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# Finite Element Methods to Optimize by Factorial Design the Solidification of Cu-5wt%Zn Alloy in a Sand Mold

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## 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 the number of alloys for which information is available is limited. 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. To overcome the lack of data and achieve a better understanding of how changes in composition within a specification 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 (Guo et al., 2005).

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. (Ferreira et al., 2005).

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 (Ferreira et al., 2005).

According to the authors Atwood and Lee (Atwood & Lee, 2003), the mechanical properties of metal products depend upon the phenomena occurring during production. Defects formed during each stage of production can persist or modify the behavior of the metal during subsequent processing steps. Therefore, ensuring that an appropriate microstructure is formed at each stage with minimal defects has always been a focus in the study of metal production. In aluminum alloy shape castings, the final microstructure is directly dependent upon the as-cast microstructure since the only post-casting processing is normally a heat treatment. One microstructural feature that can affect the final properties of aluminum alloy

shape castings is microporosity, formed due to the combined effects of volumetric shrinkage upon solidification. Developing a model to predict the formation of microporosity in solidifying metal castings is one way of helping. Porosity in castings is a defect that results from the interaction of a number of processes: volume change, nucleation and growth of the solid phase, diffusion of dissolved species, and the interaction of interphase surficial. Although some of these individual processes may be treated analytically, combining the processes into a predictive tool requires the numerical calculation power that has only become available over the last few decades due to the development of digital computers

The use of multivariate experimental design techniques is becoming increasingly widespread in analytical chemistry. Multivariate experimental design techniques, which permit the simultaneous optimization of several control variables, are faster to implement and more cost-effective than traditional univariate (one at a time) approaches (Khajeh, 2009). One of the most popular multivariate design techniques is two level full/fractional factorial, in which every factor is experimentally studied at only two levels. Due to their simplicity and relatively low cost, full factorial design techniques are very useful for preliminary studies or in the initial steps of an optimization, while fractional factorial designs are almost mandatory when the problem involves a large number of factors (Khajeh, 2009). On the other hand, since only two levels are used, the models that may be fit to these designs are somewhat restricted. If a more sophisticated model is needed, as for the location of an optimum set of experimental conditions, then one must resort to augment response surface designs, which employ more than two factor levels. Among these, Box-Behnken is a second-order multivariate design technique based on three-level incomplete factorial designs that received widespread application for evaluation of critical experimental conditions, that is, maximum or minimum of response functions (Khajeh, 2009).

Experimental design is a systematic, rigorous approach to engineering problem solving that applies principles and techniques at the data collection stage so as to ensure the generation of valid, precise, and accurate engineering conclusions (Xiao & Vien, 2004). 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 (Kincl et al., 2005). Different experimental designs are used for different objectives. For example, randomized block designs can be used to compare data sets, full or fractional factorial design can be used for screening relevant factors (Xiao & Vien, 2004).

The design of mixture experiments configures a special case in response to surface 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 response surface might be calculated; having the response surface, a prediction of the property value can be obtained for any design, from the changes in the proportions of its components (Aslan, 2007). The other important issue is for engineering experimenters who wish to find the concentration conditions under which a certain process attains the optimal results. That is, they want 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 (Aslan, 2007). 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 (Ferreira et al., 2005; Santos et al., 2005; Shi & Guo, 2004; Dassau et al., 2006).

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

where  $\rho$  is density [ $\text{kgm}^{-3}$ ];  $c$  is specific heat [ $\text{J kg}^{-1} \text{K}^{-1}$ ];  $k$  is thermal conductivity [ $\text{Wm}^{-1}\text{K}^{-1}$ ];  $\partial T/\partial t$  is cooling rate [ $\text{K s}^{-1}$ ],  $T$  is temperature [ $\text{K}$ ],  $t$  is time [ $\text{s}$ ],  $x$  and  $y$  are space coordinates [ $\text{m}$ ] 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,  $L$  ( $\text{J/kg}$ ) or  $\Delta H$  ( $\text{J/kg}$ ).  $\dot{Q}$  is proportional to the changing rate of the solidified fraction,  $f_s$ , as follow (Ferreira et al, 2005; Santos et al, 2005; Shi & Guo, 2004).

