Heat diffusion in a homogenous slab with an arbitrary periodical heat source: The case of heat source with square wave modulation function

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Abstract
As it has been mentioned in a previous work, the starting point in the study of heat transfer problems is the heat diffusion equation, and their solution reflects not only the boundary conditions consistent to the experimental setup, but also the kind of modulation considered for the heat source. There, the solutions of the heat diffusion equation were found for Dirichlet, Neumann and Robin boundary conditions type, and for an arbitrary modulation function, which the only requirement that the modulation function had an expansion in Fourier basis. From these general solutions, the temperature distributions (as function of relative frequency and relative position) were calculated, under the assumption that the heat source had the sinusoidal modulation inherit from the modulation of the optical excitation, and for all three boundary conditions mentioned before, since this kind of modulation is usually used in the standard models in Photothermal Science and Techniques. However, this kind of modulation is in fact an approximation for the real experimental conditions, since mechanical modulators (choppers) are frequently used in Photothermal experiments with modulated light. In this present work, the temperature distributions are calculated, considering a square wave modulation for Dirichlet, Neumann and Robin boundary conditions, and in the case of Robin boundary conditions, the influence of different Biot numbers in the thermal response, are also presented and discussed.

Keywords: Diffusion equation, homogenous solid, Photothermal techniques, square wave modulation, thermal diffusivity, thermal wave.

Resumen
Como se ha mencionado en trabajos previos, el punto de partida en el estudio de los problemas de transferencia de calor es la ecuación de difusión de calor, y su solución no solo refleja las condiciones de frontera compatibles con el sistema experimental, sino también el tipo de modulación tomado en cuenta para la fuente de calor. Así, las soluciones de la ecuación de difusión de calor fueron calculadas para las condiciones de frontera de los tipos Neumann, Dirichlet, y Robin, y para una función de modulación arbitraria, con el único requisito de que la función de modulación tuviera una expansión en base de Fourier. A partir de estas soluciones generales, la distribución de temperatura (como la función de la frecuencia relativa y la posición relativa) fueron determinadas, bajo la suposición de que la fuente de calor tuviera una modulación sinusoidal heredada de la excitación óptica, y para las tres condiciones de frontera antes mencionadas, ya que este tipo de modulación se utiliza generalmente en los modelos estándar en las Ciencias y Técnicas Fototérmicas. Sin embargo, este tipo de modulación es una aproximación a las condiciones experimentales reales, ya que los moduladores mecánicos (choppers) se utilizan frecuentemente en experimentos Fototérmicos con luz modulada. En el presente trabajo, las distribuciones de temperatura son calculadas, considerando una modulación de onda cuadrada para las condiciones de frontera Neumann, Dirichlet y de Robin, y en el caso de condiciones de frontera de Robin, la influencia de diferentes números de Biot en la respuesta térmica, también se presentan y discuten.

Palabras clave: Ecuación de difusión, sólidos homogéneos, técnicas Fototérmicas, modulación de onda cuadrada, difusividad térmica, onda térmica.

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I. INTRODUCTION

When an experiment that involves heat transfer phenomena [1, 2], such as Photothermal (PT) measurement techniques does [3], is conceived to use modulated light as excitation, there are many ways to accomplish a useful modulation, *i.e.* a controllable modulation. In several measurement systems, photodiodes and laser diodes controlled by a signal generator are used to generate a modulated optical excitation, with the convenience of having various options in the kind of modulation for the amplitude (even a very good approximation to a sinusoidal modulation). Nevertheless, the most common way to generate modulated optical excitation still is by means of a mechanical modulator (chopper), since it is a cheap option and easy to implement in any laboratory. The continuous light beam, becoming from the light source, emerges from the chopper as a square pulse train, this is, as a square wave. In Fig. 1, a comparison between the sinusoidal and the square wave modulations is presented.

To include the square wave (SW) modulation into the heat diffusion equation (HDE), an expansion in Fourier basis can be carried out, and so, the coefficients C_m of the Fourier series of the SW were calculated to be:

$$C_m = \frac{\mathrm{Sinc}(m/2)}{2} \cdot \exp(-\mathrm{i}m\pi/2). \tag{1}$$

Where the Sinc function, is the cardinal sine function [4]. From Eq. (1), is clear that only the odd harmonics will contribute to the SW function, and therefore, only the odd harmonics are relevant in the thermal response, for the SW case, calculated from the general solutions of the HDE by the Green's function technique [2, 4].

