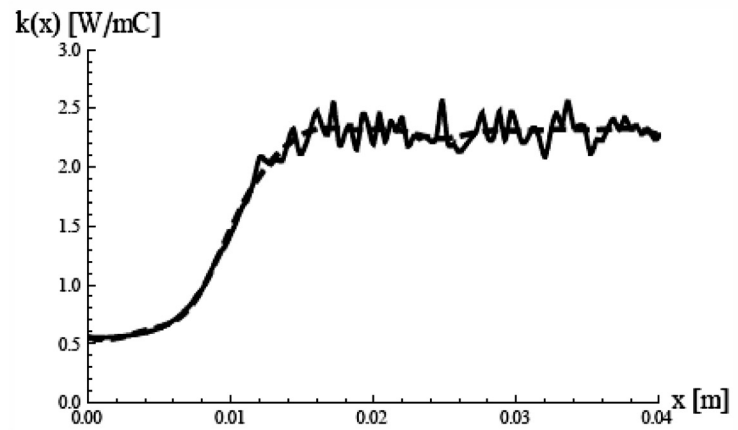
Assuming a burn in period of 10,000 states in the Markov chains and a total of 50,000 states in the whole chains, estimates



(*a*)



(*b*)



(*c*)

Fig. 3 Behavior of priors: (*a*) filler concentration distribution with 20% standard deviation and resulting function (solid) and expansion (dashed) of (*b*) thermal capacity and (*c*) thermal conductivity

of the parameters for each case were obtained from the sample average of the remaining 40,000 states. The acceptance rates reached in the cases analyzed are around 15% to 20%. Case 1 was aimed at validating the computational procedure and expected to provide the best estimates, since the same size of expansions were employed in both the simulation and the inverse analysis, and the uncertainty of the simulated temperature data is the lower value of 0.1°C. In case 2, the expansions truncation orders are different for the simulated data and the inverse problem solution. In addition, the standard deviation of the simulated measurements was increased to 0.5°C; hence, the estimated results are expected to be not as accurate as for case 1. Case 3 also involves the uncertainty of 0.5°C in the simulated data, but now the number of parameters has been increased.

Figures 4–6 present the estimated functions found for the two properties, their exact original and expanded relations, as well as the curves constructed for the 99% confidence intervals. Clearly, case 1 (Fig. 4) provides the best set of results, offering further evidence of the algorithm validation. It is noticeable from Figs. 4(*a*) and 4(*c*) that the exact functions, $k(x)$ and $w(x)$, expanded with four terms, are fully recovered by the estimated function, also with $N_w = N_k = 4$. The thin solid line represents the exact original function for the coefficients, which is shown just for reference purposes, since the simulated data were obtained with its

Table 2 Exact values, initial guesses, search step, and the search bounds for the inverse analysis

Parameter	Exact	Initial guess	Step	P_{min}	P_{max}
h_{eff} , W/m^{2}C	16.694	18.364	0.0334	10.	20.
$k_{x=0}$, W/mC	0.5490	0.604	0.00220	0.545	5.786
$k_{x=L}$, W/mC	2.2929	2.522	0.00909	0.545	5.786
$\bar{k}_1$, W/mC	0.1097	0.121	0.000455	-0.944	0.944
$\bar{k}_2$, W/mC	0.00204	0.00225	$4.167\ 10^{-6}$	-0.236	0.236
$\bar{k}_3$, W/mC	−0.02825	−0.0311	0.000111	−0.315	0.315
$\bar{k}_4$, W/mC	−0.02661	−0.0293	0.000122	−0.118	0.118
$\bar{k}_5$, W/mC	−0.01328	−0.0146	0.0000443	−0.189	0.189
$\bar{k}_6$, W/mC	−0.00107	−0.00118	$1.700\ 10^{-6}$	−0.0786	0.0786
$\bar{k}_7$, W/mC	0.00485	0.00534	0.0000185	−0.135	0.135
$w_{x=0}$, J/m^{3}C	$2.229\ 10^6$	$2.452\ 10^6$	4457.6	$2.226\ 10^6$	$2.938\ 10^6$
$w_{x=L}$, J/m^{3}C	$2.582\ 10^6$	$2.841\ 10^6$	5161.9	$2.226\ 10^6$	$2.938\ 10^6$
$\bar{w}_1$, J/m^{3}C	25047.5	27552.2	50.516	−128155.	128155.
$\bar{w}_2$, J/m^{3}C	4370.2	4807.2	8.607	−32038.7	32038.7
$\bar{w}_3$, J/m^{3}C	−2701.1	−2971.2	5.362	−42718.2	42718.2
$\bar{w}_4$, J/m^{3}C	−4449.0	−4893.9	9.375	−16019.3	16019.3
$\bar{w}_5$, J/m^{3}C	−3613.8	−3975.2	6.924	−25630.9	25630.9
$\bar{w}_6$, J/m^{3}C	−1955.3	−2150.8	3.680	−10679.6	10679.6
$\bar{w}_7$, J/m^{3}C	−512.22	−563.44	1.024	−18307.8	18307.8