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

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 relationship between the solid fraction and the temperature. One of the simple forms is a linear relationship (Shi & Guo, 2004; Pericleous et al., 2006):

$$f_s = \begin{cases} 0 & T > T_l \\ (T_l - T)/(T_l - T_s) & T_s \leq T \leq T_l \\ 1 & T < T_s \end{cases} \quad (3)$$

where  $T_l$  and  $T_s$  are, respectively, the liquid and solid temperature ( $\text{K}$ ). Another relation is the widely used Scheil relationship, which assumes uniform solute concentration in the liquid but no diffusion in the solid (Shi & Guo, 2004):

$$f_s = 1 - \left( \frac{T_s - T}{T_s - T_l} \right)^{\frac{-1}{1-k_0}} \quad (4)$$

where  $k_0$  the equilibrium partition coefficient of the alloy.

Eq. (1) defines the heat flux (Radovic & Lalovic, 2005), 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 have showed that lattice defects and vacancy are condensed in the already solidified part of the crystal and the enthalpy of the solid increases and thus the latent heat will decrease (Radovic & Lalovic, 2005). Due to this fact, another way to represent the change of the solid fraction during solidification can be written as (Radovic & Lalovic, 2005):

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

Considering  $c'$ , as pseudo specific heat, as  $c' = c - L \frac{\partial f_s}{\partial T}$  and combining Eqs. (1) and (2), one obtains (Shi & Guo, 2004 ; Radovic & Lalovic, 2005):

$$\frac{\partial(\rho c' T)}{\partial t} = \nabla(k \nabla T) \quad (6)$$

The boundary condition applied on the outside of the mold is:

$$-k \frac{\partial T}{\partial n} = h(T - T_o) \quad (7)$$

Here  $h$  is the heat transfer coefficient for air convection and  $T_o$  is the external temperature.

## 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 response surface that is influenced by various process parameters. Response surface methodology also quantifies the relationship between the controllable input parameters and the obtained response surfaces (Kwak, 2005). The design procedure of response surface methodology is as follows (Gunaraj & Murugan, 1999):

- i. Designing of a series of experiments for adequate and reliable measurement of the response of interest.
- ii. Developing a mathematical model of the second-order response surface 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 response surface can be expressed as follows (Aslan, 2007; Yetilmezsoy et al., 2009; Pierlot et al., 2008; Dyshlovenko et al. 2006):

$$y = f(x_1, x_2, x_3, \dots, x_k) \quad (8)$$

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 response variable  $y$ . 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 relationship between independent variables (or factors) and the response surface. Usually a second-order model is utilized in response surface methodology:

$$y = \beta_0 + \sum_{i=1}^m \beta_i x_i + \sum_{i=1}^m \beta_{ii} x_i^2 + \sum_{i=1}^{m-1} \sum_{j=2}^m \beta_{ij} x_i x_j + \varepsilon \quad (9)$$

where  $x_1, x_2, \dots, x_k$  are the input factors which influence the response  $y$ ;  $\beta_0, \beta_{ii}$  ( $i=1, 2, \dots, m$ ),  $\beta_{ij}$  ( $i=1, 2, \dots, m; j=1, 2, \dots, m$ ) are unknown parameters and  $\varepsilon$  is a random error. The  $\beta$  coefficients, which should be determined in the second-order model, are obtained by the least square method.



The model based on Eq. (9), if  $m=3$  (three variables) this equation is of the following form:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \varepsilon \quad (10)$$

where  $y$  is the predicted response,  $\beta_0$  model constant;  $x_1$ ,  $x_2$  and  $x_3$  independent variables;  $\beta_1$ ,  $\beta_2$  and  $\beta_3$  are linear coefficients;  $\beta_{12}$ ,  $\beta_{13}$  and  $\beta_{23}$  are cross product coefficients and  $\beta_{11}$ ,  $\beta_{22}$  and  $\beta_{33}$  are the quadratic coefficients (Kwak, 2005).

In general Eq. (9) can be written in matrix form (Aslan, 2007).

$$Y = \mathbf{b}X + \varepsilon \quad (11)$$

where  $\mathbf{Y}$  is defined to be a matrix of measured values,  $\mathbf{X}$  to be a matrix of independent variables. The matrixes  $\mathbf{b}$  and  $\varepsilon$  consist of coefficients and errors, respectively. The solution of Eq. (11) can be obtained by the matrix approach (Kwak, 2005; Gunaraj & Murugan, 1999).