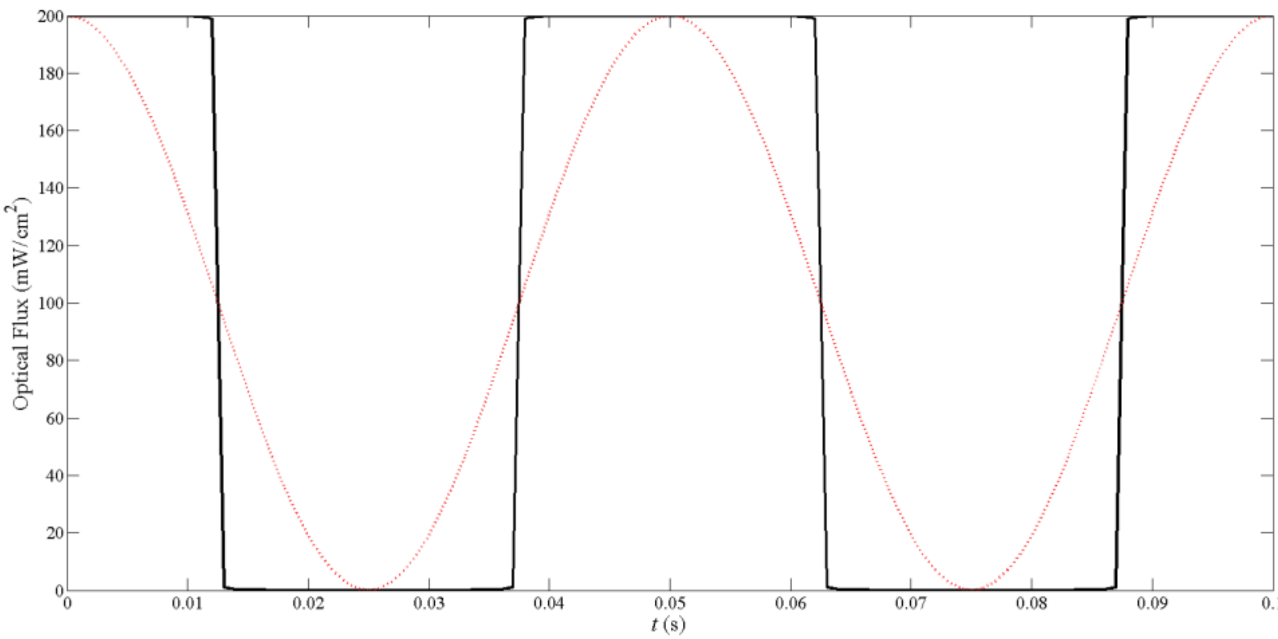


FIGURE 1. Comparison between the sinusoidal modulation (red dotted line) and the square wave modulation (black solid line) of an optical excitation flux.

II. SOLUTIONS OF THE HEAT DIFFUSION EQUATION

Be a lineal, homogenous and isotropic slab, such that its geometry and the flux's direction of the incident light beam sustain a cylindrical symmetry, as Fig. 2 schematizes.

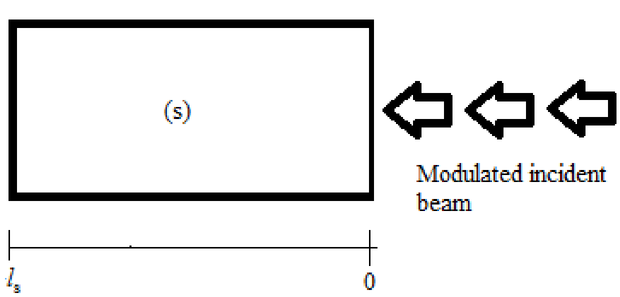


FIGURE 2. Scheme of the geometry of the system.

Referring us to our previous work [5], where the method of solving the heat diffusion equation is described in detail, at next, the solutions under Dirichlet, Neumann and Robin boundary type conditions are described for the SW modulation. As well as the previous work, relative position $z^* = z/l_s$ and relative frequency $\nu = f/f_c$ are used to discuss the theoretical predictions, being l_s the thickness of the slab, and f_c the characteristic frequency [6].

A. Dirichlet boundary condition

In this case $A_f = A_r = 1$ y $B_f = B_r = 0$. The restriction implies the continuity of the temperature distribution across the interfacial surfaces, therefore, the response on the frequency domain to be:

$$\theta_D(\omega', z^*) = \sum_m \frac{A_m r_s}{(r_s^2 - 1)} \left[H(\omega', z^* - l_s) F(\omega', z^*) - \ldots \right. \qquad (2)$$
$$\left. \ldots - H(\omega', z^*) F(\omega', z^* - l_s) \exp(-\beta l_s) \right]$$

Where:

$$H(\omega', \varsigma) \equiv \frac{\mathrm{Sinh}\,\sigma_s \varsigma}{\sigma_s \mathrm{Sinh}\,\sigma_s l_s},$$