Table 3 Definition of input data for test cases in the inverse analysis

Input data	Case 1	Case 2	Case 3
NT, N_w, N_k (simul. data)	15, 4, 4	50, 14, 14	50, 14, 14
NT, N_w, N_k (inverse sol.)	15, 4, 4	15, 4, 4	15, 7, 7
NP (inverse sol.)	13	13	19
Step, δ	1%	1%	1%
White noise std. dev. (priors)	0%	20%	20%
Std. dev. priors (w, k, h_{eff})	40%, 40%, 20%	40%, 40%, 20%	40%, 20%, 20%
Exp. Error (temperature)	0.1°C	0.5°C	0.5°C

approximation expanded in the series (15*a*) and (15*b*) (thick lines in Figs. 4(*a*) and 4(*c*)). For case 2 (see Fig. 5) when the simulated data uncertainty is increased to 0.5°C, the thermal conductivity estimation shows some deviation at the boundary $x=L$, and besides, the thermal capacity is slightly less adherent at the neighborhood of the opposing boundary, $x=0$, but with a sufficiently wide confidence interval. The exact value for $k_{x=L}$ is 2.293 W/m°C, while the estimation provides the value 2.422 W/m°C, with the 99% confidence interval [2.339, 2.505] W/m °C, which does not include the exact boundary thermal conductivity. For the thermal capacity, the exact value for $w_{x=0}$ is 2.229×10^6 J/m^3°C, while the estimation provides the value 2.277×10^6 J/m^3°C, with the 99% confidence interval $[2.210\times10^6,\ 2.344\times10^6]$ J/m^3°C, which clearly includes the exact boundary value.

In Figs. 6(*a*)–6(*d*), related to case 3, we illustrate the behavior of the estimation of the properties with expansions of $N_w=N_k=7$, which clearly provides a much better reproduction of the original functions (thin solid line), practically overwritten by the exact expansions at this same order. Fairly large standard deviations of 40% and 20% were provided for the priors on both $k(x)$ and $w(x)$, so as to challenge the proposed approach, and quite reasonable estimates were achieved. The estimation of the thermal capacity boundary values now provides 2.247×10^6 J/m^3°C and 2.595×10^6 J/m^3°C, with the 99% confidence intervals $[2.213\times10^6,\ 2.281\times10^6]$ J/m^3°C and $[2.570\times10^6,\ 2.619\times10^6]$ J/m^3°C, at $x=0$ and $x=L$, respectively. The estimation of the thermal conductivity function is fairly accurate in case 3, similarly to case 2, while the estimates for the heat transfer coefficient were all very accurate in the three cases analyzed.