$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} \quad (12)$$

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

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<sup>2</sup>.K. For the generation of heat, three models of the solid fraction were considered: the linear relationship, Scheil's equation and the equation proposed by Radovic and Lalovic (Radovic & Lalovic, 2005). 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. Also, 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 (Su, 2001; Shi & Guo, 2004; Janik & Dyja, 2004; Grozdanic, 2002). Software program Ansys version 11 (Handbook Ansys, 2010) 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). Some material properties of Cu-5 wt %Zn alloy were taken from the reference Miettinen (Miettinen, 2001), the other properties were taken from Thermo-calc software (Thermo-calc software, 2010), and in Figure 2 the enthalpy and the phase diagram of alloy Cu-Zn are presented (Thermo-calc software, 2010). Three pseudo specific heat ( $c'$ ) obtained from the equations (3), (4) and (5) were used and these equations were denoted respectively by models A, B and C, and the sand thermo-physical properties was given by Midea and Shah (Midea and Shah, 2002).

In this study, the Box-Behnken factorial design in three levels (Aslan, 2007; Paterakis et al., 2002; Montgomery, 1999) was chosen to find out the relationship between the response

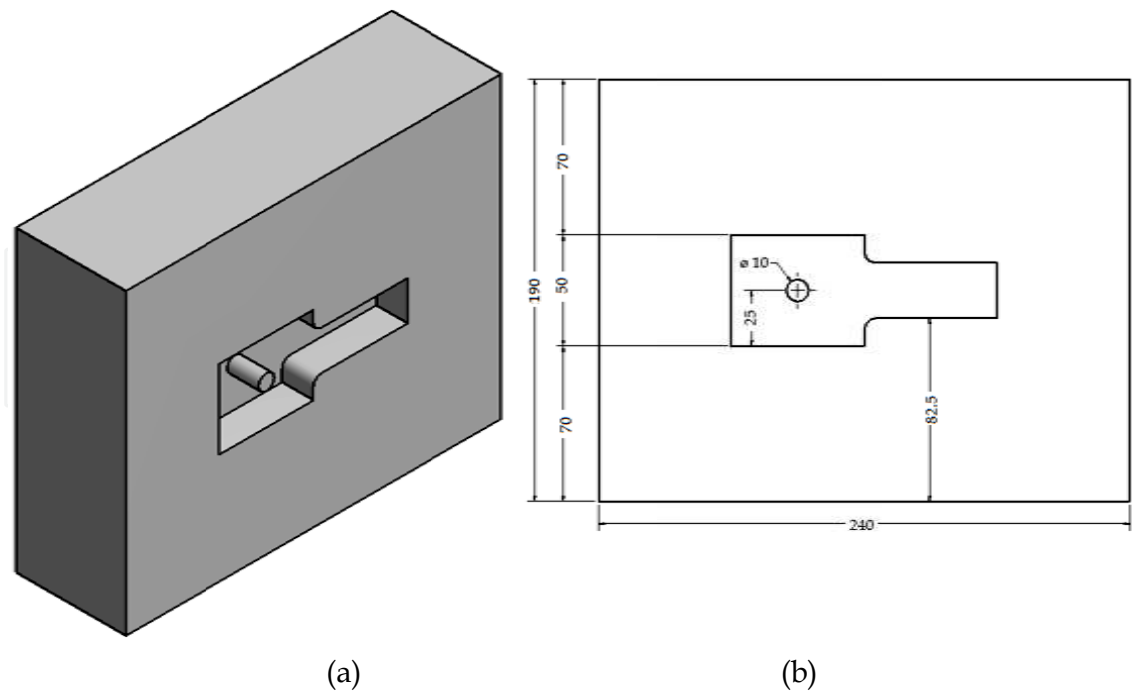


Fig. 1. The cast part and mold in (a) three dimensional and (b) bi dimensional

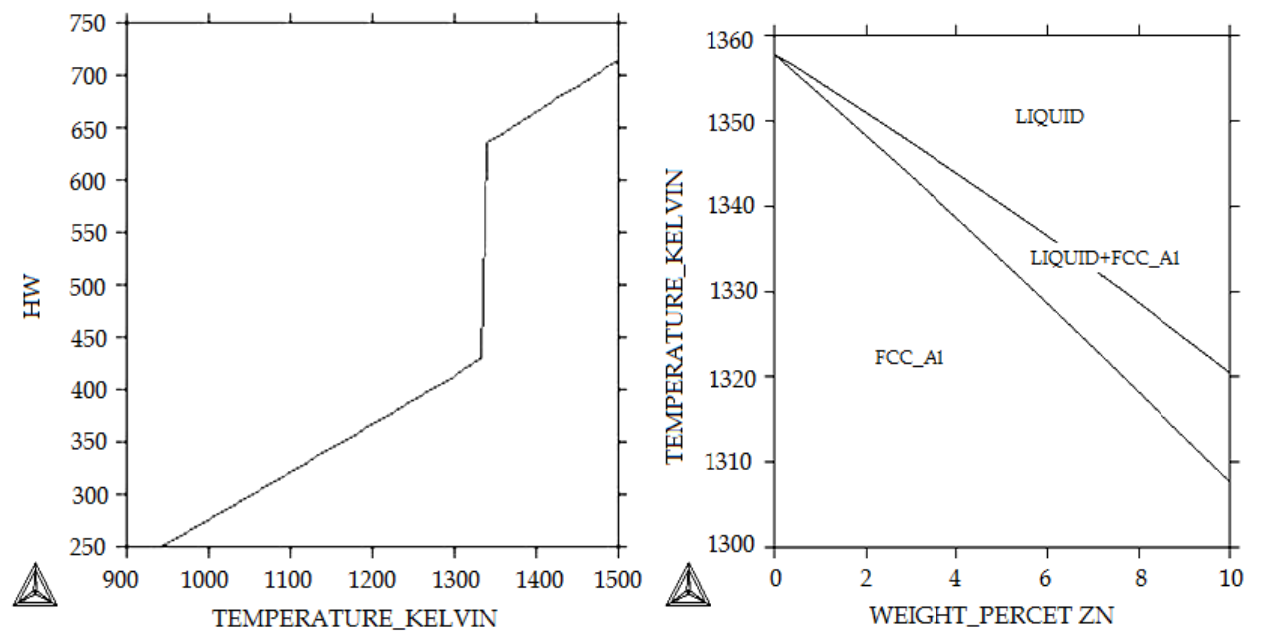