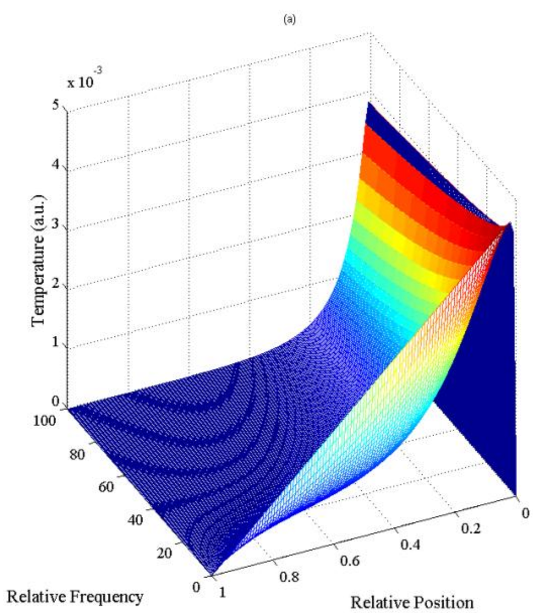
$$F(\omega', \varsigma) \equiv 1 - \exp(-\beta\varsigma)\left[r_s \mathrm{Sinh}\,\sigma_s \varsigma + \mathrm{Cosh}\,\sigma_s \varsigma \right], \qquad (3)$$

$$r_s \equiv \frac{\beta}{\sigma_s} \quad ; \quad A_m = \sqrt{2\pi}\, \frac{(1-R) I_0 \eta}{\kappa_s} C_m .$$

In the previous equations, $\sigma_s \equiv (1+i)/\mu_s$ is the complex thermal diffusion coefficient, defined by means of the thermal diffusion length [6, 7] $\mu_s \equiv (2\alpha_s/\omega')^{1/2}$, being α_s the thermal diffusivity of the sample (s). By means of the Inverse Unitary Fourier Transform of Eq. (2), the temperature distribution (under Dirichlet boundary conditions) in time domain is given by:

$$\Theta_D(t, z^*) = \sum_m \frac{\theta_D(\omega_m, z^*)}{\sqrt{2\pi}} \exp(i\omega_m t) . \qquad (4)$$

In the calculations values of βl_s = 300 (*i.e*. the sample is optically opaque) and were considered, and the results are presented in Fig. 3 for the SW modulation, and in order to make a comparison between the behavior of the thermal response for sinusoidal and the SW modulations, Fig. 4 shows the theoretical calculations at z^* = 0.5, in relative frequency domain.



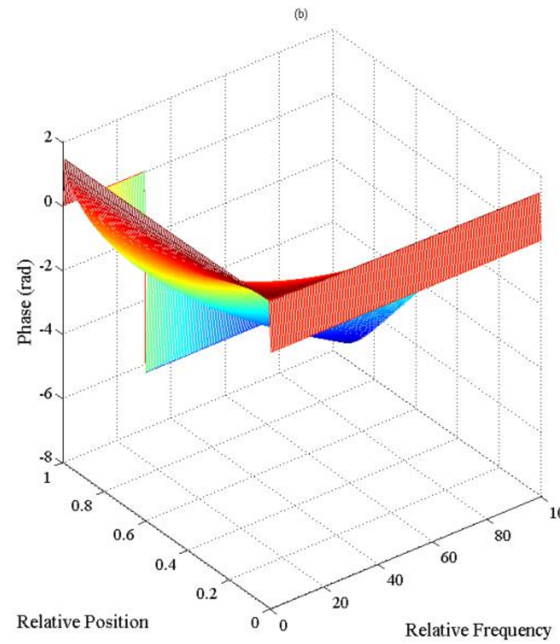
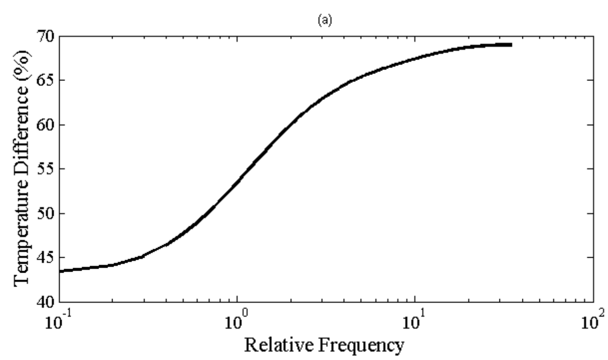
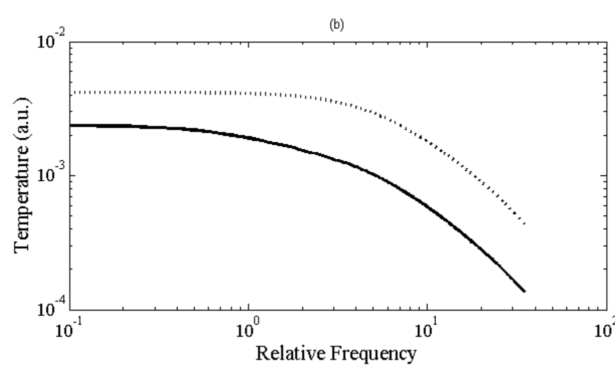
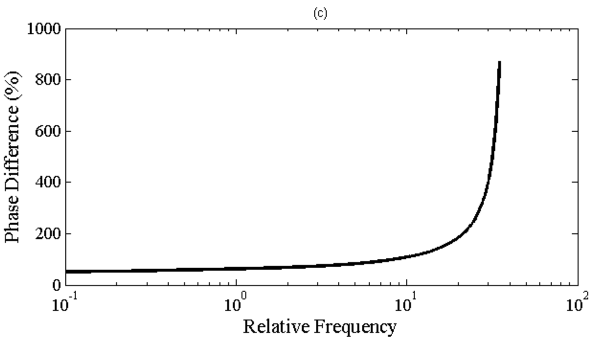


