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THERMAL CONTACT RESISTANCE ESTIMATION USING FUTURE TIME REGULARIZATION

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Abstract. *In mechanical engineering, some critical parameters are hard to measure directly. For example, estimating the friction heat flux in a machining tool processing involves calculating high temperatures, something almost impossible with conventional equipment. Another good example could be the measurement of the aerodynamic heat flux on the nose of a space vehicle in a reentry condition. This heat flux can generate temperatures bigger than 10^4 °C in some cases. However, the estimation of these parameters can be done indirectly using inverse techniques. These techniques are in the scope of optimization problems. This work aims to solve an inverse problem by applying a Future Time Regularization combined with two minimization techniques: The Quadrilateral Optimization Method and Bayesian Inference (Metropolis-Hastings algorithm). The reason behind using a regularization method is that inverse problems are ill-posed. Thus, the estimation of the parameters can be highly harmed by errors in the data measurements. This work aims to estimate the thermal contact resistance in a one-dimensional heat conduction problem. The Finite Volumes method is applied using Parallel Cyclic Reduction for solving the direct problem. The problem is solved using an in-house algorithm developed using Python language, and the performance of the different inverse methods will be compared. Furthermore, different roughness conditions will be analyzed in order to determine the Thermal Contact Resistance behaviour.*

Keywords: *Inverse Problems, Time Traveling Regularization, Thermal Contact Resistance, Quadrilateral Optimization Method, Bayesian Inference.*

1. INTRODUCTION

Nowadays, optimization techniques are widely used in both industrial and academic scenarios. An important subgroup of optimization techniques deserves some attention in this context: the inverse methods. An inverse technique is focused on determining hard-to-measure parameters, while the most popular optimization techniques are used to determine design variables.

Fundamentally, an inverse problem is formulated to estimate the causes of a phenomenon and know its effects. In contrast, a direct problem is formulated to determine the impact of known causes. A relevant difference between direct and inverse problems is that, in general, the direct problem is well-posed. In contrast, according to Hadamard's criteria, the inverse problem is ill-posed, Hadamard, (1902). The criteria are settled by the three statements: 1) existence of the solution; 2) uniqueness of the solution; and 3) The solution must behave continuously according to the inputs of the problem. Related to these criteria, the most critical point about inverse problems is that their solutions are unstable. In other words, their solutions do not behave continuously. The leading cause for that is the introduction of noise on the data points, which leads to more considerable fluctuations in the determination of parameters.

Because of this behavior, regularization techniques were developed to stabilize the responses. The most traditional method is Tikhonov Regularization described in Beck *et al.* (1958), which minimizes an objective function added to a regularization parcel associated with previous information about the parameters.

Orlande *et al.* (2006) presents several optimization techniques that can coupled with Inverse Problems like Conjugate Gradient Method, Newton-Raphson Method, Simulated Annealing, and Genetic Algorithms. Furthermore, their work presented some results for Inverse Estimation in forced and natural convection heat estimation, electric potential determination in electrodynamical optimization, and source therm and diffusion coefficient in diffusion problems.

Thiachacht *et al.* (2021) performs an evolutionary algorithm named Marine Predator Algorithm for the determination of the location and amount of structural vulnerabilities in a building. The algorithm is based on the ablest survivor principle and works on maximizing the encounter rate between predators and prey, represented by positional matrices.

In the heat conduction case, the inverse techniques fulfill the determining parameters that are difficult to measure due to the high temperatures involved or spatial inaccessibility. In the particular case of spatial inaccessibility, the work Ribeiro *et al.* (2013) applied the Specified Function technique to estimate the heat flux caused by friction on a machining tool. This approach allows the operator to measure the temperature history on appropriate points and then minimize an objective function using Sensitivity Coefficients.

Ferreira (2009), uses Tikhonov Regularization and maximum entropy as alternatives in determining the heat flux on the thrust camber of the L15 liquid propulsion rocket engine, develod at the Institute of Space Aeronautics. The autor uses L-curve method to determine the most adequate regularization parameter. Similarly, Martins (2012), employs Ordinary Conjugate Gradient and Adjount Problem and Conjugate Gradient in order to determine the wall temperature and heat flux in an cooper plate heated by butane torch.