Fig. 2. (a) Enthalpy and phase diagram of Cu-5 wt %Zn alloy and (b) phase diagram of Cu-5wt%Zn alloy (Thermo-calc software, 2010)

functions. Independents variables (factors) and their coded/actual levels considered 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).

	x <sub>1</sub> Mold Temperature	x <sub>2</sub> Convection phenomenon (h <sub>f</sub> )	x <sub>3</sub> Mathematic model	Z - Temperature after 1.5 h of solidification (K)
-1	298 K	5 W/m <sup>2</sup> K	A	
0	343 K	70 W/m <sup>2</sup> K	B	
+1	423 K	150 W/m <sup>2</sup> 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

Table 1. Factorial design of the solidification process parameters



The initial and boundary conditions were applied to geometry of Figure 1 according to Table 1. The boundary condition was the convection phenomenon and this phenomenon was applied to the outside walls of the sand mold, as shown in Table 1. The convection transfer 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 gassing 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), in applied boundary condition and in controlling the convergence condition. Heat transfer is analyzed in 2-D form, as well as the heat flux, the thermal gradient, and in addition, the thermal history for some points in the cast metal and in the mold is discussed.

3. Result and discussion

The result for solidification was discussed for some particular cases, at condition given in lines 7, 8 and 9 from Table 1, which correspond respectively to the lowest temperatures for each mathematical model of latent heat release. Each one of the lines corresponds to the temperature of the mold for the lower state (-) and for convection phenomenon for the higher state (+).