FIGURE 3. Calculation of: (a) Amplitude of the temperature variations, and (b) Phase of the temperature variations, as function of relative position and frequency. Dirichlet boundary conditions were considered.







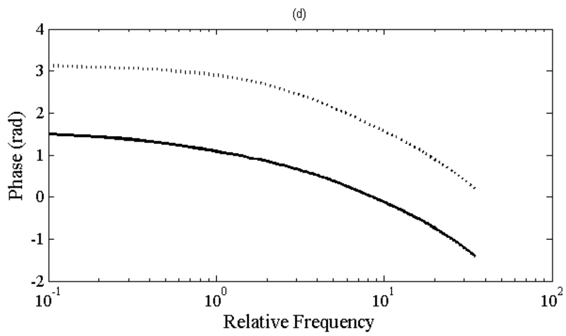


FIGURE 4. Percentage difference in (a) Amplitude and (c) Phase difference of the temperature, as function of relative frequency, between the sinusoidal and SW modulations. Comparison between the thermal responses in: (b) Amplitude and (d) Phase Difference, as function of relative frequency, for sinusoidal (dotted line) and SW (solid line) modulations. Dirichlet boundary conditions were considered.

From Fig. 4 it can be seen that for very small and very large values of the relative frequency, the behavior of the thermal response under the sinusoidal and SW modulations differs almost by a constant factor. This can be explained because the two models converge to each other when the thermal response of the sample lies in the thermally thin or thick regimes, since the contribution of the higher harmonics in the SW modulation are negligible. However, for values of 0.37 to 3.7 for the relative frequency, the higher harmonics contribute to the temperature distribution in such way that their influence cannot be neglected. This range for the relative frequency can be associated to a transition from the thermally thin regime to the thermally thick regime. Also, from Fig. 4(a) it follows that the temperature difference reaches its greatest rate of change, with a change in its concavity, around f_c, highlighting the importance of the characteristic frequency in the thermal response.

B. Neumann boundary conditions

In this second case, $A_f = A_r = 0$ y $B_f = B_r = k_s$, and so, the continuity of the heat flux across the interfacial surfaces is guarantee. In such case, the response on the frequency domain will be:

$$\theta_N(\omega', z^*) = \sum_m \frac{A_m r_s}{(r_s^2 - 1)} \Big[M(\omega', z^* - l_s)\, S(\omega', z^*) - \ldots \qquad (5)$$
$$\ldots - M(\omega', z^*)\, S(\omega', z^* - l_s) \exp(-\beta l_s) \Big].$$

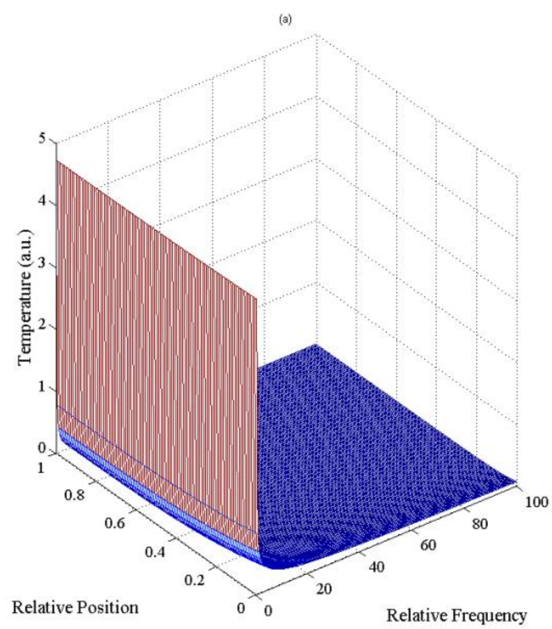
Where:

$$M(\omega', \zeta) \equiv \frac{\mathrm{Cosh}\,\sigma_s \varsigma}{\sigma_s \mathrm{Sinh}\,\sigma_s l_s},$$
$$S(\omega', \zeta) \equiv r_s - \exp(-\beta\zeta)\big[\mathrm{Sinh}\,\sigma_s\varsigma + r_s \mathrm{Cosh}\,\sigma_s\varsigma\big]. \qquad (6)$$

In similar way, applying the Inverse Unitary Fourier Transform to Eq. (5), the temperature distribution (under Neumann boundary conditions) in time domain is given then by:

$$\Theta_N(t, z^*) = \sum_m \frac{\theta_N(\omega_m, z^*)}{\sqrt{2\pi}} \exp(\mathrm{i}\omega_m t). \qquad (7)$$

In the calculations a value of $\beta l_s = 300$ was considered.