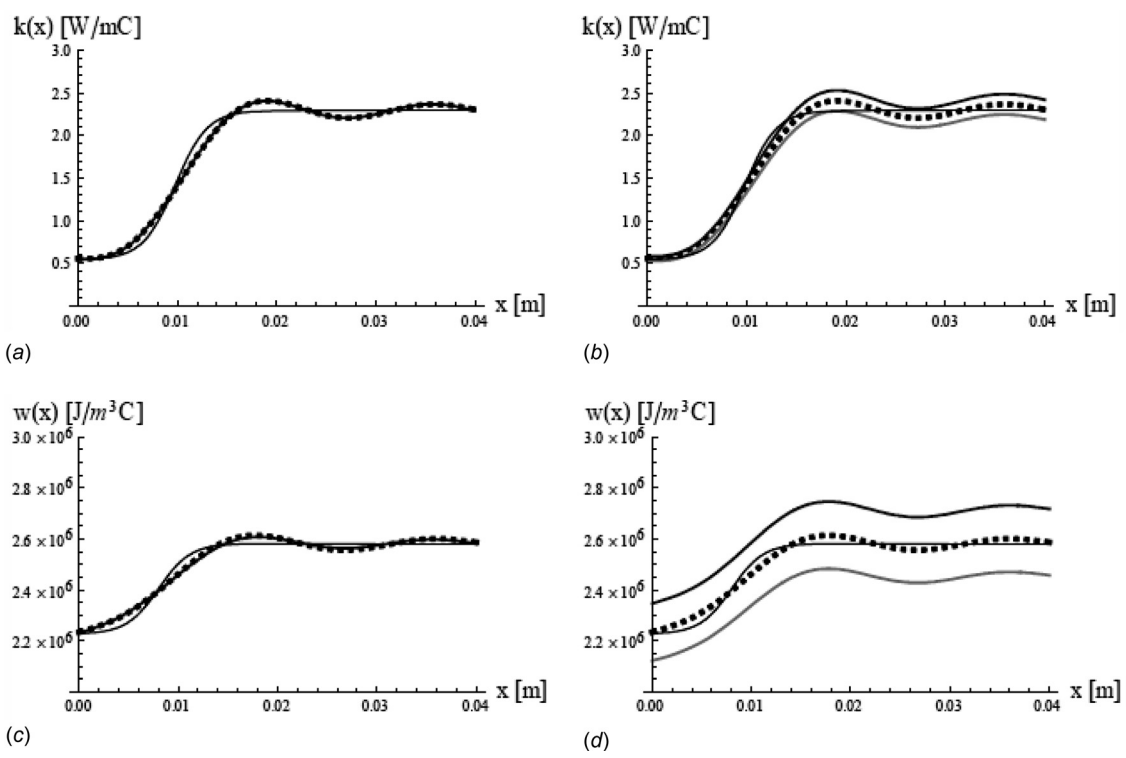


Fig. 4 (*a–d*)—Estimated functions in case 1: (*a*) *k*(*x*)—exact (solid thin), exact expanded (solid thick), and estimated (dashed); (*b*) *k*(*x*)—exact (solid thin), confidence bounds (solid thick), and estimated (dashed); (*c*) *w*(*x*)—exact (solid thin), exact expanded (solid thick), and estimated (dashed); (*d*) *w*(*x*)—exact (solid thin), confidence bounds (solid thick), and estimated (dashed)

