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# Explicit scheme based on integral transforms for estimation of source terms in diffusion problems in heterogeneous media

# Esquema explícito com transformações integrais para estimativa de termos fonte em problemas de difusão em meios heterogêneos

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**Resumo**
A estimativa dos termos-fonte presentes em equações diferenciais possui diversas aplicações, que vão desde a avaliação estrutural, monitoramento de processos industriais, detecção de falhas em equipamentos, identificação de fontes de poluição ambiental até aplicações na medicina. Nos últimos anos, houve progresso significativo em metodologias capazes de estimar esse parâmetro. Este trabalho utiliza uma metodologia baseada em uma formulação explícita da transformação integral para caracterizar o termo-fonte desconhecido, reconstruindo-o por meio da expansão em autofunções conhecidas do problema de autovalor de Sturm-Liouville. Para alcançar isso, um modelo linear é considerado em um meio heterogêneo com propriedades físicas conhecidas e variáveis espacialmente, e duas fontes de calor, com dependências temporais e espaciais, sendo que a dependência é apenas espacial. O problema de autovalor contém informações sobre as propriedades heterogêneas e é resolvido usando a técnica generalizada de transformação integral. Além disso, é proposta uma interpolação inicial dos dados do sensor para cada tempo de observação, tornando o problema inverso computacionalmente mais leve. As soluções do problema inverso apresentam desempenho ótimo, mesmo com dados de entrada ruidosos e fontes com descontinuidades abruptas. As temperaturas recuperadas pelo problema direto, considerando a fonte recuperada, coincidem de perto com dados experimentais sintéticos, mostrando erros inferiores a 1%, garantindo a robustez e confiabilidade da técnica para a aplicação proposta.
**Palavras-chave:** Problemas inversos. Transformadas integrais. Termo fonte. Meios heterogêneos.

**Abstract**
The estimation of source terms present in differential equations has various applications, ranging from structural assessment, industrial process monitoring, equipment failure detection, environmental pollution source detection to identification applications in medicine. Significant progress has been made in recent years in methodologies capable of estimating this parameter. This work employs a methodology based on an explicit formulation of the integral transformation to

characterize the unknown source term, reconstructing it through the expansion in known eigenfunctions of the Sturm-Liouville eigenvalue problem. To achieve this, a linear model is considered in a heterogeneous medium with known and spatially varying physical properties and two heat sources, with both temporal and spatial dependencies, and only spatial dependence. The eigenvalue problem contains information about the heterogeneous properties and is solved using the generalized integral transformation technique. Additionally, an initial interpolation of the sensor data is proposed for each observation time, making the inverse problem computationally lighter. The solutions of the inverse problem exhibit optimal performance, even with noisy input data and sources with abrupt discontinuities. The temperatures recovered by the direct problem considering the recovered source closely match synthetic experimental data, showing errors less than 1%, ensuring the robustness and reliability of the technique for the proposed application.
**Keywords:** Inverse problems. Integral transforms. Source term. Heterogeneous media.

## 1. Introduction

Estimating source terms in diffusion problems is a classic instance of an inverse heat conduction problem (IHCP), which has been thoroughly investigated over the years (Alifanov, 1994; Beck and Arnold, 1997; Beck *et al*., 1985; Özisik and Orlande, 2021). This field has found a large range of applications (Negreiros *et al*., 2020; Lugão *et al*., 2022; Mital and Scott, 2006; Nelson and Yoon, 2000; Yoon *et al*., 2023; Mehrabanian and Nejad, 2023; Alosaimi and Lesnic, 2023). The inverse problem of heat source identification can be formulated as either parameter estimates or function estimation, considering some IHCP classifications found in the literature. In particular, for three-dimensional inverse problems involving function estimates, computational data processing is increased, posing a challenging problem, especially for some methods like Monte Carlo with Markov Chains in Bayesian inference (Orlande *et al*., 2014; Kaipio and Somersalo, 2006; Cao *et al*., 2022; Sajedi *et al*., 2021).

The use of GITT in inverse problems has proven to be a consistent approach, and the results and applications obtained so far are quite exciting. It is worth noting that, for example, the use of measurements in the transformed domain can not only lead to lower computational costs but also provide regularization for the ill-posed nature that is typical of inverse problems (Naveira-Cotta *et al*. 2011a, b; Abreu *et al*, 2018; Özisik and Orlande, 2021).