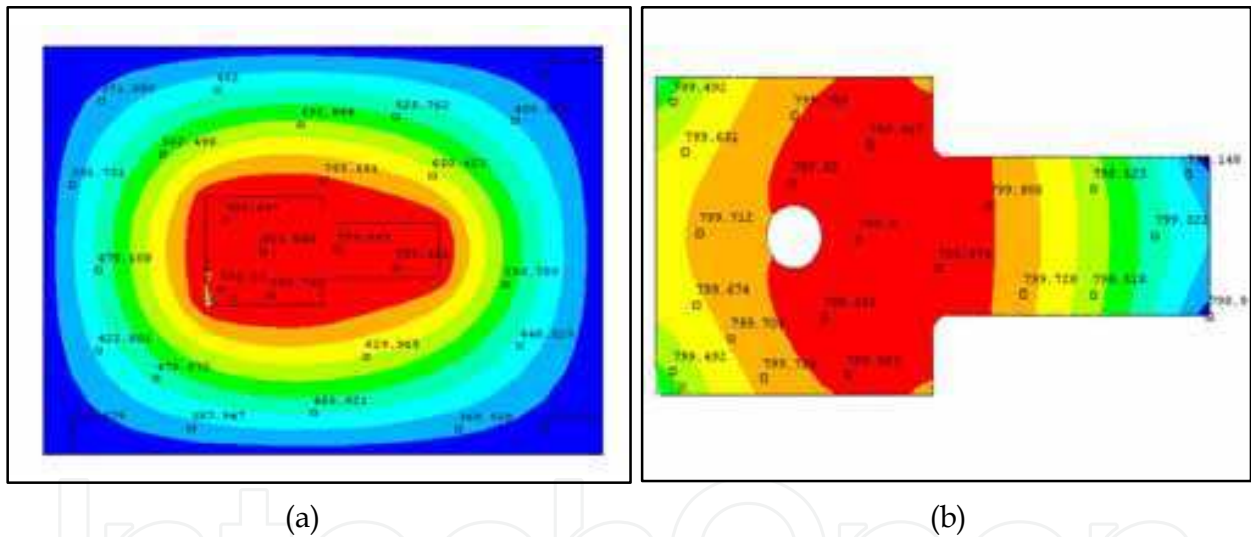


Fig. 3. Temperature distribution in (a) sand mold system, (b) cast metal (line 9 of Table 1)

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 Houzeaux and Codina (Houzeaux & Codina, 2004).

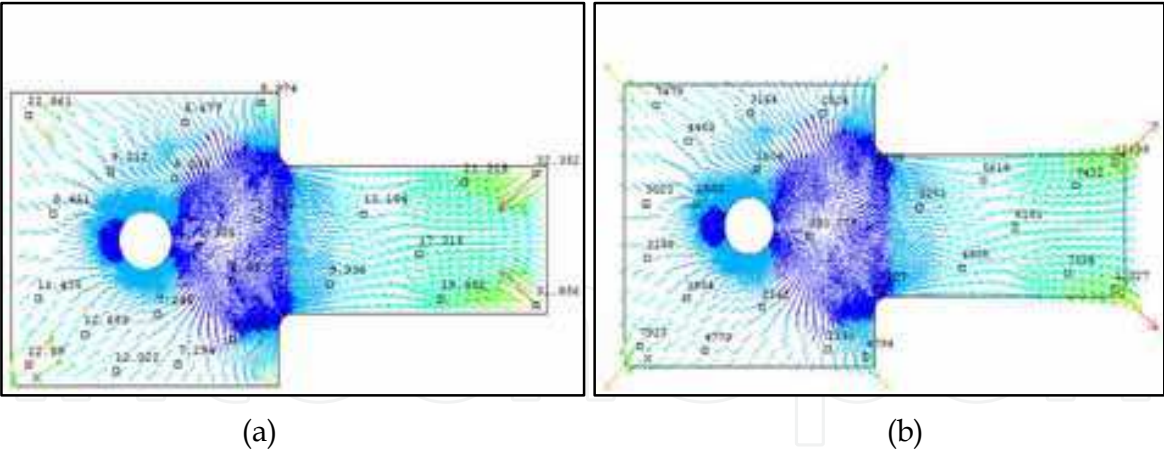


Fig. 4. (a) Thermal gradient (K/m) in vector form and (b) Heat flux (W/m<sup>2</sup>) in vector form (line 9 of Table 1)

