BAYESIAN ESTIMATION OF THERMO-PHYSICAL PROPERTIES IN A TWO-DIMENSIONAL SEMI-TRANSPARENT MEDIUM

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Abstract. *Semi-transparent materials are largely used on industrial applications, as the manufacturing of optic fibers, electronic components, glasses, thermal protection devices, etc. In order to describe how the heat transfer occurs in such cases, it is necessary to determine the values of the related thermo-physical properties. In a static, semi-transparent material, heat is transferred at the same time by conduction and radiation, and such phenomenon is described by a coupled conduction-radiation mathematical model. In the present work, a Bayesian approach is applied to simultaneously estimate the parameters related to the coupled heat transfer model from simulated temperature measurements, taken at observation points of a two-dimensional semitransparent surface. Mean values and confidence intervals are calculated for the physical parameters. The estimated properties are then used to calculate the temperature at the observation points and these results are compared to the simulated temperatures. The robustness of the estimation method is verified, since the mean values obtained for the parameters agree with the reference values used to generate the simulated measurements.*

Keywords: *Bayesian estimation, heat transfer, two-dimensional, coupled model, semi-transparent.*

1. INTRODUCTION

The identification of physical properties plays an important role in today's research and development in engineering, which deeply relies on computational simulation of physical phenomena for analysis and design. The solution of parameter estimation problems (Beck and Arnold, 1977) is capable of providing accurate estimates for unknown physical properties and can cope with the physical phenomena of such complex experiments.

A Bayesian estimator is concerned with the analysis of the posterior probability density, which is our model for the conditional probability distribution of the unknown parameters given the measurements. The measurement error model and the related uncertainties is called the likelihood, that is, the conditional probability of the measurements given the unknown parameters. The model for the unknowns that reflects all the uncertainty of the parameters without the information conveyed by the measurements, is called the prior model (Beck and Arnold, 1977, Kaipio and Somersalo, 2004, Tan et al., 2006, Lee, 2004).

The Bayesian approach for parameter estimation has been used before by the leading author in applications concerning water flow and mass transfer in non-saturated porous media (Orlande et al., 2009, Moreira, 2016), when the involved parameters were estimated by using the Metropolis-Hastings algorithm of the Markov Chain Monte Carlo (MCMC) method (Kaipio and Somersalo, 2004, Tan et al., 2006, Lee, 2004). In the present work, such method is applied to estimate the thermo-physical properties of a semi-transparent plate, which is subjected to a radiative heat flux (Wellele, 2007).

2. PHYSICAL PROBLEM AND MATHEMATICAL FORMULATION

The physical problem considered here is the conduction and radiation heat transfer in a semi-transparent plate, covered by graphite ink with emissivity ε equal to 1 and surrounded by a medium with temperature T_∞. A low power CO_2 laser flux is applied at the center of the top plate surface, so that it is symmetrically heated by a radiative heat flux, q_l (x,y,t). The outside surfaces of the plate are subjected to radiative and convective boundary conditions. In the present study, a two-dimensional mathematical formulation was used to describe a simplified version of the original three-dimensional problem. The mathematical domain was then taken as the *xz* plane, with dimensions (a x c), where a = $5x10^{-3}$ m and c = $1x10^{-3}$ m. The temperature measurements were assumed available on the surface exposed to the radiative hear flux, at the positions A= 0 m, B=$1.3x10^{-3}$m and C=2 $x10^{-3}$m, as presented in Figure 1.