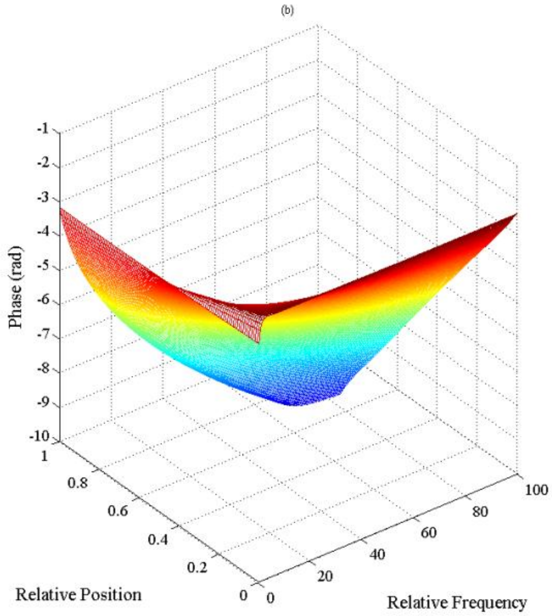
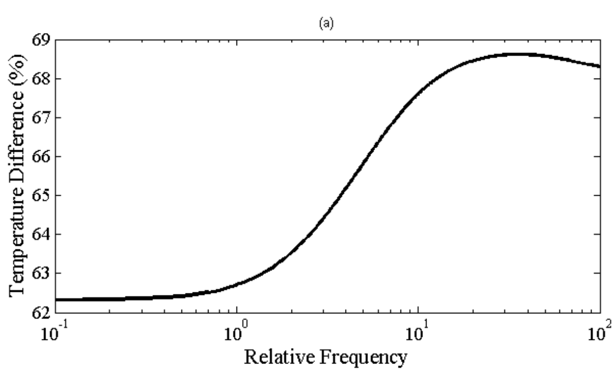


FIGURE 5. Calculation of: (a) Amplitude of the temperature variations, and (b) Phase of the temperature variations, as function of relative position and frequency. Neumann boundary conditions were considered.

In order to make a comparison between the behavior of the thermal response for sinusoidal and the SW modulations, Fig. 6 shows the theoretical calculations at $z^* = 0.5$, in relative frequency domain. Also, it shows that for values around of 1 to 10 for the relative frequency, the contributions of higher harmonics must be taken into account. In this range for the relative frequency, a transition from the thermally thin to thermally thick regimes occurs, and the difference of the model under the sinusoidal and SW modulations strongly depends on the frequency. Thus, for the Neumann boundary conditions, the transition interval between the thermally thin regime and the thermally thick regime is broader than the Dirichlet case.

Also, from Fig. 6(a) it follows that the temperature difference reaches its greatest rate of change, with a change in its concavity, around $v = 3.7$.