A new explicit approach for identifying boundary source terms was proposed by Knupp and Abreu (2016), using a regularization scheme through the truncation of terms in a series and an associated eigenvalue problem. This proposal was experimentally validated and compared with the MCMC method in Sanches *et al*. (2021), where the same explicit method utilized an explicit formulation with the assistance of an integral transform to address the actual experimental data for estimating time-varying boundary heat fluxes in thin thermally plates using temperature measurements obtained through infrared thermography. Knupp (2021) presented an approach where direct and simultaneous estimation of thermal conductivity and thermal capacity in heterogeneous media is carried out, employing transformed temperatures in the transformed equation. The methodology is based on a minimization problem that does not require an iterative solution of the direct problem, making it a computationally lightweight cost process.

Recently, Negreiros *et al*. (2020) proposed a methodology for estimating source terms in diffusion models using the classical integral transformation technique (CITT), more details about the technique at Cotta (1993). They evaluated the methodology using simulated measurements with different noise levels, and the results, employing a basis of eigenfunctions and eigenvalues from the eigenvalue problem, proved to be robust. The technique was tested on classical one-dimensional and two-dimensional diffusion models, considering constant coefficients in the differential equations. However, models involving variable coefficients are common, introducing complexity, especially in the eigenvalue problem of the integral transformation.

In this work, the goal is to apply the same technique proposed by Negreiros *et al*. (2020), but with the inclusion of a more complex model involving spatially varying coefficients in the eigenvalue problem. This problem is solved using the Generalized Integral Transformation

Technique (GITT), as described by Cotta (1993). Additionally, linear interpolation is employed on the sensor data to avoid the self-cost of semi-analytical interval integration, reducing the computational cost of the problem.

## 2. Direct problem

Consider the one-dimensional transient diffusion equation, presented in a general form in Naviera-Cotta *et al*. (2011 a, b) and Knupp (2021). This model describes the heat conduction in a thermally thin plate with length $L$ and thickness $l_e$, where $\mathcal{K}(x)$ and $\rho(x)c_p(x)$ represent spatially varying thermal conductivity and thermal capacity, respectively. The plate experiences an imposed heat flux $q(x,t)$ on one surface, while the opposite surface exchanges heat with the surrounding environment at $\theta_\infty$.

$$\rho(x)c_p(x)\frac{\partial\theta_m(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\mathcal{K}(x)\frac{\partial\theta_m(x,t)}{\partial x}\right) - \frac{h}{l_e}(\theta_m(x,t)-\theta_\infty) + \frac{q(x,t)}{l_e},\ x\in[0,L],\ t>0 \quad (1a)$$
$$\mathcal{K}(x)\frac{\partial\theta_m(x,t)}{\partial\boldsymbol{\eta}} = 0,\ \text{at } x=0 \text{ and } x=L \quad (1b)$$
$$\theta_m(x,0) = \theta_\infty,\ x\in[0,L] \quad (1c)$$

Before presenting the solution to the model represented by Eq. (1), a linear filter is applied to filter the initial condition of the problem. This filtering methodology, which can occur in the initial condition or boundary conditions, aims to homogenize the problem, demonstrating convergence benefits in terms of solution truncation, (Cotta, 1993; Cotta, 2013). Therefore:

$$\theta_m(x,t) = \theta^*(x,t) + \theta_\infty \quad (2)$$

where $\theta^*$ represents the filtered temperatures, and $\theta_\infty$ is the filter temperature. The equation for the filtered temperatures is then represented by:

$$\mathcal{W}(x)\frac{\partial\theta^*(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\mathcal{K}(x)\frac{\partial\theta^*(x,t)}{\partial x}\right) - d(x)\theta^*(x,t) + P(x,t) \quad (3a)$$
$$k(x)\frac{\partial\theta^*(x,t)}{\partial\boldsymbol{\eta}} = 0, \text{ at } x=0 \text{ and } x=L \quad (3b)$$
$$\theta^*(x,0) = 0 \quad (3c)$$

where $\mathcal{W}(x) = \rho(x)c_p(x)$ and $\mathcal{K}(x)$ are the terms responsible for the heterogeneous information of the problem, with the source term $P(x,t) = \frac{q(x,t)}{l_e}$ and $d(x) = \frac{h}{l_e}$.