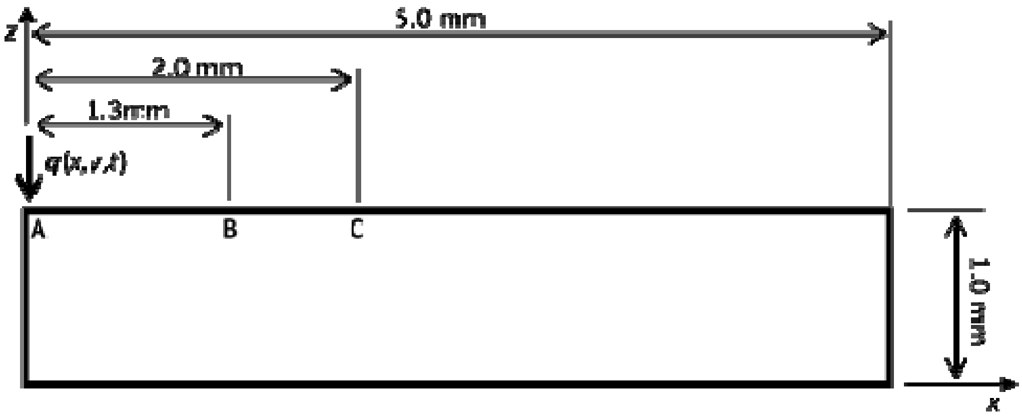

Figure 1: Scheme of the mathematical domain

The coupled conduction and radiation model consists of the Radiative Transfer Equation (RTE) and the conduction equation. The RTE was defined for a known wavelength, λ, as (Modest, 1993):

$$\Omega \cdot \nabla I_\lambda(\mathbf{r},\Omega) = -(\kappa_{a\lambda} + \sigma_{s\lambda}) I_\lambda(\mathbf{r},\Omega) + S_\lambda(\mathbf{r},\Omega) \tag{1}$$

where I_λ ($\mathbf{r}$,Ω) is the radiative intensity irradiating from a point $\mathbf{r}$ in a direction sustained by the vector Ω. S_λ ($\mathbf{r}$,Ω) is the radiative source term and $\kappa_{a\lambda}$ and $\sigma_{s\lambda}$ are the monochromatic absorption and scattering coefficients, respectively. It is assumed that the radiative intensity field is symmetric on the physical domain.

Conduction heat transfer is modeled by the balance between the cumulative energy in an elemental volume of semi-transparent material and the energy transferred by conduction and radiation (Modest, 1993):

$$C\frac{\partial T(\mathbf{r},t)}{\partial t} = -\nabla\cdot(\mathbf{q}^{cond} + \mathbf{q}^{rad}) \tag{2}$$

where $\mathbf{r}$ is the coordinates of the elemental volume, t is the time variable, C is the volumetric thermal capacity. The conduction heat flux vector is given by Fourier's Law, so that:

$$\nabla \cdot q^{\text{cond}} = -\nabla \cdot \left(k \nabla T(\mathbf{r},t)\right) \tag{3}$$

where k is the thermal conductivity. The radiation flux is obtained by integrating the RTE source term, S_λ.
The boundary conditions for the heat conduction model are defined by taking into account the incident heat fluxes from the environment and the medium over the surfaces of the plate, as well as the heat flux emitted from the surfaces. As small variations of temperature are considered in the present problem, the radiative heat transfer term between the surface and the environment is linearized, making it possible to define a generalized heat transfer coefficient, h^{rad}, which includes both convective and radiative heat losses. On the surfaces that are not subjected to the laser flux, the boundary conditions are defined as:

$$k\frac{\partial T}{\partial n} + h^{rad}T + \sum_{m=1}^{N_f} \varepsilon_m F_m(T) n_r^2 \sigma T^4 = h^{rad}T_\infty + \sum_{m=1}^{N_f} \varepsilon_m \int_{\vec{n}.\Omega>0} I_m(\mathbf{r}_c,\Omega)\vec{n}\cdot\Omega \, d\Omega \tag{4.a}$$

where h^{rad} is obtained from:

$$h^{rad} = h + 4\varphi T_\infty^3 = h + 4\sigma T_\infty^3 \left(\sum_{m=1}^{N_f} \varepsilon_m F_m(T_\infty) \right) \tag{4.b}$$

On the heated surface, the laser flux term, $q^{rad} = \varepsilon_l q_l$, where ε is the emissivity of the graphite ink for the wavelength of 10.6 µm of the laser. The boundary condition for such surface is then written as:

$$k\frac{\partial T}{\partial n} + h^{rad}T + \sum_{m=1}^{N_f}\varepsilon_m F_m(T)n_r^2\sigma T^4 = h^{rad}T_\infty + \sum_{m=1}^{N_f}\varepsilon_m\int_{\vec{n}.\Omega>0} I_m(\mathbf{r}_c,\Omega)\vec{n}\cdot\Omega\, d\Omega + \varepsilon_l q_l \tag{5}$$

