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Application of the factorial design and finite element methods to optimize the solidification of Cu-5wt%Zn alloy in a sand mold

M.M. Pariona[1], G.A. Salem[2] and N. Cheung[3]

[1,2]Department of Mathematics and Statistics, State University of Ponta Grossa, UEPG Campus Uvaranas, Block CIPP, Laboratory LIMAC, CEP:84030900, Ponta Grossa, PR, Brazil. mmpariona@uepg.br, moisespariona@uol.com.br

[1,3]Department of Materials Engineering, University of Campinas - UNICAMP, PO Box 6122, 13083-970, Campinas-SP, Brazil. cheung@fem.unicamp.br

Abstract

In the study reported in this work, two-dimensional numerical simulations were accomplish for the solidification of the Cu-5 wt %Zn alloy in industrial greensand. The latent heat release during the solidification using different mathematical models was incorporated. In order to accomplish this work, the finite elements technique and the ANSYS software program were used. The thermo-physical properties of the alloy Cu-5 wt %Zn were considered temperature-dependent, while for sand were considered constant. In addition, a full three-level Box-Behnken factorial design has been employed in order to investigate the effect of the three factors on the casting process, namely initial temperature of the mold, the convection in the external mold and the latent heat release during the phase change. The results of the heat transfer shown throughout the 2D system, such as thermal flow, thermal gradient and the cooling curves at various points of the cast metal/mold were determined. It was verified that the mold temperature and the mathematical model of the latent heat realease are the most important parameters in the solidification process.

Key words: Numerical simulation, finite elements, factorial design in three levels, solidification of alloy Cu-5wt%Zn, sand mold, latent heat release.

Aplicación de la técnica de diseño factorial y del método de elementos finitos para optimizar la solidificación de la aleación Cu-5wt%Zn en un molde de arena

Resumen

En este trabajo fue realizada la simulación numérica en 2-D para la solidificación de la aleación Cu-5wt%Zn en molde de arena industrial a verde. Fue incorporada en esta investigación la liberación del calor latente durante la solidificación usando diferentes modelos matemáticos. Para realizar este trabajo, la técnica de elementos finitos y el software ANSYS fueron usados. Para este finalidad las propiedades termofísicas de la aleación Cu-5wt%Zn fueron consideradas dependientes con la temperatura, entre tanto, para la arena fueron considerados constantes. Además, el planeamiento factorial de Box-Behnken en tres niveles fue empleado para investigar el efecto de los tres factores sobre el proceso de la fundición, fueron entre ellos: la temperatura del molde, la convección en la parte externa del molde y la liberación del calor latente durante el cambio de fase. Los resultados de la transferencia de calor se presentaron en el sistema 2D para el flujo de calor, el gradiente térmico, las curvas de enfriamiento en la pieza solidificada y en el molde. Fue verificado que la temperatura del molde y el modelo matemático de la liberación del calor latente durante el cambio de fase son los más importantes parámetros del proceso de la solidificación.

Palabras clave: Simulación numérica, elementos finitos, planeamiento factorial en tres niveles, solidificación de la aleación Cu-5wt%Zn, molde de arena, generación de calor.

1. Introduction

Throughout the manufacturing industry, casting process simulation has been widely accepted as an important tool in product design and process development to improve yield and casting quality. Casting simulation requires high-quality information concerning thermo-physical and physical properties during solidification. Some properties have been measured for specific alloys, but these data are generally reduced. Furthermore, the information may be incomplete in the sense that not all properties have been measured and sometimes, disparate information from a variety of sources is used to build up the database for one specific alloy. In order to overcome the lack of data and achieve a better understanding of how changes according to composition range of an alloy may affect solidification properties, it is highly desirable to develop experimental techniques or computer models for calculation of the thermo-physical and physical properties of multi-component alloys for the process of reliable solidification [1].

The computer simulation of cooling patterns in castings has done much to broaden our understanding of casting and mold system design. The structural integrity of shaped castings is closely related to the time-temperature history during solidification, and the use of casting simulation could do much to increase this knowledge in the foundry industry [2].

The ability of heat to flow across the casting and through the interface from the casting to the mold directly affects the evolution of solidification and plays a notable role in determining the freezing conditions within the casting, mainly in foundry systems of high thermal diffusivity such as chill castings. Gravity or pressure die castings, continuous casting and squeeze castings are some of the processes where the product's soundness is more directly affected by heat transfer at the metal/mold interface [2].

Experimental design is a systematic, rigorous approach to solve engineering problem that applies principles and techniques at the data collection stage so as to ensure the generation of valid, precise, and accurate engineering conclusions [3]. It is a very economic way of extracting the maximum amount of complex information and saving a significant experimental time and the material used for analyses and personal costs as well [4]. Different experimental designs are used for different objectives. For example, randomized block designs can be used to compare data sets, and full or fractional factorial design can be used for screening relevant factors [3].