The integral transform technique consists, first and foremost, in defining the transform-inverse pair and normalized eigenfunctions:

$$\bar{\theta}_i^*(t) = \int_0^L \mathcal{W}(x)\tilde{\Upsilon}_i(x)\theta^*(x,t)dx, \text{ transform} \quad (5a)$$
$$\sum_{i=1}^{\infty}\tilde{\Upsilon}_i(x)\,\bar{\theta}_i^*(t), \text{ inverse} \quad (5b)$$
$$\tilde{\Upsilon}_i(x) = \frac{\Upsilon_i(x)}{\sqrt{N_i}}, \text{ normalized eigenfunctions} \quad (5c)$$
$$N_i = \int_0^L \mathcal{W}(x)[\Upsilon_i(x)]^2dx, \text{ normalization integrals} \quad (5d)$$

with $\bar{\theta}_i^*$ representing the transformed filtered potential, $\xi_i$and $\Upsilon_i$ are, respectively, eigenvalues and eigenfunctions originating from the eigenvalue problem (see Naviera-Cotta *et al*., 2009), which contains information about the heterogeneous medium:

$$\frac{\partial}{\partial x}\left(\mathcal{K}(x)\frac{\partial\Upsilon_i(x)}{\partial x}\right) + \left(\xi_i^2\mathcal{W}(x) - d(x)\right)\Upsilon_i(x) = 0,\ x\in[0,L] \quad (6a)$$

$$\frac{\partial \Upsilon_i(x)}{\partial \boldsymbol{\eta}} = 0, \text{ at } x = 0 \text{ and } x = L \tag{6b}$$

The problem given by Eq. (6) is solved using the GITT technique, see Cotta (1993), proposing a simpler Sturm-Liouville eigenvalue problem with a closed-form solution. The unknown eigenfunctions $\Upsilon_i$ are expanded around this base, as detailed in (Naviera-Cotta *et al*., 2009; Naviera-Cotta *et al*., 2010).

Thus, with the eigenfunctions and eigenvalues in hand, the operator $\int_0^L \mathcal{W}(x)\tilde{\Upsilon}_i(x,\xi_i)(\cdot)dx$ is applied to (3), transforming the potential and yielding the following transformed differential equation:

$$\frac{\partial \bar{\theta}_i^*(t)}{\partial t} + \xi_i^2 \bar{\theta}_i^*(t) = \bar{p}_i(t) \tag{7a}$$

$$\bar{\theta}_i^*(0) = 0 \tag{7b}$$

where $\bar{p}_i$ is the transformed source term, given by:

$$\bar{p}_i(t) = \int_0^L \mathcal{W}(x)\tilde{\Upsilon}_i(x)P(x,t)dx \tag{8}$$

The solution to the differential equation (7) determines the transformed potentials $\bar{\theta}_i^*$. Subsequently, the solution to the filtered problem can be determined by applying the inverse, as defined by Eq. (5b). Therefore, the final solution to the problem (1) is given by:

$$\theta_m(x,t) = \theta_\infty + \sum_{i=1}^{\infty} \tilde{\Upsilon}_i(x) \int_0^t \bar{p}_i(t) e^{-\xi_i^2(t-t')} dt' \tag{9}$$

## 2. Inverse problem

In this work, the focus is on estimating the unknown source term function $q(x,t)$ using measurements of transient temperatures assumed to be available at equally spaced locations in the domain. For this purpose, an explicit formulation is proposed based on the transformed equation Eq. (7a) to estimate the transformed source term $\bar{p}_i(t)$, and by utilizing the inverse Eq. (5b), the source term $P(x,t)$ is found, controlling the number of eigenfunctions in the expansion Negreiros *et al.* (2020). Therefore:

$$P(x,t) = \sum_{i=1}^{N_T} \mathcal{W}(x)\tilde{\Upsilon}_i(x)\, \bar{p}_i(t) \tag{10}$$

where the normalized eigenfunctions originate from the eigenvalue problem Eq. (6).