This work intends to apply inverse formulation in determining consistent results for the Thermal Contact Resistance (TCR) in an one-dimensional heat conduction problem. Although one can estimate this variable by inverse techniques, it could be complex to do by a direct approach. The TCR between two walls depends on several variables like contact pressure, heat flux direction, interstitial medium, roughness, and hardness, as is said by Tang *et al.* (2015) and Gill *et al.* (2009). Another important assumption about contact resistance is that it can vary spatially. Because of this, it would be complex to choose an explicit correlation between the TCR and the mentioned variables.

This work presents results obtained with an in-house Python program and a heat conduction experiment in two roughness configurations to achieve these goals. Future Time Regularization is applied to solve the inverse problem, Magalhães (2018). The optimization of the unknown parameters involved in the objective function is performed using Quadrilateral Optimization Method (QOM), Magalhães (2021), and MCMC Metropolis-Hastings algorithm, Chib *et al.* (1995). The direct problem for the one-dimensional heat conduction equation will be solved using a Finite Volumes discretization.

The value of this works consists in developing an effective TCR estimation tool, which is an important variable on aerospace projects due to its sensitive nature. In addition, this work shows a comprehensive design for inverse problems solutions by appling optimization techniques based on different concepts, deterministic and probabilistc. It can be useful when the required parameter behaves sensitively.

2. MATERIAL AND METHODS

2.1 Direct problem solution via Finite Volumes discretization

It is necessary to solve the direct problem several times for each iteration involving the inverse technique. For this, it is used the Finite Volumes Method discretization, Versteeg and Malalasekera (1995). The integral form for the heat equation is presented in Eq. (1). An advantage of this formulation is that it does not make assumptions about smoothness, which is not previous information.

$$\int_{t_0}^{t_0+\Delta t} \int_{CV} \rho c \frac{\partial T}{\partial t} dV dt = \int_{t_0}^{t_0+\Delta t} \int_{CV} \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) dV dt \tag{1a}$$

$$-k \frac{\partial T(y,t)}{\partial y}\bigg|_{y=0} = q''(t) \tag{1b}$$

$$-k \frac{\partial T(y,t)}{\partial y}\bigg|_{y=\frac{L}{2}^-} = -k \frac{\partial T(y,t)}{\partial y}\bigg|_{y=\frac{L}{2}^+} = \frac{T\left(\frac{L}{2}^-,t\right)-T\left(\frac{L}{2}^+,t\right)}{R_C} \tag{1c}$$

$$-k \frac{\partial T(y,t)}{\partial y}\bigg|_{y=L} = 0 \tag{1d}$$

$$T(y,0) = T_0 \tag{1e}$$

where ρ is the material specific mass, c is the specific heat, k is the material conductivity and R_C is the TCR.

In this work, the time integration in Eq. (1) is made using a fully implicit scheme. After implementing this Equation, one can obtain the coefficients of a tridiagonal matrix. This matrix is solved for each time step using Parallel Cyclic Reduction, as described by Bini and Meini (2009).

It is essential to mention that Parallel Cyclic Reduction only solves meshes with a length equal to 2^k. Because of this, the method operates k reductions until it reaches 2^k equations with one unknown variable.

2.2 Inverse Model – Future Time Regularization

This method is presented in (Magalhães, 2018) as a generalization of the Sequential Specified Function Method, Beck *et al.* (1985). For each time step, one estimates a temporal function for the unknown variable, the heat flux, and the TCR, for the r future times and then applies an optimization technique to fit the measured temperatures to the estimated temperatures. This process is iterated from time $jj = 0$ until $jj = jj_{máx} - r$. Figure 2 shows a flowchart for the method.