The design of experimental mixtures configures a special case of surface response methodologies using mathematical and statistical techniques, with important applications not only in new products design and development, but also in the improvement of the design of existing products. In short, the methodology consists firstly to select the appropriate mixtures from which the surface response might be calculated; and, further, having the surface response, a prediction of the property value can be obtained for any design, from the changes in the proportions of its components [5]. The other important issue is for engineering experimenters who wish to find the conditions under which a certain process attains the optimal results. In other words, it is aimed to determine the levels of the operational factors at which the response reaches its optimum. The optimum could be either a maximum or a minimum of a function of the design parameters [5].

Factorial design is a useful tool in order to characterize multivariable processes. It gives the possibility to analyze the important influent factors of the process, and to identify any possible interactions among them.

1.1. Mathematical solidification heat transfer model

The mathematical formulation of heat transfer to predict the temperature distribution during solidification is based on the general equation of heat conduction in the unsteady state, which is given in two-dimensional heat flux form for the analysis of the present study [2, 6-8].

$$\frac{\partial}{\partial t}(\rho \cdot c \cdot T) = \frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right) + \dot{Q} \qquad (1)$$

where ρ is density [kgm^{-3}]; c is specific heat [$J\ kg^{-1}\ K^{-1}$]; k is thermal conductivity [$Wm^{-1}K^{-1}$]; $\partial T / \partial t$ is cooling rate [$K\ s^{-1}$], T is temperature [K], t is time [s], x and y are space coordinates [m] and $\dot{Q}$ represents the term associated to the latent heat release due to the phase change. In this equation, it was assumed that the thermal conductivity, density, and specific heat vary with temperature.

In the current system, no external heat source was applied and the only heat generation was due to the latent heat of solidification, L (J/kg) or ΔH (J/m^3). $\dot{Q}$ is proportional to the changing rate of the solidified fraction, f_s, as follows [2, 6, 7].

$$\dot{Q} = \Delta H \frac{\partial f_s}{\partial t} = \rho L \frac{\partial f_s}{\partial t} = \rho L \frac{\partial f_s}{\partial T}\frac{\partial T}{\partial t} \qquad (2)$$

where $\partial f_s / \partial t$ is the rate of the solid fraction along the solidification.

Therefore, Eq. (2) is actually dependent on two factors: temperature and solid fraction. The solid fraction can be a function of a number of solidification variables. But in many systems, especially when undercooling is small, the solid fraction may be assumed as being dependent on temperature only. Different forms have been proposed to the relation between the solid fraction and the temperature. One of the simple forms is a linear relation [7]:

$$f_s = \begin{cases} 0 & T > T_\ell \\ (T_\ell - T)/(T_\ell - T_s) & T_s \le T \le T_\ell \\ 1 & T < T_s \end{cases} \qquad (3)$$

where T_ℓ and T_s are, respectively, the liquid and solid temperature (K). Scheil is another widely used relation, which assumes uniform solute concentration in the liquid but no diffusion in the solid [7]:

$$f_s = 1 - \left(\frac{T_s - T}{T_s - T_\ell}\right)^{-1/1-k_o} \qquad (4)$$

where k_o the equilibrium partition coefficient of the alloy.

Eq. (1) defines the heat flux [9], which is released during liquid cooling, solidification and solid cooling in classical models. The heat evolved after solidification was assumed to be equal zero, i.e. for $T < T_s$, $\dot{Q} = 0$. However, experimental investigations [9] show that lattice defects energy, during solidification increase solid free energy, proportionally to defects type. Lattice defects and vacancy are condensed in the already solidified part of crystal and increase enthalpy of the solid and thus the latent heat will decrease. Due to this fact, another way to represent the change of the solid fraction during solidification can be written as [9].

$$f_s = \frac{(T_\ell - T) + \frac{2}{\pi}(T_s - T_\ell)\left(1 - \cos\left[\frac{\pi(T - T_\ell)}{2(T_s - T_\ell)}\right]\right)}{(T_\ell - T_s)(1 - 2/\pi)} \qquad (5)$$

Considering c´, as pseudo specific heat, as $c' = c - L\frac{\partial f_s}{\partial T}$ and combining Eqs. (1) and (2), one obtains [7, 9]

$$\frac{\partial(pcT)}{\partial t} = \nabla(k\nabla T) \qquad (6)$$

1.2. The factorial design technique

The factorial design technique is a collection of statistical and mathematical methods that are useful for modeling and analyzing engineering problems. In this technique, the main objective is to optimize the surface response that is influenced by various process parameters. Surface response methodology also quantifies the relation between the controllable input parameters and the obtained response surfaces [10]. The design procedure of surface response methodology is as follows [11]:

i. Designing a series of experiments for adequate and reliable measurement of the surface response.