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

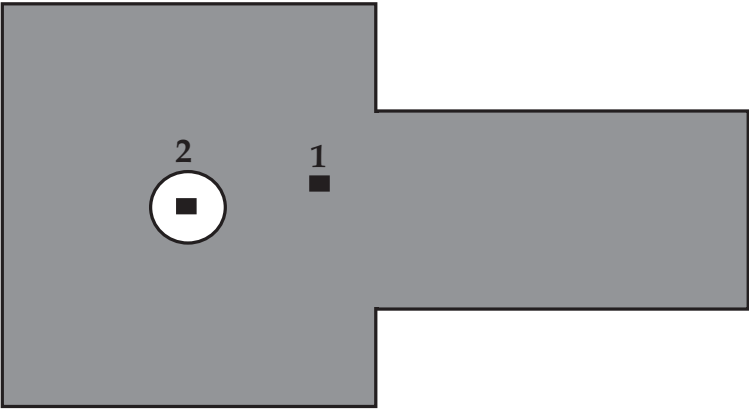


Fig. 5. Reference points for the mold/metal system

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 point (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 other positions in the casting. Chen and Tsai (Chen and Tsai, 1990) 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(b), 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 ( $t_{SL}$ ) are well known in the literature (Rosa et al., 2008). Investigations correlating ultimate tensile strength ( $\sigma_U$ ) and secondary (SDAS) or primary (PDAS) dendrite arm spacings have shown that ( $\sigma_U$ ) increases with decreasing (SDAS) or (PDAS) (Quaresma et al., 2000).

Figure 6 (b) shows a comparison of temperature evolution at point (1) 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 points in the mold.

The significant variables indicated by the Pareto chart (which was obtained after multiple linear regression and analysis of variance) were optimized using a Box-Behnken design, which is a response surface methodology, based on a highly fractionalized three-level factorial design.

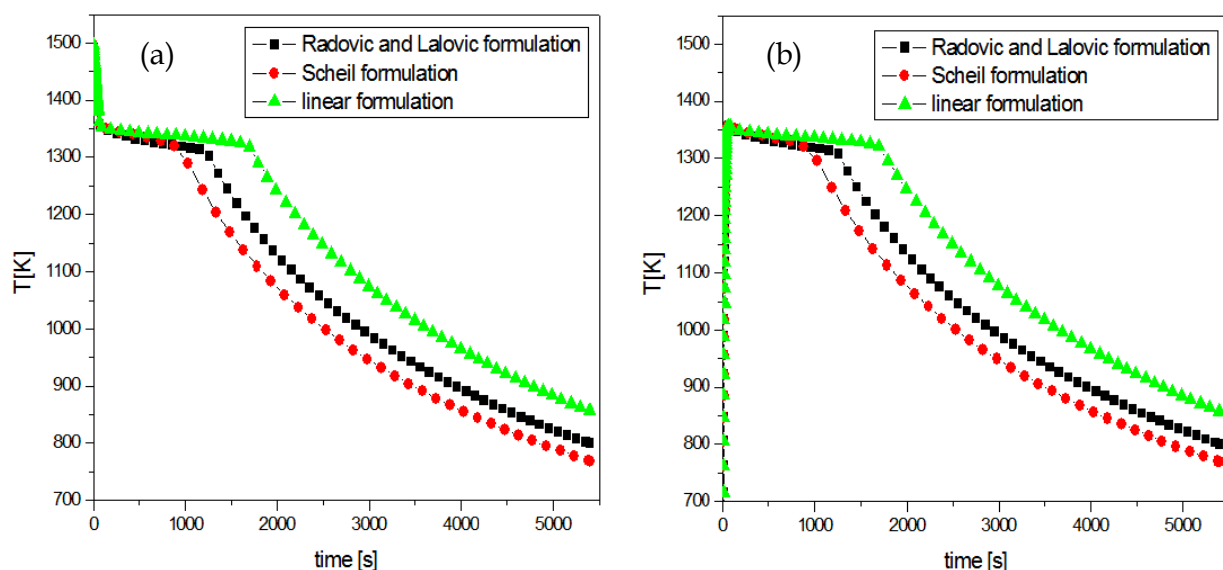


Fig. 6. Thermal profiles for the mold/metal system concerning condition 7, 8 and 9 of Table 1. (a) Inside of the cast – point 1, (b) Inside of the mold – point 2

A three level Box-Behnken design (Aslan, 2007; Paterakis et al., 2002; Montgomery, 1999; Yetilmezsoy et al., 2009) was used to determine the responses of the three variables  $x_1$ ,  $x_2$  and  $x_3$ , based in Table 1. The result of this analysis is shown in the Pareto's diagram of 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 significant influences. 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. To clarify more this analysis, other type of standard graph was accomplished, and it is shown in Figure 8. This