It is important to note the regularization aspect of this method. The regularization minimizes the instabilities of an estimation, which results in solutions with fewer sensitives to the input data error. In choosing r future time steps, a specific function to heat flux and a constant value for TCR to be able to fit the estimated temperatures to the measured ones, this method introduces some previous assumptions to the unknown variables, minimizing the range for the solutions and stabilizing them.
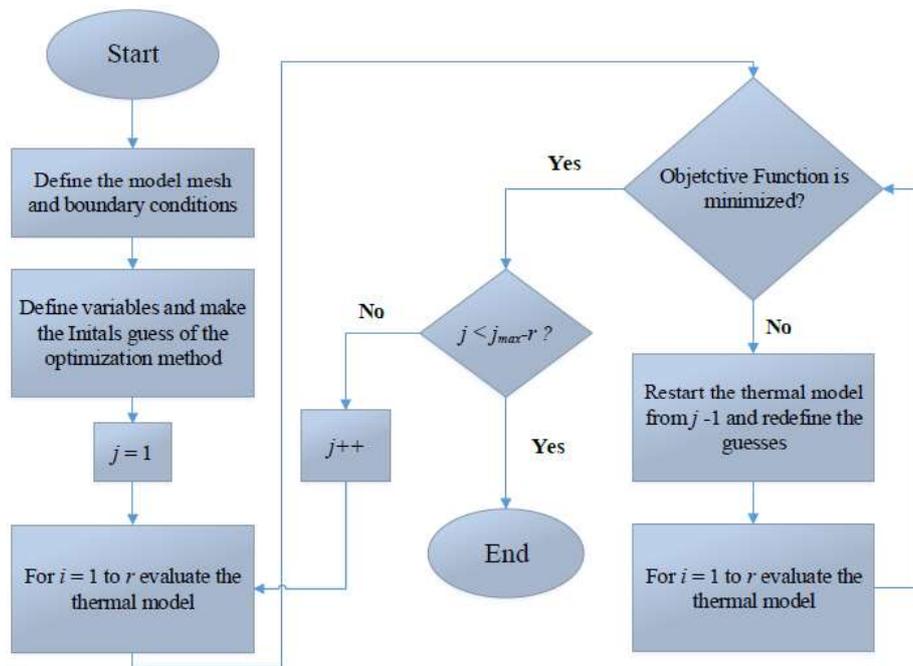

Figure 2. Flowchart for the Future Time Regularization method, adapted from Magalhães (2018).

2.3 Quadrilateral Optimization Method

This optimization method starts by proposing a range of values for k unknown parameters. The coupling between these ranges defines a quadrilateral domain of search performed by the algorithm. In each iteration, the range of values is divided into 3^k homogeneous subdomains. The objective function is evaluated for all of them to find the best subdomain for that iteration. After finding the best value, another domain is defined around the found one, but now with size reduced by $(1-\tau)^k$, i.e., each parameter range is multiplied by $(1-\tau)$, that is the compression factor.

This process is iterated until it reaches one convergence criteria. Equation (3) defines a matrix containing the range of values for each unknown parameter for a two-variable optimization problem. The first column is the lower bound, and the second column is the upper bound.

$$X_{2,2} = \begin{Bmatrix} X_{1,0} & X_{1,1} \\ X_{2,0} & X_{2,1} \end{Bmatrix}$$
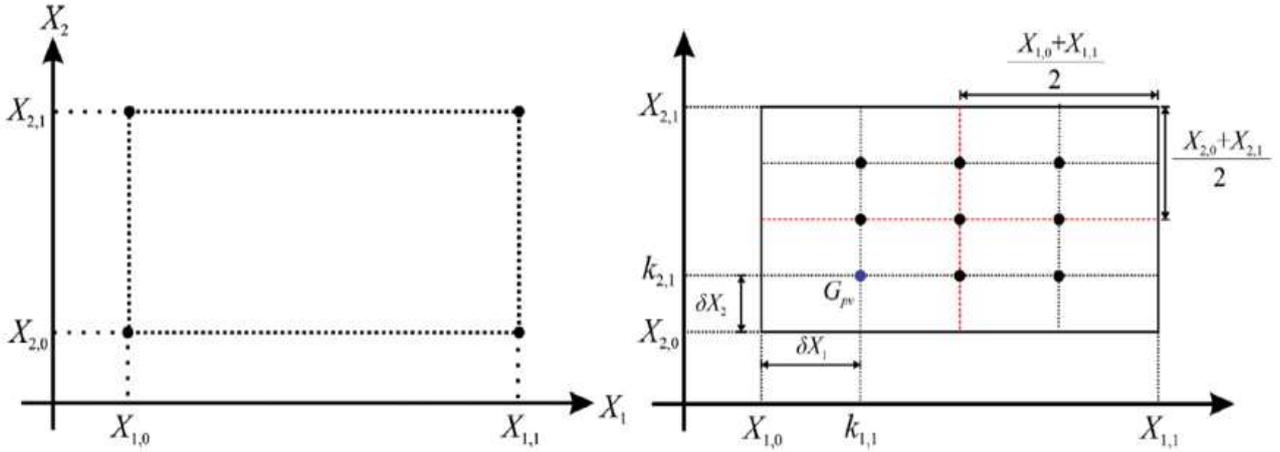
(2)

Figure 3. (a) First domain of search – (b) Segmentation of first domain of search, Magalhães (2021).