ii. Developing a mathematical model of the second-order surface response with the best fittings.

iii. Finding the optimal set of experimental parameters that produce a maximum or minimum value of response.

iv. Representing the direct and interactive effects of process parameters through two and three-dimensional plots. If all variables are assumed to be measurable, the surface response can be expressed as follows [5]:

$$y = f(x_1, x_2, x_3, \ldots x_k) \quad (7)$$

where y is the answer of the system, and x_i the variables of action called variables (or factors).

The goal is to optimize the variable response y. It is assumed that the independent variables are continuous and controllable by experiments with negligible errors. It is required to find a suitable approximation for the true functional relation between independent variables (or factors) and the surface response. Usually a second-order model is utilized in surface response methodology:

$$y = \beta_o + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum_{i=1}^{m-1} \sum_{j=2}^{m} \beta_{ij} x_i x_j + \varepsilon \quad (8)$$

where $x_1, x_2, \ldots, x_k$ are the input factors which influence the response y; β_o, β_{ii} (i=1, 2,…,m), β_{ij} (i=1, 2,…,m; j=1,2,…,m) are unknown parameters and ε is a random error. The β coefficients, which should be determined in the second-order model, are obtained by the least square method.

The model based on Eq. (8), if m=3 (three variables) this equation is of the following form:

$$y=\beta_o + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \varepsilon \quad (9)$$

where y is the predicted response, β_o model constant; x_1, x_2 and x_3 independent variables; β_1, β_1 and β_3 are linear coefficients; β_{12}, β_{13} and β_{23} are cross product coefficients and β_{11}, β_{22} and β_{33} are the quadratic coefficients [Kwak, 2005].

In general Eq. (8) can be written in matrix form [5].

$$\mathbf{Y=bX} + \varepsilon \quad (10)$$

where **Y** is defined to be a matrix of measured values, **X** to be a matrix of independent variables. The matrixes **b** and å consist of coefficients and errors, respectively. The solution of Eq. (10) can be obtained by the matrix approach [10; 11].

$$\mathbf{b=(X'X)^{-1}X'Y} \quad (11)$$

where **X'** is the transpose of the matrix **X** and $(\mathbf{X'X})^{-1}$ is the inverse of the matrix **X'X**.

The objective of this work was to study the solidification process of the alloy Cu-5 wt %Zn during 1.5 h of cooling. It was optimized through the factorial design in three levels, where the considered parameters were: temperature of the mold, the convection in the external mold and the generation of heat during the phase change. The temperature of the mold was initially fixed in 298, 343 and 423 K, as well as the loss of heat by convection on the external mold was fixed in 5, 70 and 150 $W/m^2.K$. For the heat generation, three models of the solid fraction were considered: the linear relationship, Scheil´s equation and the equation proposed by Radovic and Lalovic [9]. As result, the transfer of heat, thermal gradient, flow of heat in the system and the cooling curves in different points of the system were simulated. In addition, a mathematical model of optimization was proposed and finally an analysis by the factorial design of the considered parameters was made.

2. Methodology of the Numerical Simulation

The finite elements method was used in this study [12-15]. Software program Ansys version 11 [16] was used to simulate the solidification of alloy Cu-5 wt %Zn in green-sand mold. Effects due to fluid motion and contraction are not considered in the present work.

The geometry of the cast metal and the greensand mold is illustrated in Figure 1(a), which is represented in three-dimensions. However, in this work the analysis was accomplish in 2-D, which is illustrated in Figure 1(b). The material properties of a Cu-5 wt %Zn alloy were taken from the reference Miettinen [17]. In Figure 2, the phase diagram of alloy Cu-Zn is presented [18].

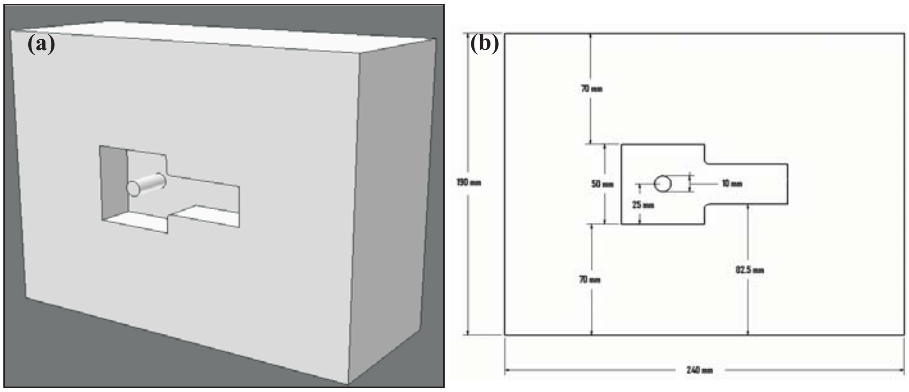

Figure 1. The cast part and mold in 3-D and 2-D.