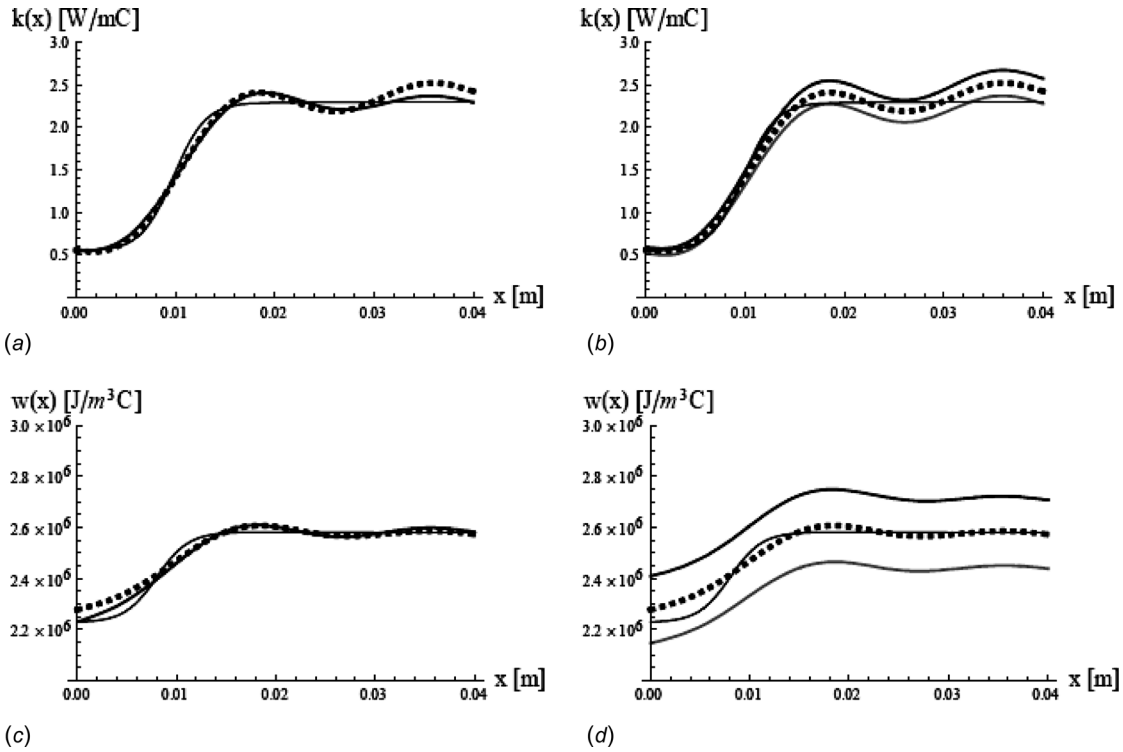


Fig. 5 (*a–d*)—Estimated functions in case 2: (*a*) *k*(*x*)—exact (solid thin), exact expanded (solid thick), and estimated (dashed); (*b*) *k*(*x*)—exact (solid thin), confidence bounds (solid thick), and estimated (dashed); (*c*) *w*(*x*)–exact (solid thin), exact expanded (solid thick), and estimated (dashed); (*d*) *w*(*x*)—exact (solid thin), confidence bounds (solid thick), and estimated (dashed)

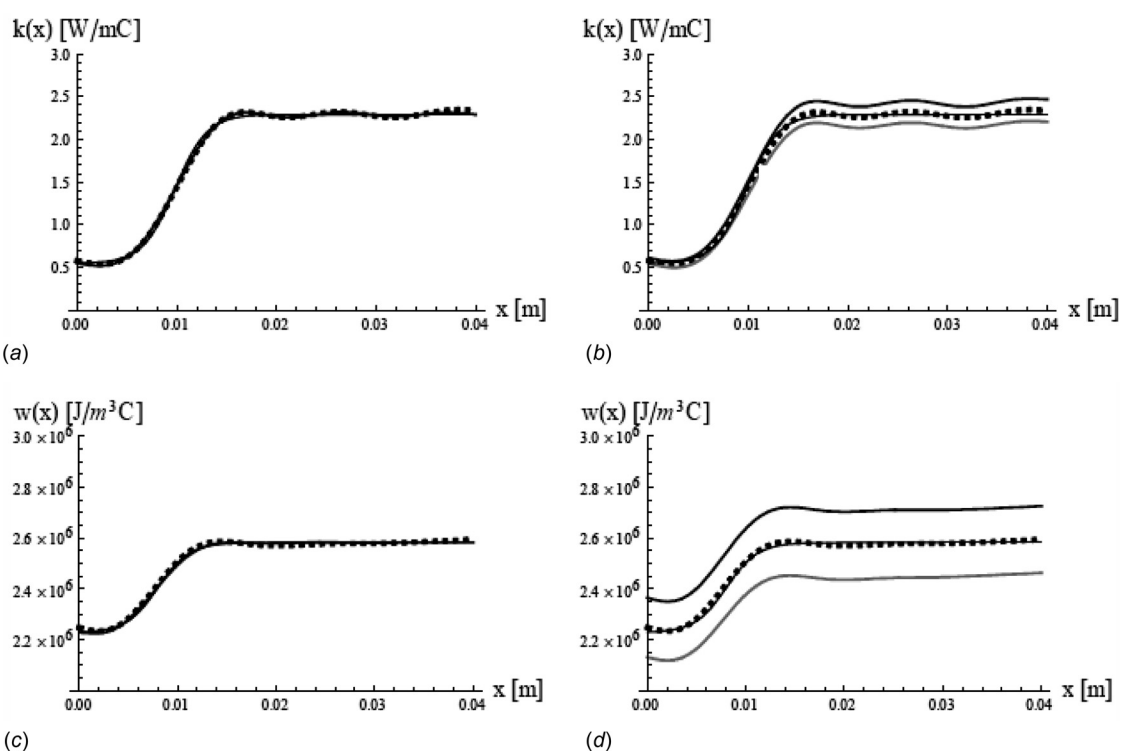


Fig. 6 (*a–d*)—Estimated functions in case 3: (*a*) *k*(*x*)—exact (solid thin), exact expanded (solid thick), and estimated (dashed); (*b*) *k*(*x*)—exact (solid thin), confidence bounds (solid thick), and estimated (dashed); (*c*) *w*(*x*)—exact (solid thin), exact expanded (solid thick), and estimated (dashed); (*d*) *w*(*x*)—exact (solid thin), confidence bounds (solid thick), and estimated (dashed)