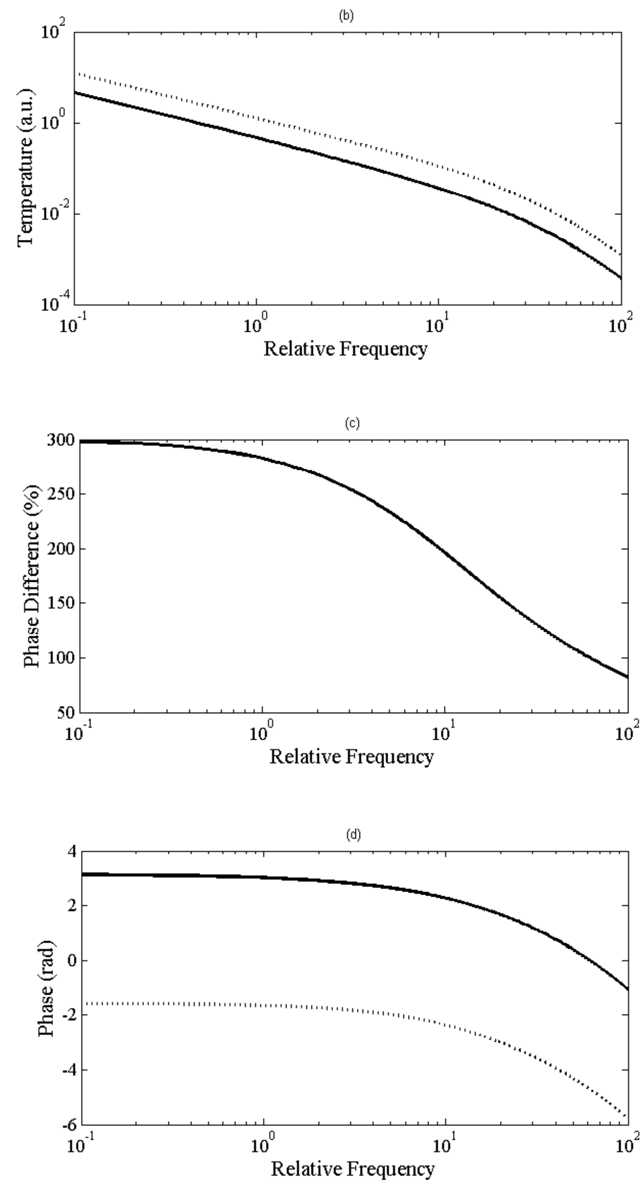


FIGURE 6. Percentage difference in (a) Amplitude and (c) Phase difference of the temperature, as function of relative frequency, between the sinusoidal and SW modulations. Comparison between the thermal responses in: (b) Amplitude and (d) Phase Difference, as function of relative frequency, for sinusoidal (dotted line) and SW (solid line) modulations. Neumann boundary conditions were considered.

C. Robin boundary conditions

This third case, also known as impedance boundary conditions, $A_r = A_f = h$, and $B_r = B_f = k_s$. In this kind of boundary conditions, h represents the overall heat exchange coefficient, and depends on the surrounding medium as well the physical properties of the sample. So, the homogenous Robin boundary condition states that the total heat flux is conserved, taking into account the conductive, convective and radiative heat fluxes.

If we considered that the Biot number $\mathrm{Bi_s} \equiv h l_s k_s^{-1}$ [8, 9] is a simple index of the ratio of the heat transfer resistance of and at the surface of the sample (and therefore qualifies the ability of it to exchange heat through their surfaces), it is possible to define a coefficient e_s as:

$$e_{\mathrm{s}} = \frac{\mathrm{Bi_s}\mu_{\mathrm{s}}}{\sqrt{2}l_{\mathrm{s}}}\exp(-\mathrm{i}\pi/4). \tag{8}$$

The coefficient e_s is a dimensionless quantity, being a function not only of the solid sample and its surroundings, but also a function of the modulation frequency, diminishing at the time that the modulation frequency gets larger. The response on the frequency domain to be:

$$\theta_{\mathrm{R}}(\omega', z^*) = \sum_m \frac{A_m r_{\mathrm{s}}}{(r_{\mathrm{s}}^2 - 1)} \left\{ \frac{\left[\left(W_{(-)} \circ V\right)(\omega', z^* - l_{\mathrm{s}})\right] Q_{(+)}(\omega', z^*) - \left[\left(W_{(+)} \circ V\right)(\omega', z^*)\right] Q_{(-)}(\omega', z^* - l_{\mathrm{s}})}{\sigma_{\mathrm{s}}[(1 - e_{\mathrm{s}}^2)\mathrm{Sinh}\sigma_{\mathrm{s}} l_{\mathrm{s}} - 2e_{\mathrm{s}}\mathrm{Cosh}\sigma_{\mathrm{s}} l_{\mathrm{s}}]} \right\}. \tag{9}$$

In Eq. (9), ⌊, denotes the function composition operator, and the following definitions were used:

$$Q_{(\pm)}(\omega', \zeta) \equiv W_{(\pm)}(r_{\mathrm{s}}, 1) - \exp(-\beta\zeta)\left[r_{\mathrm{s}}\left(W_{(\pm)} \circ V\right)(\omega', \zeta) + \left(W_{(\pm)} \circ U\right)(\omega', \zeta)\right],$$

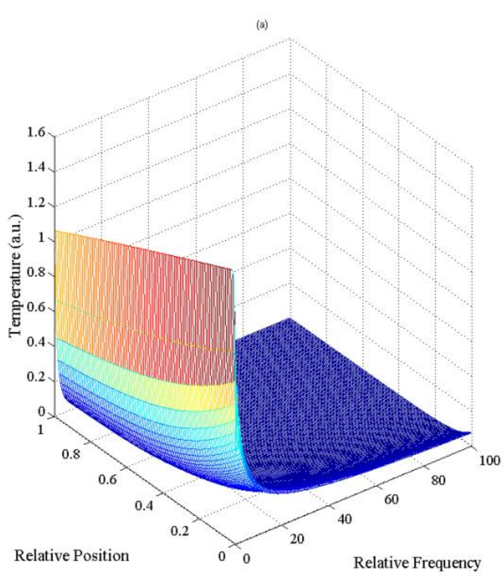
$$W_{(\pm)}(X, Y) \equiv X \pm e_{\mathrm{s}} Y, \tag{10}$$

$$U(\omega', \zeta) \equiv \left(\mathrm{Sinh}\sigma_{\mathrm{s}}\zeta, \mathrm{Cosh}\sigma_{\mathrm{s}}\zeta\right) \quad ; \quad V(\omega', \zeta) \equiv \left(\mathrm{Cosh}\sigma_{\mathrm{s}}\zeta, \mathrm{Sinh}\sigma_{\mathrm{s}}\zeta\right).$$