Considering the measurements over the domain $\theta^e$ at each position $(x_n, t_j)$, they are transformed using Eq. (5b). In the methodology proposed by Negreiros *et al.* (2020), these measurements are transformed using semi-analytic interval integration. However, simple linear interpolation of the sensor data $x_n$ for each time unit allows for a single integration, reducing computational cost, as follows:

$$\theta^e(t_j) = \int_0^L \left(\theta^e(x,t_j) - \theta_\infty\right)\mathcal{W}(x)\tilde{\Upsilon}_i(x)dx \tag{11}$$

Thus, using finite differences to approximate the derivative of the potential represented by Eq. (7a), one can estimate $\bar{p}_i(t)$, as per Eq. (12). To distinguish the notations, we denote $\hat{p}_i(t)$ as the estimated source term through experimental measurements.

$$\frac{\theta^e(t_{j+1}) - \theta^e(t_{j-1})}{2\Delta t} + \xi_i^2 \theta^e(t_j) = \hat{p}_i(t) \tag{12}$$

hence, applying the inverse formulation to $\hat{p}_i(t)$ the flux of the source term $\hat{q}(x,t)$ is determined as follows:

$$\hat{q}(x,t) = l_e \sum_{i=1}^{N_T} \mathcal{W}(x)\tilde{\Upsilon}_i(x)\,\hat{p}_i(t) \tag{13}$$

The truncation $N_T$ is chosen by the principle of discrepancy, where the optimal truncation of the series in the solution of the inverse problem is the one for which the variance of the recovered data ${\sigma^2}_{rec}$ best approximates the variance of the uncertainties in the experimental data ${\sigma^2}_e$, see (Knupp and Abreu, 2016; Özisik and Orlande, 2021; Beck and Arnold, 1997; Beck *et al*., 1985).

**3. Numerical results**

For numerical simulations, the parameter values presented in Knupp (2021) were considered. This scenario represents a nanocomposite consisting of a high-density polyethylene matrix with a concentration of 45%. The parameter data are represented in Table 1. The properties vary spatially at positions $x = 0$ and $x = L$. In this work, the exponentially smoothed transition will be considered, as given by the following equations, where $\mathcal{K}_0$ and $\mathcal{W}_0$ represent values at $x = 0$, and $\mathcal{K}_L$ and $\mathcal{W}_L$ represent values at $x = L$.

$$\mathcal{K}(x) = \mathcal{K}_0 + (\mathcal{K}_L - \mathcal{K}_0)\mathcal{W}(x) \tag{14}$$
$$\mathcal{W}(x) = \mathcal{W}_0 + (\mathcal{W}_L - \mathcal{W}_0)\mathcal{H}(x) \tag{15}$$

with

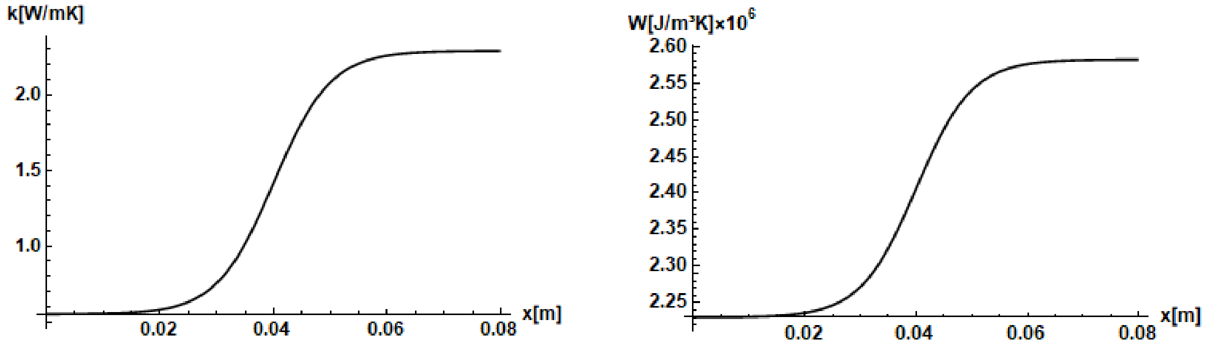
$$\mathcal{H}(x) = \frac{1}{1+exp[-200(x-0.04)]} \tag{16}$$

The function $\mathcal{H}$ allows for a smooth transition between abrupt changes in the system, as illustrated in Figure 1, providing a graphical representation of the smoothed variation of parameters $\mathcal{K}(x)$ and $\mathcal{W}(x)$, representing the conductivity and thermal capacity, respectively. The values of these parameters correspond to those in Table 1. These parameters contain the heterogeneous information of the model.