The G_{pv} value is the pivot point for each iteration, i.e., it is the point that minimizes the objective function for the current domain.

2.4 MCMC Metropolis-Hastings Algorithm

Another approach chosen to solve the inverse problem is the Metropolis-Hastings algorithm, whose objective is to estimate the parameters of a statistical distribution. This method maximizes the likelihood of a distribution offering each new iteration a new parameter, which can result in a higher likelihood than the previous one or not. The new parameter is accepted if it increases the likelihood, and if it decreases the likelihood, it is accepted with a certain probability.

It is important to mention that each new candidate is randomly selected from a distribution that depends on the previously accepted candidate. This method belongs to the Markov Chain Monte Carlo methods family because it creates a dependent sequence. The steps used are,

1. Choose an arbitrary point x_1 as the first candidate and arbitrary symmetric probability density $g(x/y)$. This probability density is used to generate the new candidate for each new iteration. In this work, $g(x/y)$ is the Gaussian distribution.
2. Generate a new candidate from the distribution $g(x^*|x_t)$.
3. Calculate $\alpha = g(x^*|data)/g(x_t|data)$. Where data is the real temperature distribution calculated.
4. If $\alpha > 1, accept\ x^* = x_{t+1}$. If $\alpha < 1$, accept $x^* = x_{t+1}$ with a probability α and reject x^* with a probability 1-α.
5. Go back to step 2 until it reaches the maximum iteration number in both cases of step 4.

2.5 Sensitivity Coefficients

A good objective function is built by choosing the mesh positions where the temperature is the most sensitive to the parameters variations. It means that the accuracy and stability of the inverse technique are better for some mesh points than others. Because of this it is necessary to choose the best points due to their sensitivity coefficient values, before the objective function formulation. It is made by Eq. (3), which considers the coefficient for an unknown parameter M.

$$\theta_M(x_i, t_j) = \frac{\partial T(x_i, t_j)}{\partial M} \tag{3}$$

In Equation (3) i represents the position of an element on the mesh, and j represents the time used to determine the sensitivity coefficient. Because of the discrete aspect of the simulation, Eq. (3) is performed by a centered finite difference scheme, represented by Eq. (4).

$$\theta_M(x_i, t_j) = \frac{T(x_i, t_j + \Delta t) - T(x_i, t_j - \Delta t)}{2\Delta t} \tag{4}$$

For the TCR case, the distribution for the sensitivity coefficients is presented in Fig. 4. The minimum values were subtracted from each value for these coefficients, and the maximum values normalized the resulting vector.
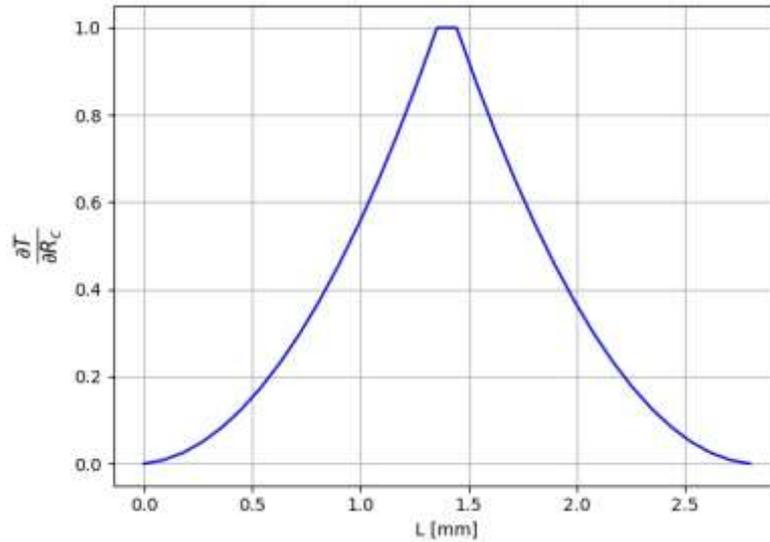
Figure 4. Normalized Sensitivity Coefficients variatons for Thermal Contact Resistante.