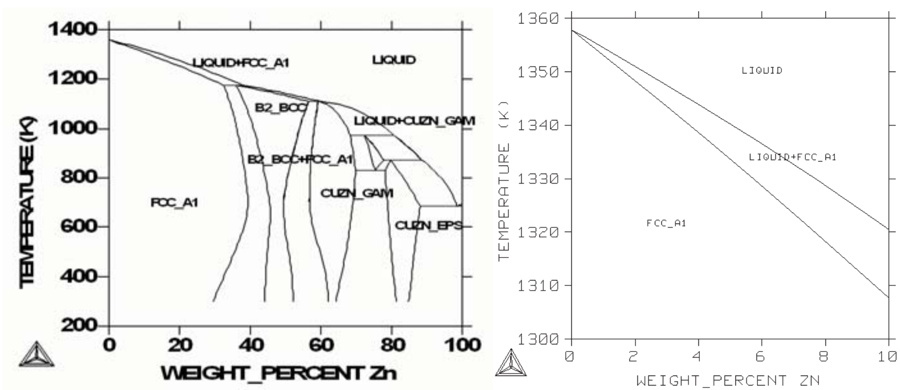

Figure 2. Phase diagram of Cu-5 wt %Zn alloy [18].

An equilibrium partition coefficient of the alloy ko=0.12 was considered in this study. Three pseudo specific heat (c´) obtained from the equations (3), (4) and (5). These equations were denoted respectively by models A, B and C, and the sand thermo-physical properties was given by Pariona and Mossi [19, 20].

In this study, the Box-Behnken factorial design in three levels [5, 21, 22] was chosen to find out the relation between the solidification parameters. Independent variables (factors) and their coded/actual levels were the mold temperature (x_1), the convection phenomenon (x_2) and the mathematical model (x_3) of the latent heat release. (Z) represents the result of the temperature after 1.5 h of solidification. The factorial design is shown in Table 1. For this design type a nomenclature was adopted, where for the inferior state of the variable it was denoted by (-1), for the intermediate state by (0) and for the superior state by (+1).

The initial and boundary conditions were applied to geometry of the Figure 1 according to Table 1. The boundary condition was the convection phenomenon, occurring at the outside walls of the sand mold, as shown in Table 1. The convection coefficient at the mold wall was considered constant in this work, due to lack of experimental data. The effects of the refractory paint and of the gassaging process were not taken into consideration either. The final step, consisted in solving the problem of heat transfer of the mold/cast metal system using Equation (6) and the convergence condition was controlled. Heat transfer is analyzed in 2-D form, as well as the heat flux and the thermal gradient. In addition, the thermal history for some points in the cast metal and in the mold is discussed.

3. Result and Discussion

The solidification results from the given conditions at the lines 7, 8 and 9 of Table 1, which correspond respectively to the lowest temperatures for each mathematical model of latent

Table 1
Factorial design of the solidification parameters

	x1 Mold Temperature	x2 Convection phenomenon (h_f)	x3 Mathematic model	Z - Temperature after 1.5 h of solidification (K)
–1	298 K	5 W/m^{2}K	A	
0	343 K	70 W/m^{2}K	B	
+1	423 K	150 W/m^{2}K	C	
1	–1	–1	–1	806.799
2	–1	–1	0	775.945
3	–1	–1	+1	862.902
4	–1	0	–1	800.301
5	–1	0	0	769.408
6	–1	0	+1	855.752
7	**–1**	**+1**	**–1**	798.197
8	**–1**	**+1**	**0**	767.562
9	**–1**	**+1**	**+1**	854.967
10	0	–1	–1	840.174
11	0	–1	0	809.199
12	0	–1	+1	897.176
13	0	0	–1	833.699
14	0	0	0	802.835
15	0	0	+1	890.279
16	0	+1	–1	832.200
17	0	+1	0	801.430
18	0	+1	+1	890.110
19	+1	–1	–1	899.860
20	+1	–1	0	868.171
21	+1	–1	+1	958.587
22	+1	0	–1	893.996
23	+1	0	0	862.277
24	+1	0	+1	953.026
25	+1	+1	–1	893.136
26	+1	+1	0	861.015
27	+1	+1	+1	952.674

heat release, were discussed. Each one of the lines corresponds to the temperature of the mold for the lower state (-) and for convection phenomenon for the higher state (+).