The radiative boundary condition on the heated surface is given in terms of the emissivity of the graphite ink, considering that the incident energy is equal to the sum of the absorbed and the reflected energies, as:

$$I_\lambda(\mathbf{r}_c) = \varepsilon_\lambda I_{b\lambda}(\mathbf{r}_c,T) + \frac{1-\varepsilon_\lambda}{\pi}\int_{\vec{n}.\Omega^*<0} I_\lambda(\mathbf{r}_c,\Omega^*)\left|\vec{n}\cdot\Omega^*\right| d\Omega^* \tag{6}$$

For the symmetry plane (y = 0), an homogeneous second kind boundary condition was used, assuming that there is no conductive heat flux:

$$\frac{\partial T}{\partial n} = 0 \tag{7}$$

A reflective boundary condition was also considered for the symmetry plane, allowing a continuous propagation of the radiative intensity. This condition is given by:

$$I_\lambda(\mathbf{r}_c,\Omega) = I_\lambda(\mathbf{r}_c,\Omega^*) \tag{8}$$

where $\mathbf{\Omega}$ is the direction of the reflected intensity and $\mathbf{\Omega}$* is the direction of the incident intensity. The initial condition is defined as the whole surface has a uniform temperature at t equal to zero, as:

$$T = T_0 \tag{9}$$

In order to calculate the temperature field over the heated semi-transparent surface, it is necessary to determine the values of the thermophysical parameters involved. Wellele (2007) estimated the values of the thermal conductivities components, as well as the volumetric thermal capacity, C, and the convective heat transfer coefficient, h, using a combination of gradient and stochastic methods, in a three dimensional problem. In the present work, a Bayesian estimator is applied in order to estimate these parameters, in a reduced two dimensional model. Thus, for the parameter estimation, the vector **P** of unknown parameters is considered as:

$$\mathbf{P} = [k_x, k_z, C, h^{rad}]^T \tag{10}$$

3. PARAMETER ESTIMATION

Bayes' theorem can then be stated as (Kaipio and Somersalo, 2004, Tan et al., 2006, Lee, 2004):

$$\pi_{posterior}(\mathbf{P}) = \pi(\mathbf{P}|\mathbf{Y}) = \frac{\pi(\mathbf{P})\pi(\mathbf{Y}|\mathbf{P})}{\pi(\mathbf{Y})} \tag{11}$$

where $\pi_{posterior}(\mathbf{P})$ is the posterior probability density, that is, the conditional probability of the parameters **P** given the measurements **Y**; $\pi(\mathbf{P})$ is the prior density, that is, a statistical model for the information about the unknown parameters prior to the measurements; $\pi(\mathbf{Y}|\mathbf{P})$ is the likelihood function, which gives the relative probability density of different measurement outcomes **Y** with a fixed **P**, and $\pi(\mathbf{Y})$ 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 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 (Kaipio and Somersalo, 2004, Tan et al., 2006, Lee, 2004):

$$\pi(\mathbf{Y}|\mathbf{P}) = (2\pi)^{-M/2}|\mathbf{W}|^{-1/2}\exp\left\{-\frac{1}{2}[\mathbf{Y}-\mathbf{T}(\mathbf{P})]^T\mathbf{W}^{-1}[\mathbf{Y}-\mathbf{T}(\mathbf{P})]\right\} \tag{12}$$

where M is the number of measurements, **W** is the covariance matrix of the measurement errors and **T**(**P**) is the solution of the direct problem obtained with the vector of parameters **P**. We note that parameters estimated through the maximization of equation (11) are referred to as *maximum likelihood estimates* (Beck and Arnold, 1977). The unknown parameters in this study were estimated by using the Metropolis-Hastings algorithm for the Markov Chain Monte Carlo (MCMC) method (Kaipio and Somersalo, 2004, Tan et al., 2006, Lee, 2004). The implementation of the Metropolis-Hastings algorithm starts with the selection of a proposal distribution $p(\mathbf{P}^*,\mathbf{P}^{(t-1)})$ which is used to draw a new candidate state $\mathbf{P}^*$, given the current state $\mathbf{P}^{(t-1)}$ of the Markov chain. Once this moving distribution has been selected, the Metropolis-Hastings sampling algorithm can be implemented by repeating the following steps:

1. Sample a *Candidate Point* $\mathbf{P}^*$ from the proposal distribution $p(\mathbf{P}^*,\mathbf{P}^{(t-1)})$.
2. Calculate the acceptance factor:

$$\alpha = \min\left[1, \frac{\pi(\mathbf{P}^* \,|\, \mathbf{Y})\, p(\mathbf{P}^{(t-1)},\mathbf{P}^*)}{\pi(\mathbf{P}^{(t-1)} \,|\, \mathbf{Y})\, p(\mathbf{P}^*,\mathbf{P}^{(t-1)})}\right] \tag{13}$$

3. Generate a random value U which is uniformly distributed on (0,1).
4. If $U \leq \alpha$, set $\mathbf{P}^t = \mathbf{P}^*$. Otherwise, set $\mathbf{P}^t = \mathbf{P}^{(t-1)}$.
5. Return to step 1 in order to generate the sequence $\{\mathbf{P}^1, \mathbf{P}^2, \ldots, \mathbf{P}^n\}$.

For more details on the theoretical aspects of the Metropolis-Hastings algorithm and MCMC methods, readers are referred to Kaipio and Somersalo (2004), Lee (2004) and Tan et al. (2006).

4. RESULTS AND DISCUSSIONS

The estimation of the thermophysical parameters was carried out using simulated temperature measurements taken on the fixed observation points. Such measurements were simulated by calculating the temperature for each point, using Eqs. (1-3), and adding a normally distributed error to each calculated value. The parameter values used for the simulation of the measurements were the same as those obtained by Wellele (2007), which are presented in Tab. 1. The Metropolis-Hastings algorithm for the Markov Chain Monte Carlo (MCMC) method (Kaipio and Somersalo, 2004, Tan et al., 2006, Lee, 2004) was then applied for the estimation of the parameters k_x, k_z, C and h^{rad}, using uniform prior distributions. T_∞ was fixed as 350K. The posterior distributions for the estimated parameters, as well as the priors considered, are shown in Tab. 1. Figure 2 shows a comparison between the simulated temperature measurements at the observation points and the temperatures calculated with the estimated parameters.

Table 1: Prior and posterior distributions for the thermophysical parameters

Parameter	**Ref. Values (Wellele,2007)**	**Prior Distribution**	**Estimated Mean**	**99% Credibility Interval**
k_x (W/m.K)	5.00	Uniform – Interval (0 , 10.00)	5.82	(5.75 , 5.89)
k_z (W/m.K)	5.00	Uniform – Interval (0 , 10.00)	4.82	(4.63 , 4.70)
C (J/m^3·K)	2.60 x10^6	Uniform – Interval (0 , 1x10^7)	2.47 x 10^6	(2.44 , 2.70) x 10^6
h^{rad} (W/m^2.K)	1.37 x 10^3	Uniform – Interval (0 , 1x10^3)	1.30 x 10^3	(1.29 , 1.31) x 10^3