The curve behavior shows that the best position for the temperature measurements is the contact region. Specifically for this problem, measuring temperatures in the contact region would significantly decrease the accuracy of the solutions because the presence of thermocouples between the two plates would decrease the number of contact points, forcing the heat flux to pass by radiation instead of conduction. Thus, due to this geometrical limitation, the temperatures were measured on the underside of the bottom plate and the upper side of the upper plate to avoid a contact problem. Specifically for this case, the absolute difference between the coefficients for the worst and the best position is small, so it will not impact the TCR estimation significantly.
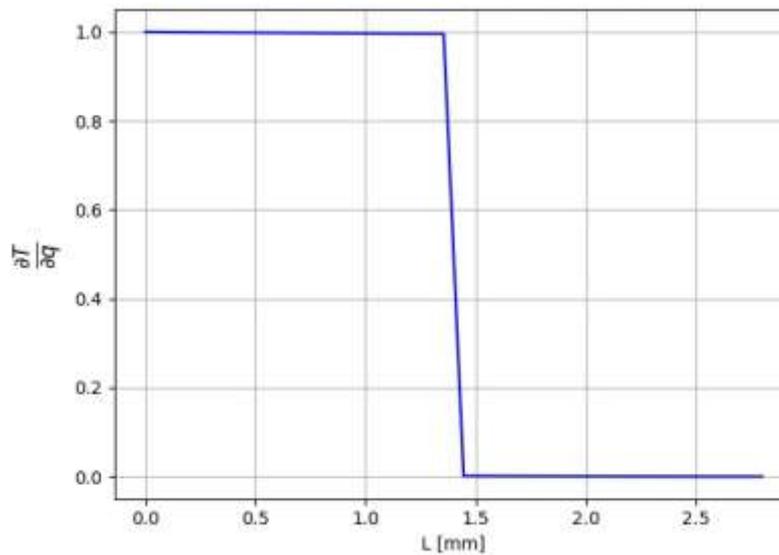

Figure 5. Normalized Sensitivity Coefficients variations for heat flux.

Figure (5) shows that the best points for heat flux estimation are the nearest ones to the heat flux application for the heat flux case. Although it was possible in this case due to the low temperatures reached by the experiment, it is not usual to estimate heat flux with temperature measurements on the heat flux application point. It happens because, in general cases, the temperatures at this point are very high and can cause damage to the thermocouples.

The coefficient analyses presented in this section are an important detail in inverse problems because they lead to a more adequate objective function. Because of this, in order to design an accurate inverse problem it is necessary to analyse the sensitivity coefficients of the problem.

2.6 Experimental Setup

The heat conduction experiment chosen to get temperature data is done as follows. Two thin 1020 steel alloy plates were heated in contact for a certain time, and two thermocouples measured the temperature data. Figure 1 presents the geometrical configuration for the experiment. The steel plates dimensions are 50.20 *mm x* 57.80 *mm x* 1.40 *mm*.
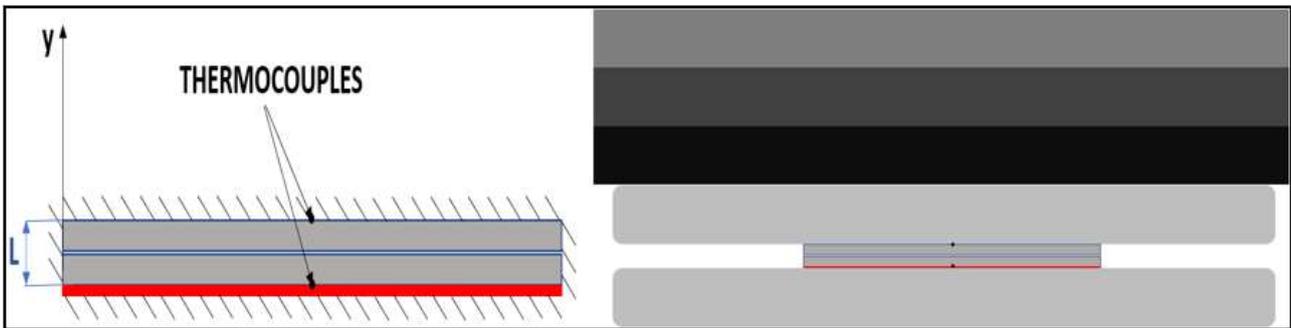

Figure 1. Geometrical representation to the heat conduction experiment.