**Table 1 - Definition of the model parameter values.**

| Parameter | Defined values |
|---|---|
| $\theta_\infty$ [°C] | 25 |
| $L[m]$ | 0.08 |
| $l_e[m]$ | 0.002 |
| $h[W/m^2K]$ | 15 |
| $\mathcal{K}_0[W/mK]$ | 0.549 |
| $\mathcal{K}_L[W/mK]$ | 2.29 |
| $\mathcal{W}_0[J/m^3K]$ | $2.23 \times 10^6$ |
| $\mathcal{W}_L[J/m^3K]$ | $2.58 \times 10^6$ |

Note: Table adapted from Knupp (2021).



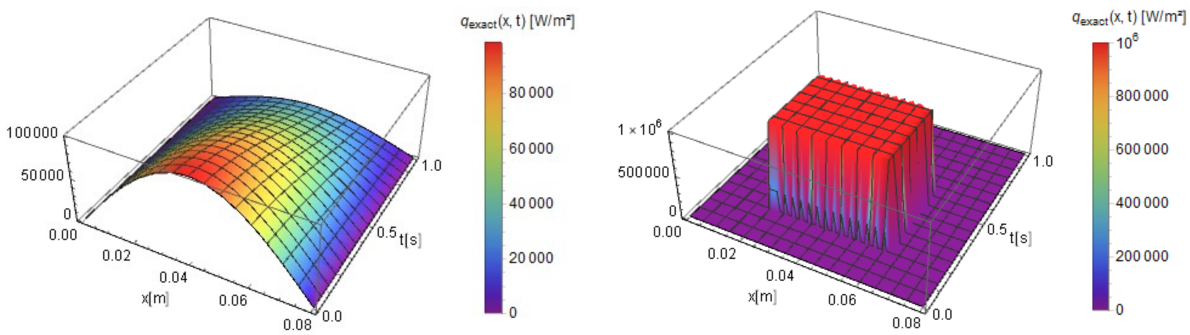

**(a)** **(b)**

**Figure 1 - Spatially varying parameters of heterogeneous properties: Spatially varying parameter $\mathcal{K}$ with exponential transition Eq. (14).; Spatially varying parameter $\mathcal{W}$ with exponential transition Eq. (15).**

Two types of heat flow are proposed for the inverse problem estimation: one continuous and transient, represented by Eq. (17); the other stationary, with discontinuity and abrupt transitions, represented by Eq. (18), graphically depicted in Figure 2. The fluxes are adapted from Yang *et al.* (2012), who proposed the inverse problem of heat flow estimation considering available measurement data in the domain.

$$q_1(x,t) = 10^4(\pi^2 - 2t)e^{-t}\sin\left(\frac{\pi x}{L}\right),\ \ (x,t) \in [0,0.08] \times [0,1] \tag{17}$$

$$q_2(x,t) = \begin{cases} 10^6, & (x,t) \in [0.02, 0.06] \times [0.2, 0.6] \\ 0, & otherwise \end{cases} \tag{18}$$




**(a)** **(b)**

**Figure 2 - Graphical representation of the heat flows to be estimated: (a) - Heat flow $q_1$; (b) - Heat flow $q_2$.**

To avoid the "inverse crime", as discussed in Kaipio and Somersalo (2006), synthetic experimental measurements are simulated using the numerical solution routine of partial differential equations available in the symbolic computing platform Wolfram Mathematica NDSolve, Wolfram (2023). This solution package has been consistently employed in scientific works such as (Freitas *et al.*, 2023; Cotta *et al.*, 2013; Knupp and Abreu, 2016), demonstrating reliability in numerical solutions. These measurements are determined considering uncertainties in the experimental data with a normal distribution of mean zero and standard deviation $\sigma_e$, as follows:

$$\theta^e(x_n, t_j) = \theta(x_n, t_j) + \epsilon; \epsilon \sim N(0, \sigma_e)$$

$$n = 1, 2, 3, \cdots, M_x; \qquad j = 1, 2, 3, \cdots, M_t \tag{19}$$

where $M_x$ and $M_t$ represent the quantity of spatial sensors and temporal measurements, respectively; $\epsilon$ is the uncertainty at each point; $N$ is the normal distribution; $\theta^e$ denotes the pointwise experimental measurement; and $\theta$ is the value of the numerical solution of the problem.