Conclusions

The combined use of integral transforms and Bayesian inference was illustrated for the inverse problem of simultaneously estimating space variable thermal capacity and conductivity in two-phase dispersed systems, undergoing a transient one-dimensional heat conduction process. The direct problem solution was analytically obtained with the classical integral transform method, while the related eigenvalue problem that carries the information on the medium heterogeneities was solved with the generalized integral transform technique (GITT).

The inverse problem solution was based on the Markov chain Monte Carlo (MCMC) method. The Metropolis-Hastings algorithm was employed for the sampling procedure, all implemented in the MATHEMATICA symbolic computation platform. Instead of seeking the function estimation in the form of a set of local values of the thermal conductivity, an alternative approach was employed in this work by using an eigenfunction expansion of the thermal conductivity itself. This approach significantly reduces the number of parameters to be estimated in comparison to the strategy of estimating local values. Gaussian distributions were used as priors with fairly large standard deviations, together with simulated experimental data with added uncertainty, in order to demonstrate the inverse analysis robustness.

The results obtained in this work reveal that the proposed inverse analysis approach can provide accurate estimation of the thermophysical properties variation and is robust with respect to measurement errors, being capable of providing accurate results even for prior distributions with significant standard deviations. The combination of the integral transform methodology with the computationally intensive inverse analysis is indeed an advantage in the proposed approach, since the only major numerical task in the direct problem solution is essentially reduced to the solution of an algebraic eigenvalue problem for each set of sampled coefficients to be estimated, i.e., only once for each state of the Markov chain. Then, the temperature solution is directly obtained as an explicit expansion, Eq. (2), and thus the overall cost is not markedly affected by the increase on the number of sensors or measurements that are made available. Also, it should be added that the approach is equally applicable to nonmonotonic filler functions, as described for the direct problem solution, even for the physical situation of a randomly distributed dispersed phase [14].

Acknowledgment

The authors would like to acknowledge the financial support provided by CNPq, CAPES, and FAPERJ, Brazilian agencies for the fostering of sciences.

Nomenclature

c_p = specific heat, Eq. (1*a*)
$d(x)$ = linear dissipation operator coefficient, Eq. (3*a*)
$h_{eff}(x)$ = effective heat transfer coefficient, Eq. (1*a*)
$k(x)$ = space variable thermal conductivity, Eq. (1*a*)
L_x = plate length
L_z = plate thickness
N = truncation order in temperature expansion
N_w, N_k = truncation orders in coefficients expansions, $w(x)$ and $k(x)$, respectively
M = truncation order in eigenvalue problem expansion
M_n = normalization integrals in auxiliary eigenvalue problem
N_P = number of parameters to be estimated, Eq. (14)
N_x = number of measurements along the spatial domain
N_t = number of measurements in time
N_m = total number of measurements
N_i = normalization integrals in original eigenvalue problem
$P(x,t)$ = source term, Eq. (3*a*)
$q(x,t)$ = applied heat flux, Eq. (1*a*)
q_w = applied heat flux in test case
t = time variable
$T(x,t)$ = temperature distribution
$w(x)$ = thermal capacity, Eq. (3*a*)
$w_f(x)$ = filter for thermal capacity expansion
x = space coordinate
$\mathbf{Y}$ = vector of measurements
$\mathbf{P}$ = vector of unknown parameters
$\mathbf{T}$ = vector of estimated temperatures
$\mathbf{W}$ = covariance matrix of the measurement errors

Greek Letters

γ = parameter in filler concentration variation
δ = function in filler concentration variation
λ = eigenvalues of the auxiliary problem
μ = eigenvalues of the original problem
$\phi(x)$ = filler concentration distribution, Eq. (11)
ψ = eigenfunctions of the original problem
Ω = eigenfunctions of the auxiliary problem
ρ = density