The condition mentioned on line 9 of Table 1 was chosen to present heat transfer results, where the temperature field is shown in Figure 3(a) in all the system mold and in the cast metal (Figure 3(b)). This last case can be visualized in more detail in part (b), where an almost uniform temperature is observed. In the geometric structure of the mold there is a core constituted of sand that is represented by a white circle in Figure 3(b), which can be verified also in Figure 1(a). In Figure 4 the results of the thermal gradient and the thermal flux are shown, where the thermal gradient goes from the cold zone to the hot zone. On the other hand, the thermal flux goes from the hot zone to the cold zone. Also the convergence of the solution was studied; this point is discussed in more detail by Pariona and Mossi [19, 20].

In order to simulate the cooling curves, two points were considered, as shown in Figure 5: one located in the core (2 point) and the other in the metal (1 point). The three forms of latent heat release were applied into the mathematical model and the resulting thermal profiles were compared.

The cooling curves were studied for condition of line 7, 8 and 9 from Table 1 as shown in Figure 6. Figure 6 (a) shows a comparison of temperature evolution at position (2) for the three formulations of latent heat release: linear (model A), Scheil (model (B) and Radovic and Lalovic (model C). It can be observed that the highest temperature profile corresponds to model A, followed by model C and last by model B, mainly after the solidification range. Although not presented, a similar behavior has occurred at

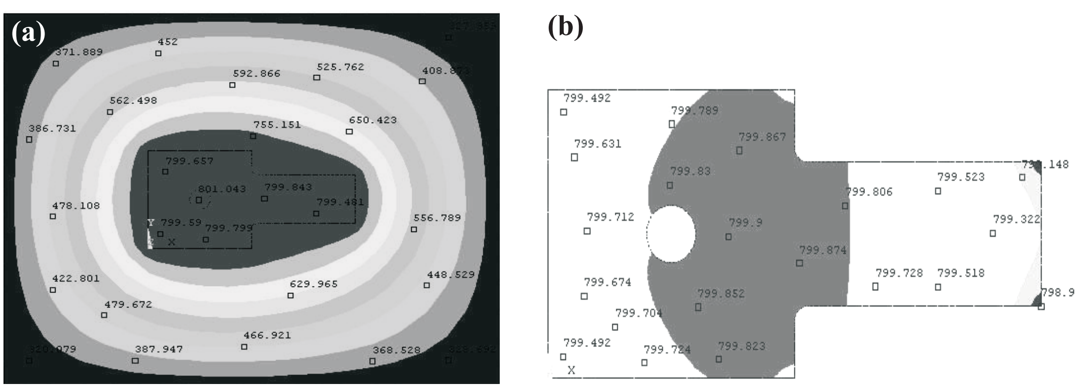

Figure 3. Temperature distribution in the (a) sand mold system, (b) cast metal (Line 9 of Table 1).

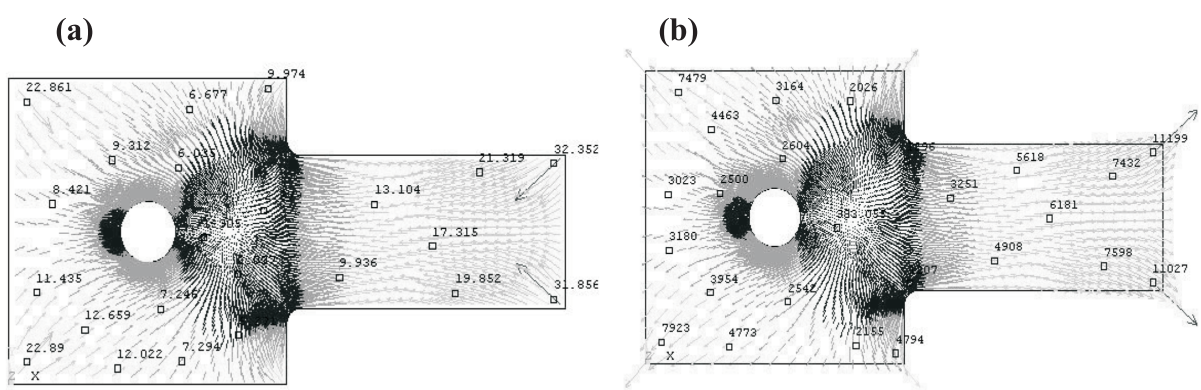

Figure 4. (a) Thermal gradient (K/m) in vectorial form and (b) Heat flux (W/m^2) in vectorial form (Line 9 of Table 1).