A low ratio between the steel plate thickness and its area was chosen to keep one-dimensional heat conduction. The red region in Fig. 1 represents the resistive heater that supplies a constant heat flux to the plates. The power applied was 10 *W*. Both the plates and the resistive heater were insulated from the environment by being pressed between two styrofoam plates. The thermocouples were positioned in the center of the bottom and upper faces of the steel plates.

This experiment was performed twice, in smooth and rough configurations. The experimental set had only two plates and both the plates had one smooth face and other considerably oxidized. So, the experiment was conducted in two contact configurations, rough-smooth and smooth-smooth. The oxidized face was considered as rough because this condition decreases the amount of contact points between the two plates, what impairs the heat conduction.

In both cases, the pressure above the plates was the same and three wooden planks were used for this. The three wooden planks were put above the upper styrofoam plate.

It is expected that the real power supply may be lower than 10 *W*. It happens because of the losses in conduction wires and because one side of the resistive heater is faced to the lower styrofoam plate.
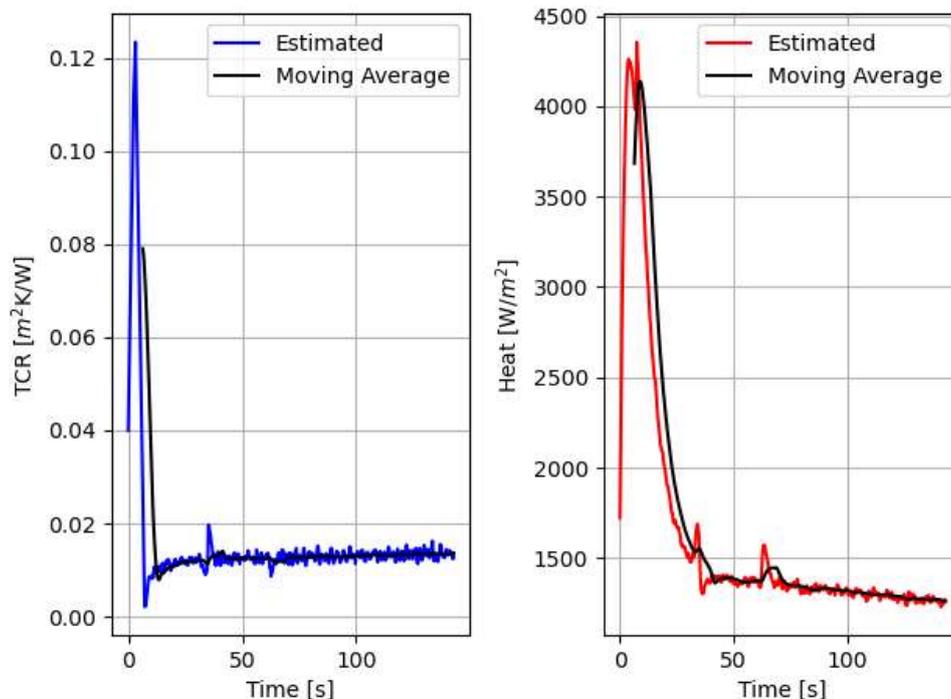
3. RESULTS AND DISCUSSIONS

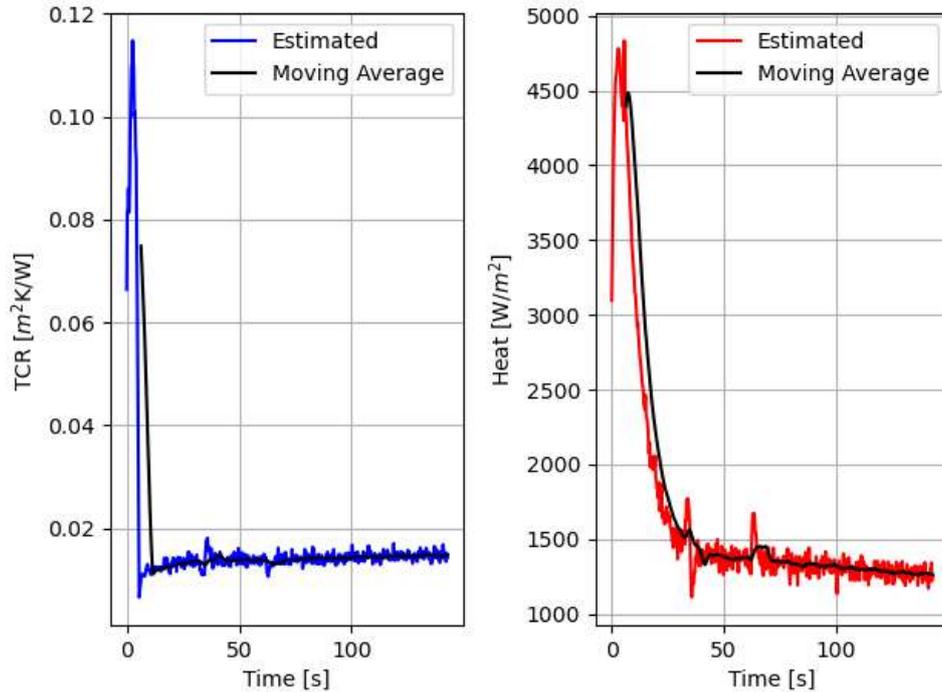Figure 6. TCR and heat flux estimations for smooth configuration and QOM optimization.