Firstly, the transient flow is estimated, represented by Eq. (17). The quantity of experimental data consisted of 36 spatial measurements and 20 temporal measurements. In the first example, experimental noise was taken into account with a standard deviation of $\sigma_e = 0.1$°C. The problem was analyzed over the range of 20 eigenvalues and eigenfunctions.

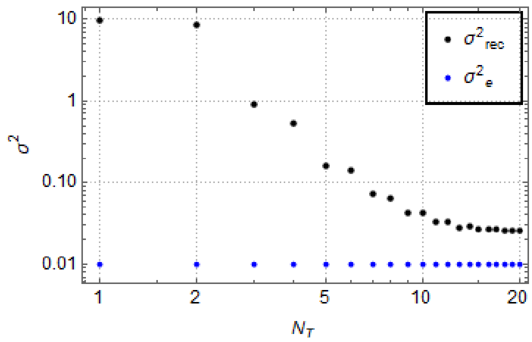



**Figure 3 - Principle of Discrepancy in the first simulation $\boldsymbol{\sigma_e = 0.1}$°C.**

Figure 3 shows the variances obtained through the principle of discrepancy. The smallest distance between the variance of experimental noise and the variance obtained by recovery at each truncation occurs when $N_T = 18$. In Figure 4, the estimation profile for time $t = 0.5[s]$, is presented, with some truncations of the inverse problem solution illustrated. Figure 5 illustrates in three dimensions the best estimate for the flow.

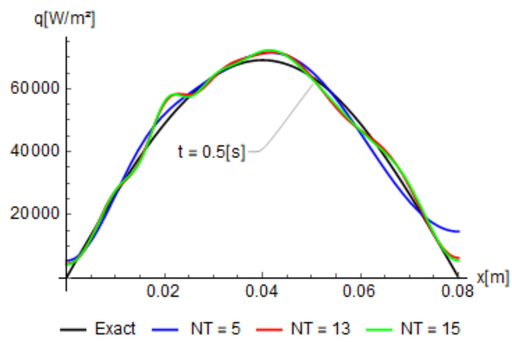



**Figure 4 - Representation of the estimation profile for various truncations of the inverse problem solution at time $\boldsymbol{t = 0.5[s]}$ with a standard deviation of uncertainty equal to $\boldsymbol{\sigma_e = 0.1}$°C.**

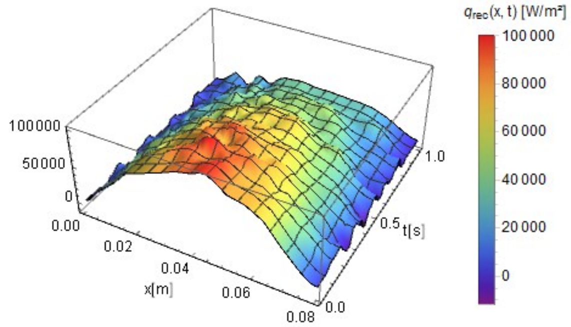
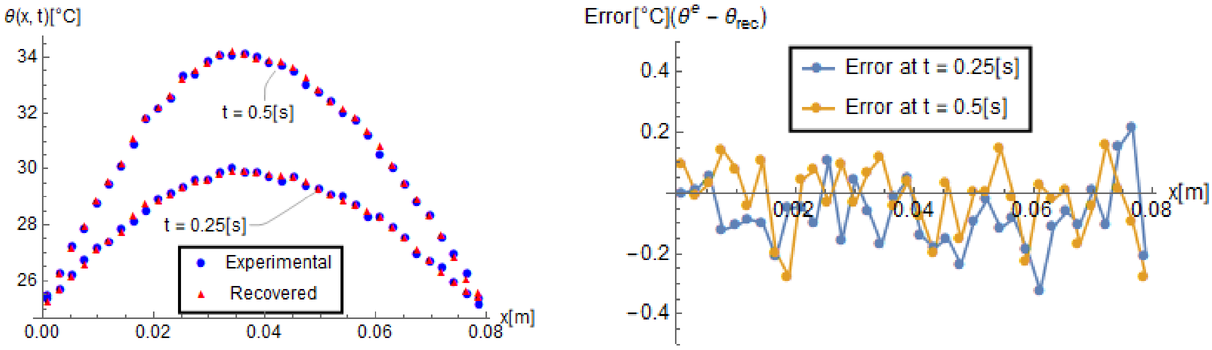