Subscripts and Superscripts

i,n,m = order of eigenquantities
$\_$ = integral transform
$\sim$ = normalized eigenfunction
d = dispersed phase (filler) properties
f = filtering function in coefficients expansion
m = matrix phase properties

References

[1] Beck, J. V., and Arnold, K., 1977, *Parameter Estimation in Engineering and Science*, Wiley, New York.
[2] Alifanov, O. M., 1994, *Inverse* Heat *Transfer Problems*, Springer-Verlag, New York.
[3] Ozisik, M. N., and Orlande, H. R. B., 2000, *Inverse Heat Transfer: Fundamentals and Applications*, Taylor and Francis, New York.
[4] Zabaras, N., 2006, "Inverse Problems in Heat Transfer," *Handbook of Numerical Heat Transfer*, 2nd ed., W. J. Minkowycz, E. M. Sparrow, and J. Y. Murthy, eds., Wiley, New York, pp. 525–557.
[5] Flach, G. P., and Ozisik, M. N., 1989, "Inverse Heat Conduction Problem of Simultaneously Estimating Spatially Varying Thermal Conduction and Heat Capacity Per Unit Volume," Numer. Heat Transfer, Part A, **16**, pp. 249–266.
[6] Huang, C. H., and Ozisik, M. N., 1990, "A Direct Integration Approach for Simultaneously Estimating Spatially Varying Thermal Conductivity and Heat Capacity," Int. J. Heat Fluid Flow, **11**(3), pp. 262–268.
[7] Lesnic, D., Elliot, L., Ingham, D. B., Clennell, B., and Knioe, R. J., 1999, "The Identification of the Piecewise Homogeneous Thermal Conductivity of Conductors Subjected to a Heat Flow Test," Int. J. Heat Mass Transfer, **42**, pp. 143–152.
[8] Divo, E., Kassab, A., and Rodriguez, F., 2000, "Characterization of Space Dependent Thermal Conductivity With a BEM-Based Genetic Algorithm," Numer. Heat Transfer, Part A, **37**, pp. 845–875.
[9] Huang, C. H., and Chin, S. C., 2000, "A Two-Dimensional Inverse Problem in Imaging the Thermal Conductivity of a Non-homogeneous Medium," Int. J. Heat Mass Transfer, **43**, pp. 4061–4071.
[10] Rodrigues, F. A., Orlande, H. R. B., and Dulikravich, G. S., 2004, "Simultaneous Estimation of Spatially Dependent Diffusion Coefficient and Source Term in a Nonlinear 1D Diffusion Problem," Math. Comput. Simul., **66**, pp. 409–424.
[11] Huttunen, J. M. J., Huttunen, T., Malinen, M., and Kaipio, J., 2006, "Determination of Heterogeneous Thermal Parameters Using Ultrasound Induced Heating and MR Thermal Mapping," Phys. Med. Biol., **51**, pp. 1011–1032.
[12] Huang, C. H., and Huang, C. Y., 2007, "An Inverse Problem in Estimating Simultaneously the Effective Thermal Conductivity and Volumetric Heat Capacity of Biological Tissue," Appl. Math. Model., **31**, pp. 1785–1797.
[13] Liu, C. S., 2008, "An LSGSM to Identify Nonhomogeneous Heat Conductivity Functions by an Extra Measurement of Temperature," Int. J. Heat Mass Transfer, **51**, pp. 2603–2613.
[14] Naveira-Cotta, C. P., Cotta, R. M., Orlande, H. R. B., and Fudym, O., 2009, "Eigenfunction Expansions for Transient Diffusion in Heterogeneous Media," Int. J. Heat Mass Transfer, **52**, pp. 5029–5039.
[15] Naveira-Cotta, C. P., Orlande, H. R. B., and Cotta, R. M., 2010, "Integral Transforms and Bayesian Inference in the Identification of Variable Thermal Conductivity in Two-Phase Dispersed Systems," Num. Heat Transfer Part B, **57**(3), pp. 1–30.
[16] Cotta, R. M., 1993, *Integral Transforms in Computational Heat and Fluid Flow*, CRC Press, Boca Raton, FL.
[17] Cotta, R. M., and Mikhailov, M. D., 1997, *Heat Conduction: Lumped Analysis, Integral Transforms, Symbolic Computation*, Wiley, New York.