The temperature distribution, under Robin boundary conditions, in time domain is written finally as:

$$\Theta_{\mathrm{R}}(t, z^*) = \sum_m \frac{\theta_{\mathrm{R}}(\omega_m, z^*)}{\sqrt{2\pi}} \exp(\mathrm{i}\omega_m t). \tag{11}$$

For Robin boundary condition, values of $\beta l_s = 300$ and $\mathrm{Bi_s} = 0.5$ were considered for the calculation of the temperature variation surface, showed in Fig. 7.



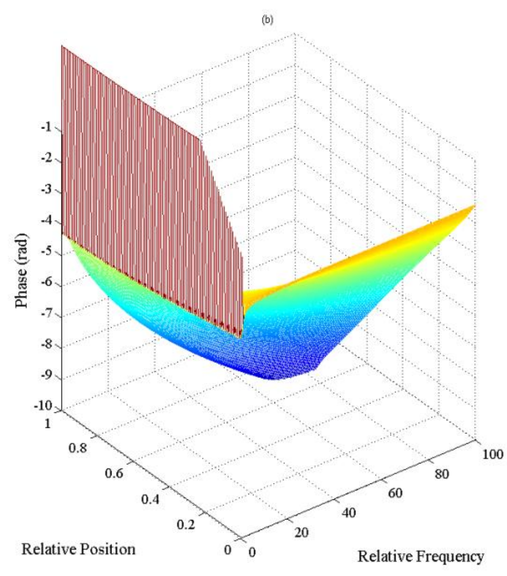


FIGURE 7. Calculation of: (a) Amplitude of the temperature variations, and (b) Phase of the temperature variations, as function of relative position and frequency. Robin boundary conditions were considered.

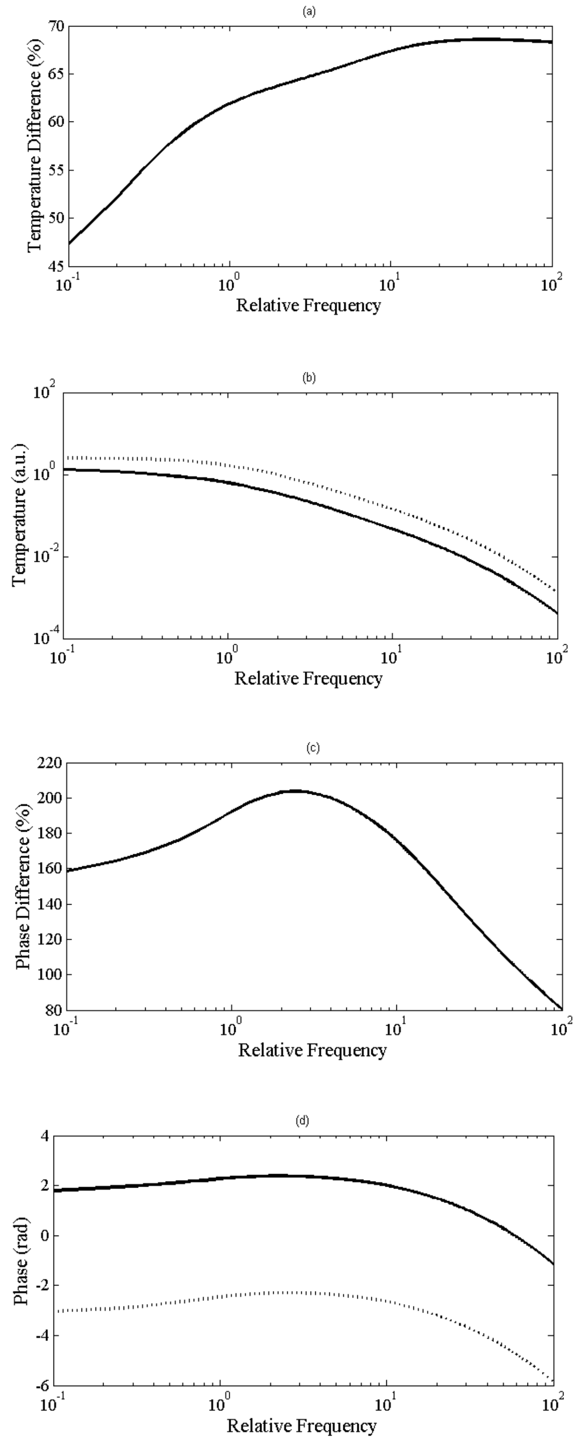


FIGURE 8. Percentage difference in (a) Amplitude and (c) Phase difference of the temperature, as function of relative frequency, between the sinusoidal modulation and SW. Comparison between the thermal responses in: (b) Amplitude and (d) Phase Difference, as function of relative frequency, for sinusoidal (dotted line) and SW (solid line) modulations. Robin boundary conditions were considered.