Figure 7. TCR and heat flux estimations for smooth configuration and MCMC optimization.

The results for TCR and heat flux obtained for each technique are presented in Fig. (6) to (9). It is important to note that these figures show the simultaneous variable estimation for each time step, considering that the initial temperature and all the others parameters are known. In addition to these data, Tab. 1 shows some errors for the estimated temperature data versus the collected data.

For Fig. (6) and (7), the results obtained are very similar for both techniques and variables. Still, both methods were capable of capturing local abrupt variations in the estimated variables that can be experimental imperfections. For these specific cases, the behavior of estimations fot the two techniques are not identical because there are no simple ways to set analogous convergence criteria for both cases. Although the local behavior is not the same, the global estimation is almost the same.

In both techniques, the initial estimations present a correlation between TCR and heat flux that causes an abrupt increase at the beginning for both variables. For TCR, one can observe that the medium value is reached in just a few seconds, but it takes more time for heat flux. The real heat flux is not constant and decreases along the time, what is expected due to the increasing in temperatures of the steel plates. Besides that, it is important to remember that one of the thermocouples was positioned on the center of the upper plate, and as discussed in session 3.6, it can harm the accuracy of the heat flux on the other face. The reasons for choosing this position were already discussed in section 3.6.

For Fig. (8) and (9), the same behavior details observed in the Fig. (6) and (7) are present. An important difference for this case is that the TCR is higher than the estimated for the smooth case. The rough configuration offers fewer contact points to the plates, so the heat flux is more irradiated than conducted. Therefore, the temperature drop between the plates, in this case, is higher than the drop in the smooth case.

Table 1. Root Mean Square Errors for temperature estimations versus collected data. Results are in ℃.

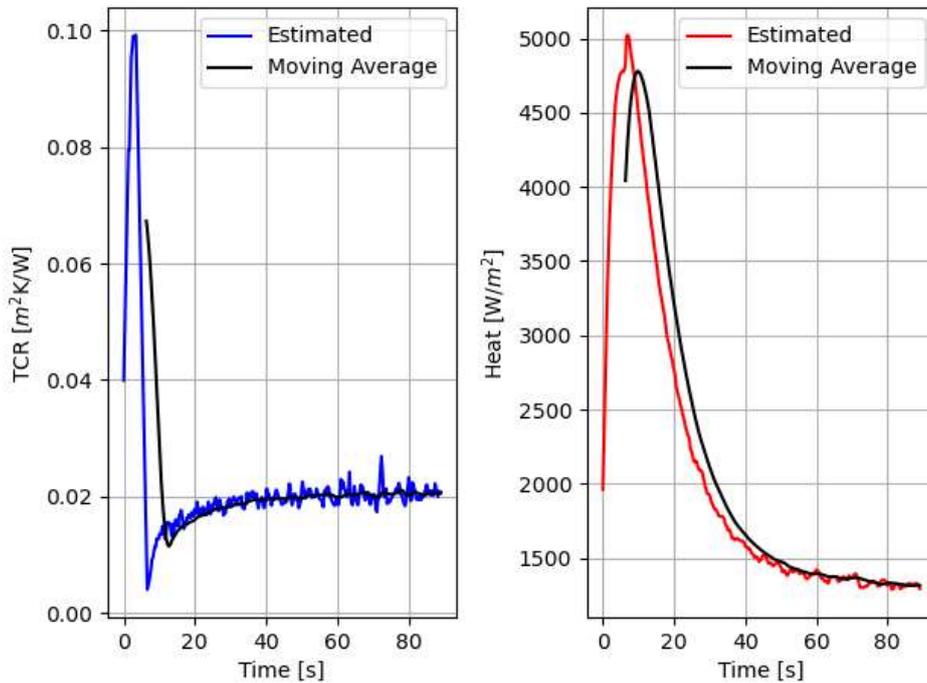| Configuration	QOM	MCMC
Smooth configuration	1.70923089e-3	6.83020142e-5
Rough configuration	2.28805635e-3	8.35997466e-5