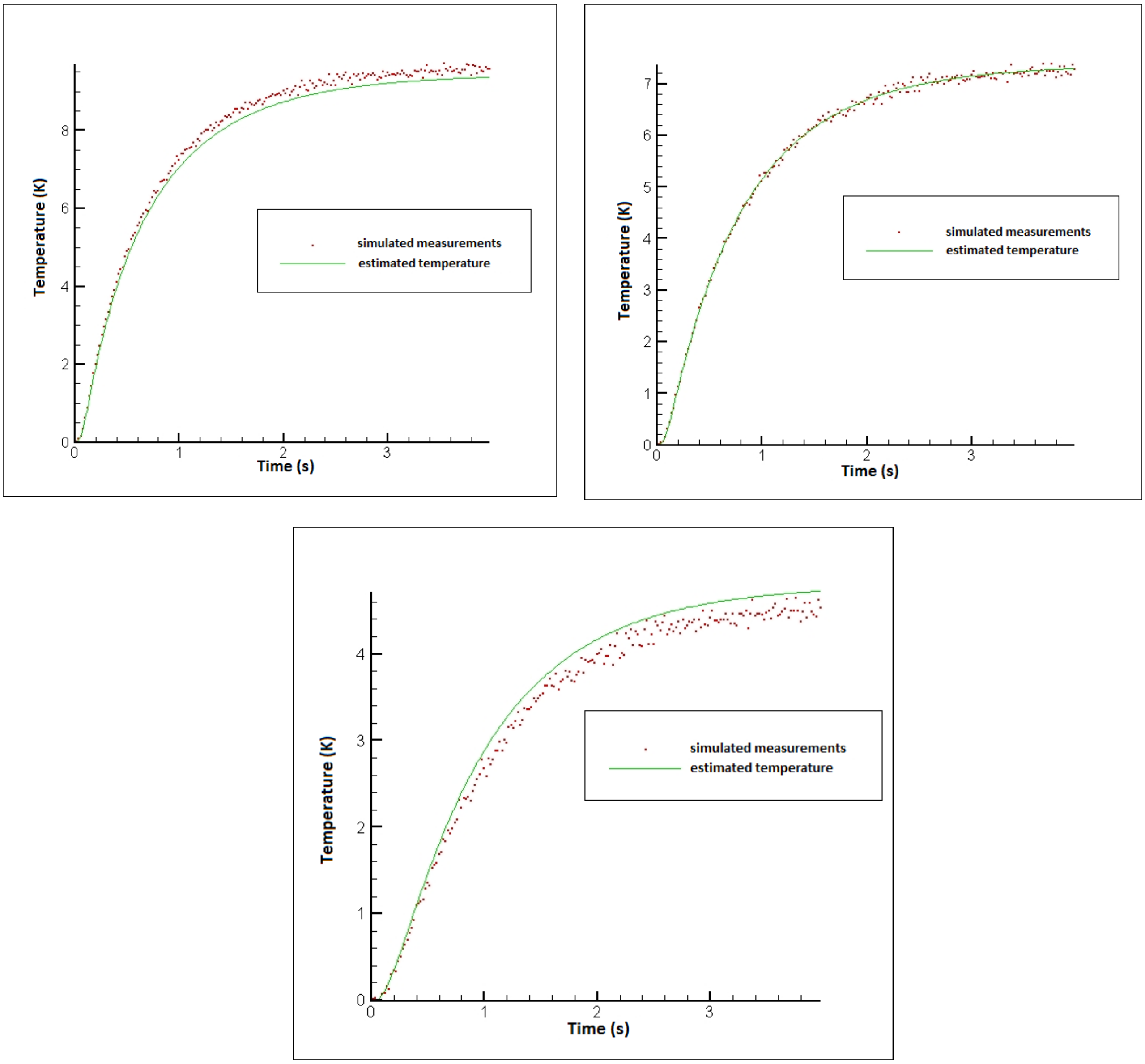

Figure 2: Comparison between the variation of the measured and estimated temperatures at observation points A (upper left), B (upper right) and C (below).

Figure 3 presents the values of the estimated thermophysical parameters at each state of the Markov chain. The Markov chains were generated with 12,000 states, where the first 10,000 states were ignored for the computation of the statistics. The chains converged for all parameters. We note that the parameters are linearly independent, as per the analysis of the sensitivity coefficients made by Wellele (2007). The acceptance ratio of the Markov chain was approximately 23%.