Figure 8 shows an even more strong dependency on the relative frequency of the percentage difference between the sinusoidal and SW modulations (especially in the phase difference calculations), since the contribution to the thermal response due to the overall heat exchange depends on the modulation frequency.

Again, the influence of Bi_s appears through the coefficient e_s, modulated by the thermal diffusion length, which is a function of the modulation frequency. In Fig. 9, different values of Bi_s number are used for the calculation of the temperature distribution (at $z^* = 0.5$), and the results are compared to the solutions under Neumann boundary condition, in the relative frequency domain, and for the SW modulation.

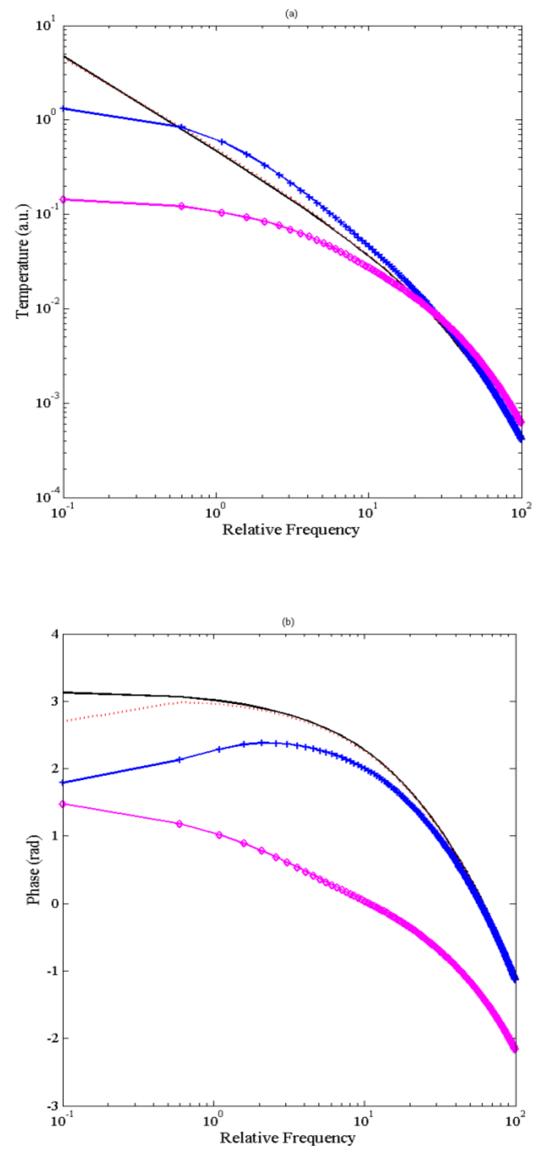


FIGURE 9. Comparison of the behavior of: (a) Amplitude and (b) Phase of the temperature variations as function of relative frequency, for Square wave modulation. The solid black line represents the solutions under Neumann boundary conditions. The calculations under Robin boundary conditions were performed for different values of Bi_s: 0.05(dotted red line), 0.5 (blued plus sign) and 5 (pink diamonds).

There are some differences in the influence of Bi_s for a SW modulation, in comparison to the sinusoidal modulation. As before, the thermal response for different Bi_s numbers tends to equalize at greater relative frequencies, but the behavior of the phase difference is quite distinctive from the calculated for the sinusoidal modulation, and these differences are strongly dependant to the relative frequency, due to the contributions of the higher harmonics for the SW results [10].

III. CONCLUSIONS

From the previous analysis, a carefully selection of the frequency range must be done in consideration to approximate the current modulation by a sinusoidal modulation, when a mechanical modulator is used in the experimental set up. If the modulation frequency guarantees that the thermal response is near or lies into one of the thermal regimes, there is not loss of reliability on the comparison between the experimental data with a model of PT generation signal based in a sinusoidal modulation. But, when there is a strong possibility that the frequency range is so that the sample makes a transition to one thermal regime to another, the correct modulation function must be used in the PT signal generation model, otherwise, the difference between the model and the experimental data will strongly depend on the modulation frequency, which is of course, an undesirable situation. Also, when the thermal response is suitable to be influenced by convective and radiative components to the heat flux, it is not sufficient to take into account the value of the Biot number alone, because its significance, speaking on terms of the thermal regime, is mixed to the thermal diffusion length, which is dependant of the modulation frequency [11].

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