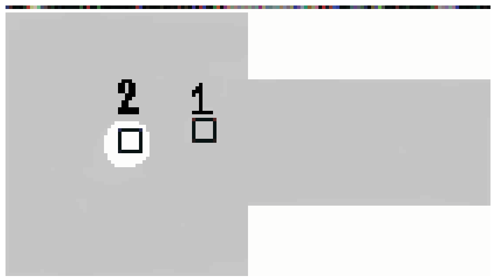

Figure 5. Reference points for the mold/metal system.

other positions in the casting. Chen and Tsai [23] analyzed theoretically four different modes of latent heat release for two of alloys solidified in sand molds: Al-4,5wt% Cu (wide mushy region, 136K) and a 1wt% Cr steel alloy (narrow mushy region, 33.3K). In their work, they conclude that no significant differences can be observed in the casting temperature for different modes of latent heat release, when the alloy mushy zone is narrow. The alloy used in the present work, Cu-5wt%Zn, as shown in Figure 2 has a narrow mushy zone (less than 10K). Figure 6(a) shows that there is a significant temperature profile difference due to the three different latent heat release modes. In addition, it is important to remark that the latent heat release form has strongly influenced the local solidification time. Such solidification parameter affects the microstructure characterized by primary and secondary dendritic arm spacings. Correlations between dendritic spacings and local time solidification (tSL) are well known in the literature [24]. Investigations correlating ultimate tensile strength (σU) and secondary (SDAS) or primary (PDAS) dendrite arm spacings have shown that (σU) increases with decreasing (SDAS) or (PDAS) [25].

Figure 6 (b) shows a comparison of temperature evolution at position (4) for the three formulations of latent heat release. It can be observed again, that the highest temperature profile corresponds to model A, followed by model C and last by model B, and this behavior is repeated for the other positions in the mold.

A three level Box-Behnken design [5, 21, 22] was used to determine the responses of the three variables x_1, x_2 and $x_{3,}$ basing in Table 1. The result of this analysis is shown in the Pareto's diagram (Figure 7). In this figure the estimated valor of the result Z is presented with the significance level (p) of 95%, showing the variables with and without influences significant. The notation adopted for this analysis was, "L" means linear, "Q" means quadratic. For example, "(1)" is the main effect of the first factor and "2L by 3Q" means the linear interaction of the parameter 2 (convection phenomenon) with the quadratic effect of parameter 3 (latent heat release form). In Figure 7, two significant influences were found: x_1 (mold temperature) with linear effect and x_3 (mathematical model) with linear and quadratic effects. The other effect of the independent variables and interactions are negligible in this figure. In order to understand better this analysis, other type of standard graph was ac-

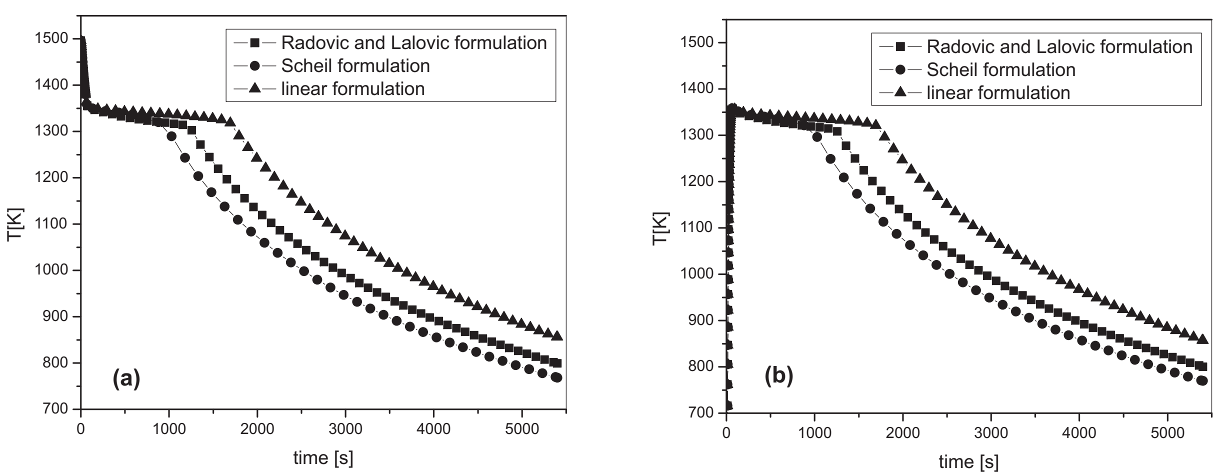

Figure 6. Thermal profiles for the mold/metal system concerning condition 7, 8 and 9 of Table 1. (a) Inside of the cast-point 1, (b) Inside of the mold-point 2.