Figure 8. TCR and heat flux estimations for rough configuration and QOM optimization.
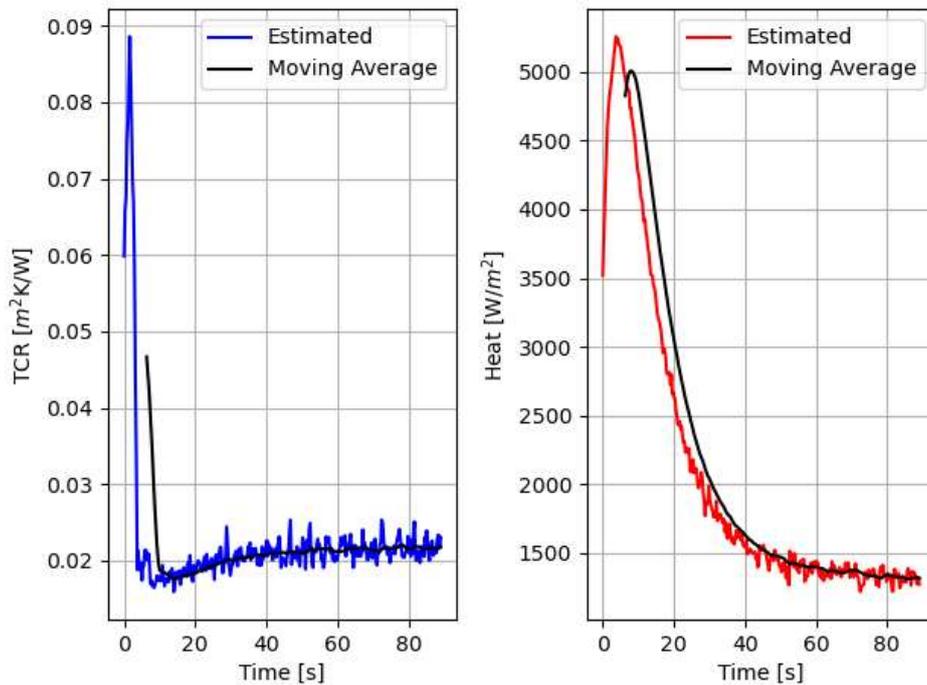

Figure 9. TCR and heat flux estimations for rough configuration and MCMC optimization.

An important detail is that the heat flux estimated leads to a power lower than 10 *W*, when multiplied by the steel plates area. As it was predicted in the experimental setup section, a significant amount of power is lost to the conduction wires and also due to one side of the resistive heater is faced to the lower styrofoam plate.

Table. 1 shows that both techniques performed fitted results to the collected data. It is observed because of the small magnitude presented. Besides that, the differences observed between the two techniques' results can be explained by the difficulty of setting analogous convergence criteria for the techniques.

4. CONCLUSION

This work performed inverse estimations for thermal contact resistance and heat flux in a conduction experiment. The inverse technique chosen was Future Time Regularization which offered stable solutions. The temperature fittings performed for each iteration were optimized by two optimization techniques for comparison and certification. These techniques were Quadrilateral Optimization Method, a deterministic algorithm, and Metropolis-Hastings Algorithm, a probabilistic Markov Chain Monte Carlo algorithm.

Despite initial conditions and paradigm differences in the update of variables, the reached values and estimations behavior for the optimization techniques were almost the same. This fact shows good stability associated to the chosen inverse technique. The estimations were made for two roughness configurations, and one could observe that the smooth configuration presents a lower TCR.

The authors consider that a complete study involving different pressure configurations could bring important insights into the TCR behavior. Besides that, a tri-dimensional analysis considering spatially differences in TCR could bring more reliable results due to the difficulty in ensuring that the pressure is distributed homogeneously on the surface of the plate.

5. ACKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE

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