**Figure 5 - Graphical representation of the estimated flow.**

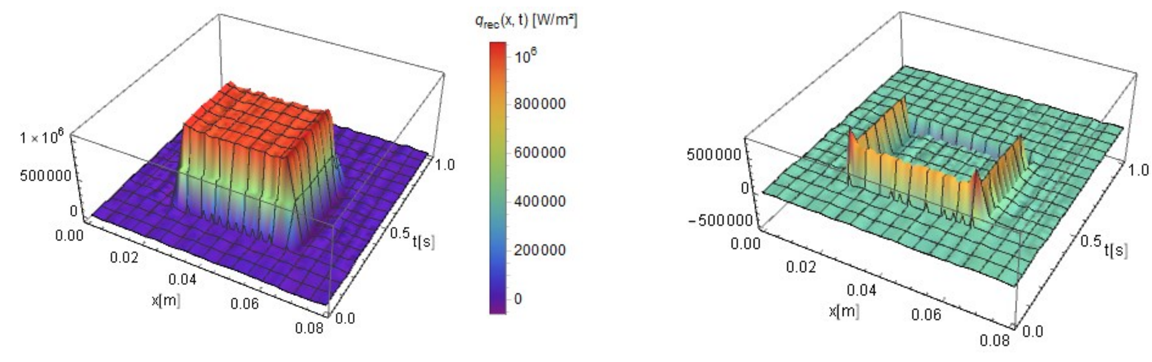



**(a)** **(b)**

**Figure 6 - Comparison between experimental temperatures and recovered temperatures, and differences among the data: (a) - Comparison between experimental temperatures and recovered temperatures; (b) - Estimation errors between experimental temperatures and recovered temperatures.**

The estimated flow is then used to solve the direct problem again. Figure 6(a) shows the comparison between the experimental temperature measurements used as input for the inverse problem and the measurements recovered by solving the direct problem using the estimated flow. It can be observed, as shown in Figure 6(b), that the difference between the measurements varies between $-0.2$[°C] and $0.2$[°C], for the considered times. The temperature range illustrated in Figure 6(a) is between $25$[°C] and $34$[°C], indicating that the errors are between 0,59% and 0,8% in relation to the experimental values. This indicates robustness in the technique and that the estimates have good results.

Now, we analyze the estimation of the steady-state flow, represented by Eq. (18). The quantity of experimental data remains at 36 spatial measurements and 20 temporal measurements. In the first example, experimental noise was taken into account with a standard deviation of $\sigma_e = 0.1$°C and $\sigma_e = 0.5$°C. The problem was analyzed over the range of 40 eigenvalues and eigenfunctions. The results are evaluated below:




**(a)** **(b)**

**Figure 7 - Graphical representation of the estimation and error for the heat flow $q_2$ with noise having a standard deviation of $\sigma_e = 0.1$°C: (a) - Estimated flow $\hat{q}_2$; (b) - Estimation error $q_2 - \hat{q}_2$.**