[18] Cotta, R. M., 1998, *The Integral Transform Method in Thermal and Fluids Sciences and Engineering*, Begell House, New York.
[19] Cotta, R. M., and Mikhailov, M. D., 2006, "Hybrid Methods and Symbolic Computations", *Handbook of Numerical Heat Transfer*, 2nd ed., W. J. Minkowycz, E. M. Sparrow, and J. Y. Murthy, eds., Wiley, New York, pp. 493–522.
[20] Mikhailov, M. D., and Cotta, R. M., 1994, "Integral Transform Method for Eigenvalue Problems," Commun. Numer. Methods Eng., **10**, pp. 827–835.
[21] Sphaier, L. A., and Cotta, R. M., 2000, "Integral Transform Analysis of Multidimensional Eigenvalue Problems Within Irregular Domains," Numer. Heat Transfer, Part B, **38**, pp. 157–175.
[22] Wolfram, S., 2005, *The Mathematica Book*, version 5.2, Cambridge-Wolfram Media.
[23] Kaipio, J. and Somersalo, E., 2004, *Statistical and Computational Inverse Problems*, Springer-Verlag, New York.
[24] Gamerman, D., and Lopes, H. F., 2006, *Markov Chain Monte Carlo: Stochastic Simulation for Bayesian Inference*, 2nd ed., Chapman & Hall/CRC, Boca Raton, FL.
[25] Migon, H. S., and Gamerman, D., 1999, *Statistical Inference: An Integrated Approach*, Arnold/Oxford, London/New York.
[26] Orlande, H. R. B., Colaço, M. J., and Dulikravich, G. S., 2008, "Approximation of the Likelihood Function in the Bayesian Technique for the Solution of Inverse Problems," Inverse Probl. Sci. Eng., **16**, pp. 677–692.
[27] Fudym, O., Orlande, H. R. B., Bamford, M., and Batsale, J. C., 2008, "Bayesian Approach for Thermal Diffusivity Mapping from Infrared Images Processing with Spatially Random Heat Pulse Heating," J. Phys. Conf. Ser., **135**, pp. 12–42.
[28] Wang, J., and Zabaras, N., 2004, "A Bayesian Inference Approach to the Inverse Heat Conduction Problem", Int. J. Heat Mass Transfer, **47**, pp. 3927–3941.
[29] Parthasarathya, S. and Balaji, C., 2008, "Estimation of Parameters in Multimode Heat Transfer Problems using Bayesian Inference—Effect of Noise and a Priori", Int. J. Heat Mass Transfer, **51**, pp. 2313–2334.
[30] Tarantola, A., 2005, *Inverse Problem Theory and Methods for Model Parameter Estimation*, Society for Industrial and Applied Mathematics, SIAM, Philadelphia.
[31] Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., and Teller, E., 1953, "Equations of State Calculations by Fast Computating Machines," J. Chem. Phys., **21**, pp. 1087–1092.
[32] Hastings, W. K., 1970, "Monte Carlo Sampling Methods Using Markov Chains and their Applications," Biometrika, **57**, pp. 97–109.
[33] Barker, A. A., 1965, "Monte Carlo Calculation of the Radial Distribution Functions for a Proton-Electron Plasma," Aust. J. Phys., **18**, pp. 119–133.
[34] Peskun, P. H., 1973, "Optimum Monte Carlo Sampling using Markov Chain," Biometrika, **60**, pp. 607–612.
[35] Tavman, I. H., 1996, "Thermal and Mechanical Properties of Aluminum Powder-Filled High-Density Polyethylene Composites," J. Appl. Polym. Sci., **62**, pp. 2161–2167.
[36] Kumlutas, D., Tavman, I. H., and Çoban, M. T., 2003, "Thermal Conductivity of Particle Filled Polyethylene Composite Materials," Compos. Sci. Technol., **63**(1), pp. 113–117.
[37] Lewis, T., and Nielsen, L., 1970, "Dynamic Mechanical Properties of Particulate-Filled Polymers", J. Appl. Polym. Sci., **14**(6), pp. 1449–1471.