complished, and it is shown in Figure 8. This figure of the factorial design was built based on the Student's probability distribution (t) [22]. In this figure the main effects and their interactions with significant influence can be observed by those dispersed points (around of the straight line). Those points that belong to the concentrated region points are of the negligible influence. It can be observed in Figure 8 that the biggest positive influence is due to the main effect of x_1 (mold initial temperature) with linear behavior, followed by the linear and quadratic effect of parameter 3 (latent heat release form). Parameter x_2 with linear behavior presents a small negative influence on the factorial design and the other effects had a negligible behavior, around zero, as presented in Figure 8. For this analysis a mathematical model was proposed, given by the following equation Z:

$$Z = 802.7889 + 46.4582x_1 - 3.9348x_2 + 28.3638x_3 + 13.0766x_1^2 + 2.5486x_2^2 + 59.2232x_3^2 + 0.4273x_1x_2 + 0.7476x_1x_3 + 0.1988x_2x_3 + 1.27212x_1x_3^2 + 0.2196x_1^2x_3 + 0.6686x_1^2x_3^2 + 0.3273x_2^2x_3 \quad (12)$$

In this equation the linear and quadratic coefficients are the most important parameters and the other coefficients are negligible (they are considered as residue). Precisely the most significant coefficients belong to the variables which

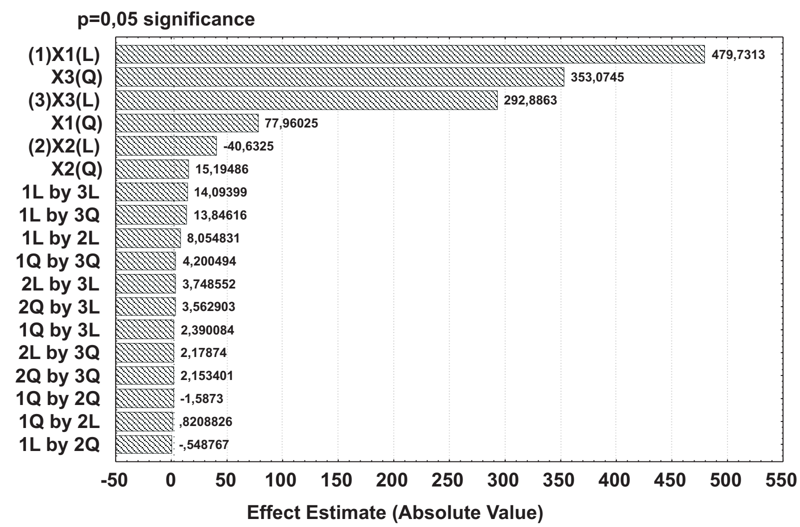

Figure 7. Pareto chart of standardized effects for the full factorial design.

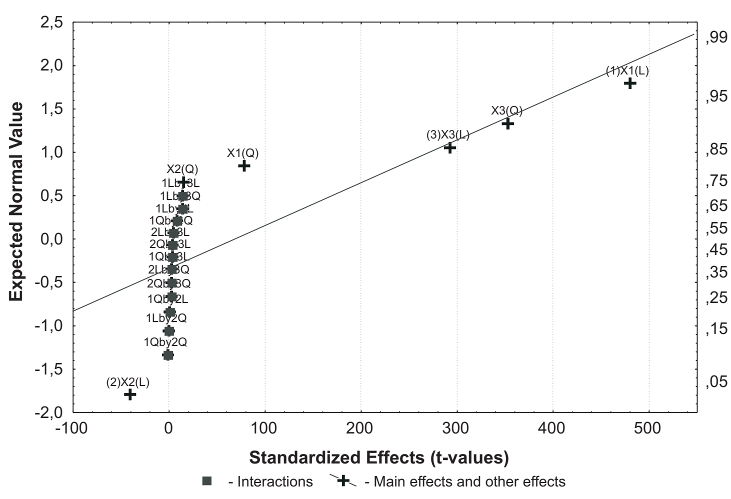

Figure 8. Curve of standardized effects of the factorial design.

strongly influence the result, as it can be observed in Figures 7 and 8.

Figure 9 presents the surface response plots [5, 21], obtained from Eq. (12), that describe the influence of the factors on the overall desirability. Fig. 9(a) shows the 3D surface response relation between convection phenomenon (x_2) and latent heat release form (x_3) at zero level of mold temperature (x_1). Note that, for a given value of x_2, as the x_3 increases and the Z decreases until a minimum value for the interval of x_3 between -0.8 and 0.2. After this minimum point, Z changes its behavior and start to increase as the x_3 increases reaching the highest value of 958.587, as can be seen in Table 1. For a given value of x_3, it can be observed that z profile is almost constant in relation to x_2 increase. Another way to visualize Z variation, is to project Z on the x_2 and x_3 plane in terms of grayscale. The region limited by the white points on this curve represents the Z confidence interval. For other levels of x_1, the surface graph behavior has same characteristic as previously mentioned.