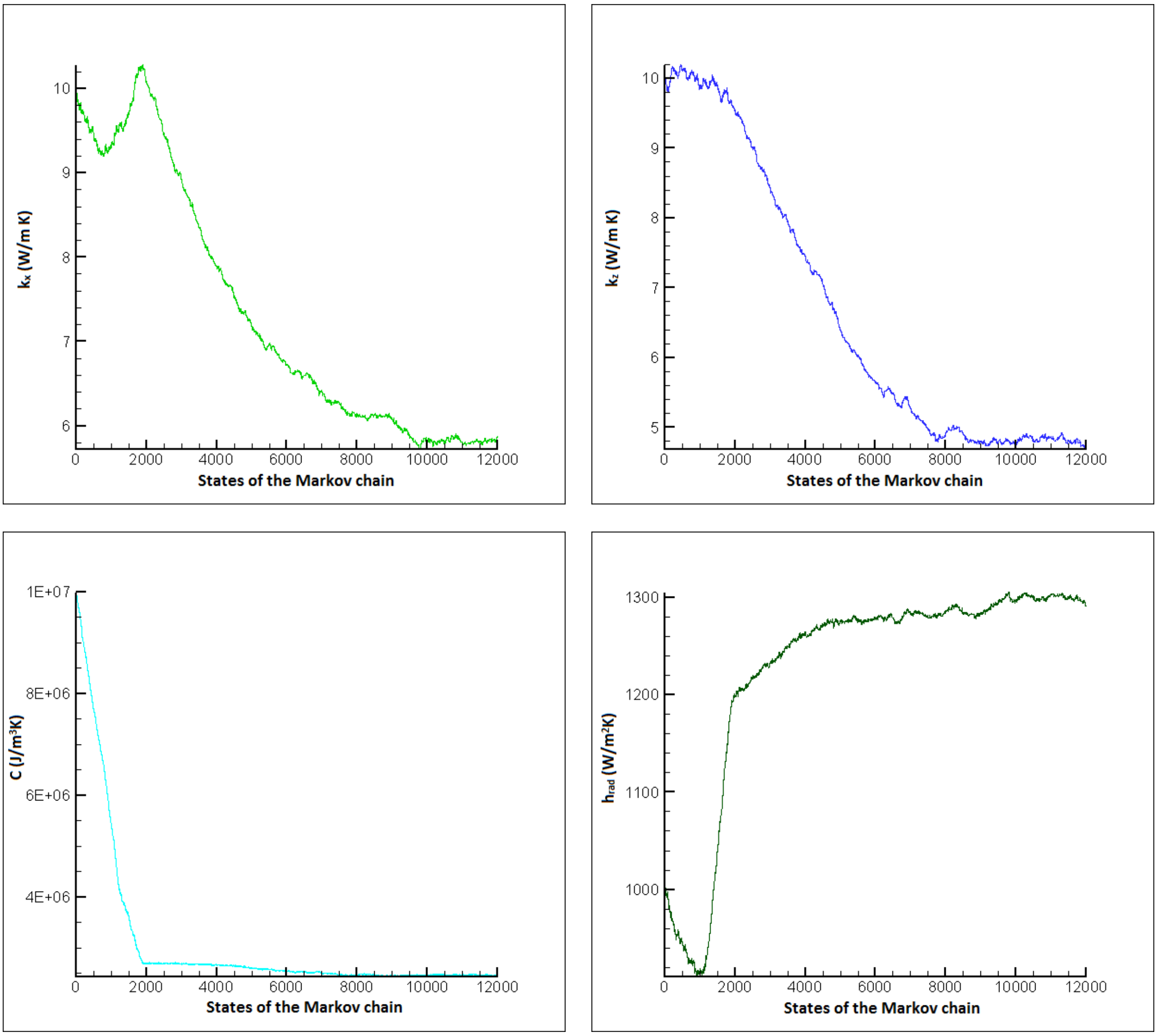

Figure 3: States of the Markov chain for k_x (upper left), k_z (upper right), C (lower left) and h^{rad} (lower right)

The convergence of the Markov chain for the parameters indicates the accuracy of the Bayesian approach for the inverse problem of parameters estimation applied in this work.

5. CONCLUSIONS

A Bayesian approach was employed to estimate thermophysical properties in a semi-transparent plate subjected to a radiative heat flux. The temperature over the plate was described by a coupled heat conduction and radiation model. Temperature measurements were simulated by adding normally distributed errors to the temperatures calculated by the model. The mean values of the posterior distributions of the parameters were obtained through the MCMC method and the reference values were inside or close to its corresponding confidence intervals. The last 2000 states of the Markov chain were considered for the computation of statistics. The chain converged for all the parameters. The MCMC method was successfully employed for the estimation of thermo-physical parameters.

6. AKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE

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