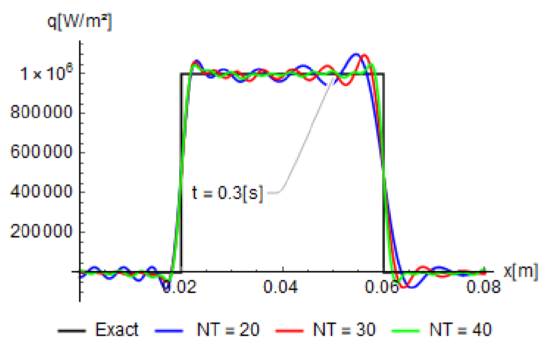
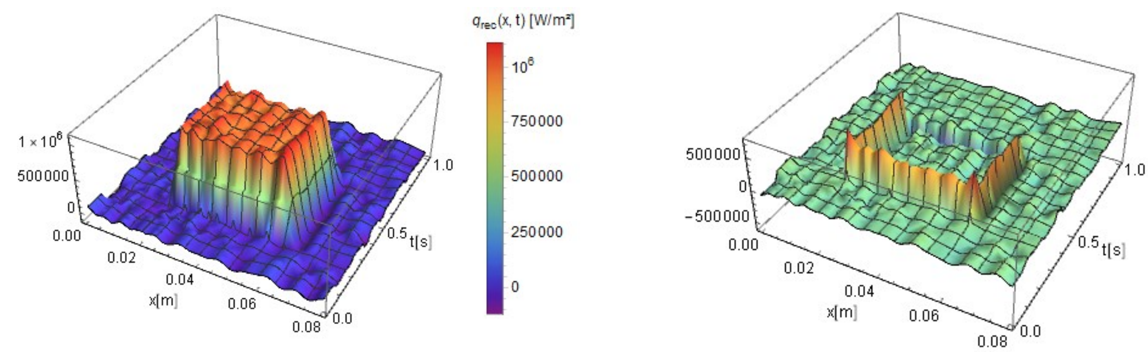



**Figure 8 - Representation of the estimation profile for various truncations of the inverse problem solution at time $t = 0.3[s]$ with a standard deviation of uncertainty equal to $\sigma_e = 0.1$°C.**




**(a)** **(b)**

**Figure 9 - Graphical representation of the estimation and error for the heat flow $q_2$ with noise having a standard deviation of $\sigma_e = 0.5$°C: (a) - Estimated flow $\hat{q}_2$; (b) - Estimation error $q_2 - \hat{q}_2$.**

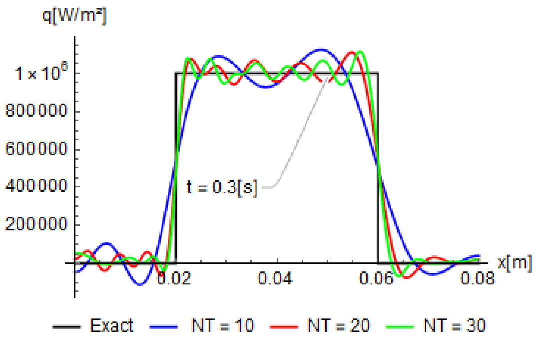



**Figure 10 - Representation of the estimation profile for various truncations of the inverse problem solution at time $t = 0.3[s]$ with a standard deviation of uncertainty equal to $\sigma_e = 0.5$°C.**

Figures 7(a) and 9(a) present, respectively, the reconstructions of heat flows and the errors in the estimates. It is observed that in both Figure 7(b) and Figure 9(b), the highest concentration of errors is at the edges where the discontinuity is encountered. Since the expansion reconstructs the term continuously, estimation errors are expected at these points of discontinuity. It is also noted that the quality of the experimental data directly affects the solution of the inverse problem. The better the quality of the data, as in the case of $\sigma_e = 0.1$°C, the better the solutions. Figures 8 and 10 show estimation profiles for some truncations of the solution, where larger oscillations are also visible when $\sigma_e = 0.5$°C. The method is able to estimate heat flow even in stationary cases with discontinuity.

## 3. Conclusions

In this work, the application of the inverse problem-solving methodology for estimating source terms applied to the reconstruction of heat flows in heterogeneous media was presented. This approach considers spatially varying physical properties within the eigenvalue expansion problem, with regularization truncation guided by the principle of discrepancy.

To verify the robustness of the technique, two examples were considered for heat flow estimation. Experimental data were subject to uncertainties, and it was observed:

- The performance of the solution is satisfactory, obtaining good estimates of the flows in both transient and steady state cases.
- Clearly the solution is more accurate when the quality of observational data is better.
- The method exhibits a good recovery of experimental measurements from the direct problem using the solution of the inverse problem as the recovered flow. In the results presented here, a difference of less than 1% was obtained.

It is concluded that the methodology is capable of establishing approximations of flow characteristics, demonstrating good accuracy and being easily implemented for the proposed application.

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