Fig 9(b) shows the effect of mold temperature (x_1) and latent heat release form (x_3) at zero level of convection phenomenon (x_2). In this case, x_1 e x_3 generated a complex surface of paraboloid type. According to the surface projection on the x_1 and x_3 plane, for a given x_3 value, it can be observed that the variation of Z is linear in relation to x_1 and this fact can be confirmed by the point x_1(L) mentioned at the graph Figure 8. On the other hand, the same cannot be affirmed in relation to x_3, if the same analysis is done. For a given value of x_1, the variation of z is parabolic in relation to x_3 and this fact can be observed by the points x_3(L) and x_3(Q) mentioned at the graph of Figure 8.

Fig 9(c) shows the effect of mold temperature (x_1) and convection phenomenon (x_2) at zero level of latent heat release (x_3). Note that, as the x_1 factor increases, the Z increases. But, for a given value of x_1, it is observed that for every x_2 value, Z is almost constant. As a result, the surface geometry is not a complex one, if we compare to the surface geometry of Figure 9b.

In this type of analysis, one can realize that the parameters x_1 and x_3 had variations more accentuated than the parameter x_2. This behavior is also verified in the Figures 7 and 8.

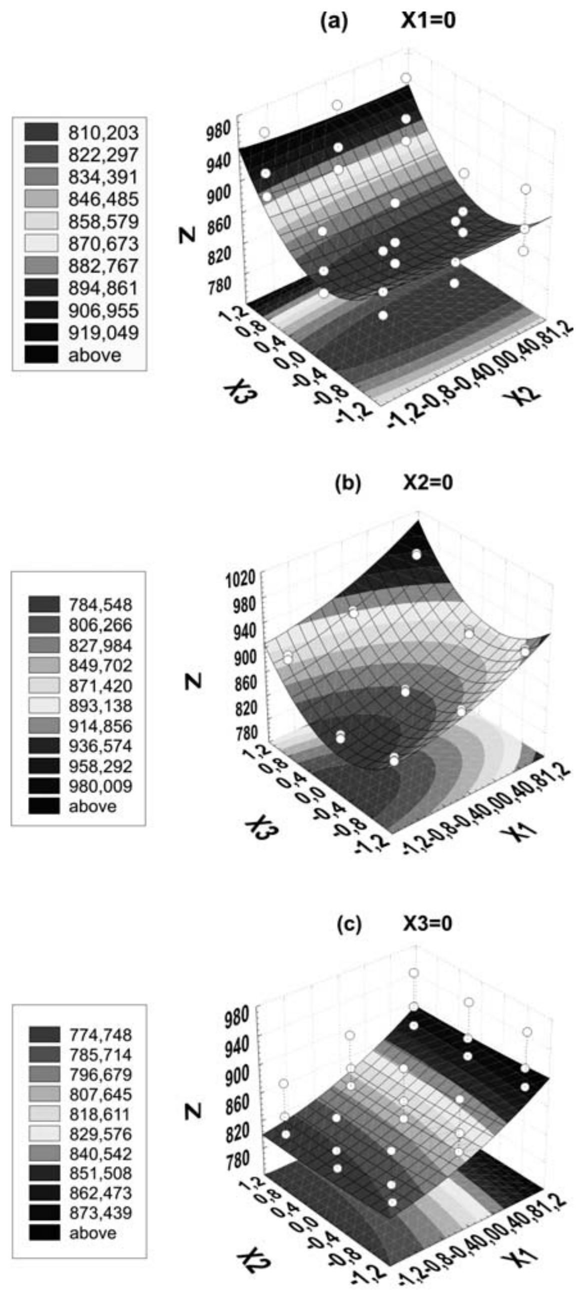

Figure 9. Surface response plots showing the effect of the (a) x_2 and x_3 factors, x_1 was held at zero level, (b) x_1 e x_3 factors, x_2 was held at zero level and (c) x_1 and x_2 factors, x_3 was held at zero level.

4. Conclusion

The three latent heat release forms implemented into the model resulted in significant different thermal responses, which contradicts a previous report in the literature.

In this study, a three-level Box-Behnken factorial design combining with a surface response methodology was employed for modeling and optimizing three operations parameters of the casting process. According to this study, it was observed that the parameters, such as, mold temperature and the mathematical model of the latent heat realease are the most important in the solidification process. The factorial design method is a useful tool to determine what factors are crucial in the solidification process and thus, a special care needs to be taken during the project elaboration of the casting.

5. Acknowledgements

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