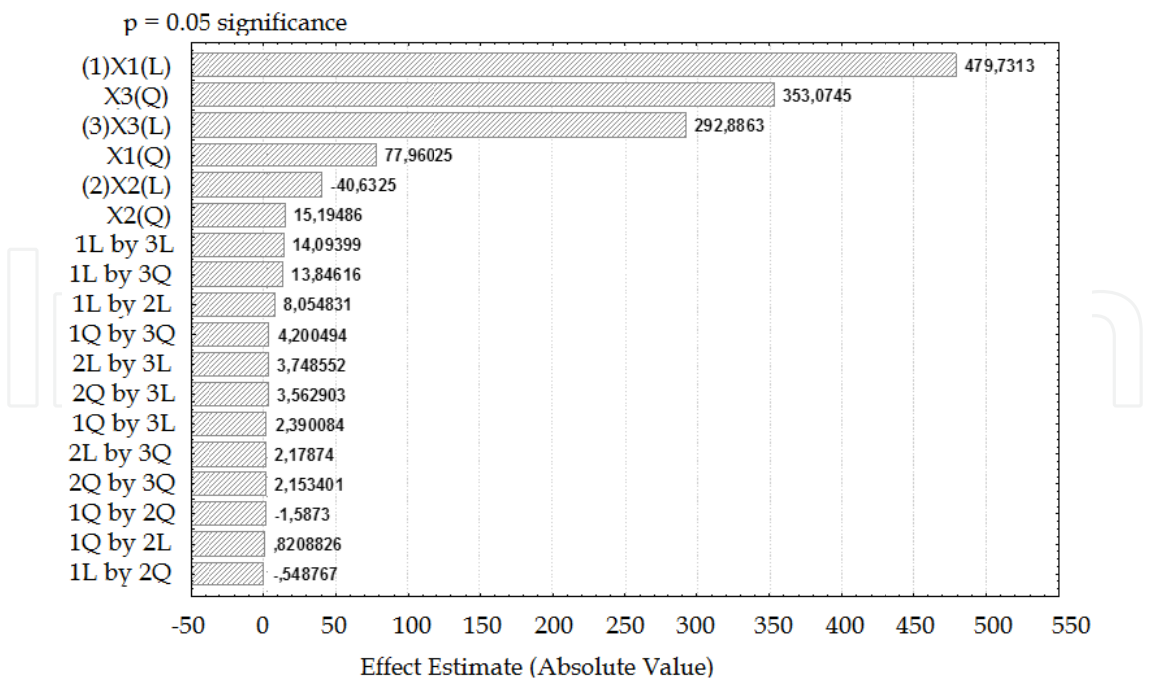


Fig. 7. Pareto chart of standardized effects for the full factorial design

figure of the factorial design was built based on the Student’s probability distribution (t) (Montgomery, 1999). 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 Z the following equation:

$$\begin{aligned} Z = & 802.7889 + 46.4582x_1 - 3.9348x_2 - 28.3638x_3 - 13.0766x_1^2 - 2.5486x_2^2 \\ & + 59.2232x_3^2 + 0.4273x_1x_2 + 0.7476x_1x_3 + 0.1988x_2x_3 \\ & + 1.27212x_1x_3^2 + 0.2196x_1^2x_3 + 0.6686x_1^2x_3^2 + 0.3273x_2^2x_3 \end{aligned} \tag{13}$$

In this equation the linear and quadratic coefficients are most important and the other coefficients are negligible (they are considered as residue). Precisely the most significant coefficients belong to the variables which strongly influence the result, as it can be observed in Figures 7 and 8. Then according to this consideration, equation (13) reduces to the following equation:

$$\begin{aligned} Z = & 802.7889 + 46.4582x_1 - 3.9348x_2 - 28.3638x_3 - 13.0766x_1^2 - 2.5486x_2^2 \\ & + 59.2232x_3^2 + 0.4273x_1x_2 + 0.7476x_1x_3 + 0.1988x_2x_3 \end{aligned} \tag{14}$$

A quadratic equation that correlates the variables and the response was obtained, and the critical points of this equation can be estimated through this mathematical relationship. Then, the derivation of this equation in relation to  $(x_1)$ ,  $(x_2)$  and  $(x_3)$  results in three new equations, being equations 15, 16 and 17:

$$\frac{dZ}{dx_1} = 46.4582 + 26.1532x_1 + 0.4273x_2 + 0.7476x_3$$

(15)

$$\frac{dZ}{dx_2} = -3.9348 + 0.4273x_1 + 5.0972x_2 + 0.1988x_3$$

(16)

$$\frac{dZ}{dx_3} = 28.3638 + 0.7476x_1 + 0.1988x_2 + 118.4464x_3$$

(17)

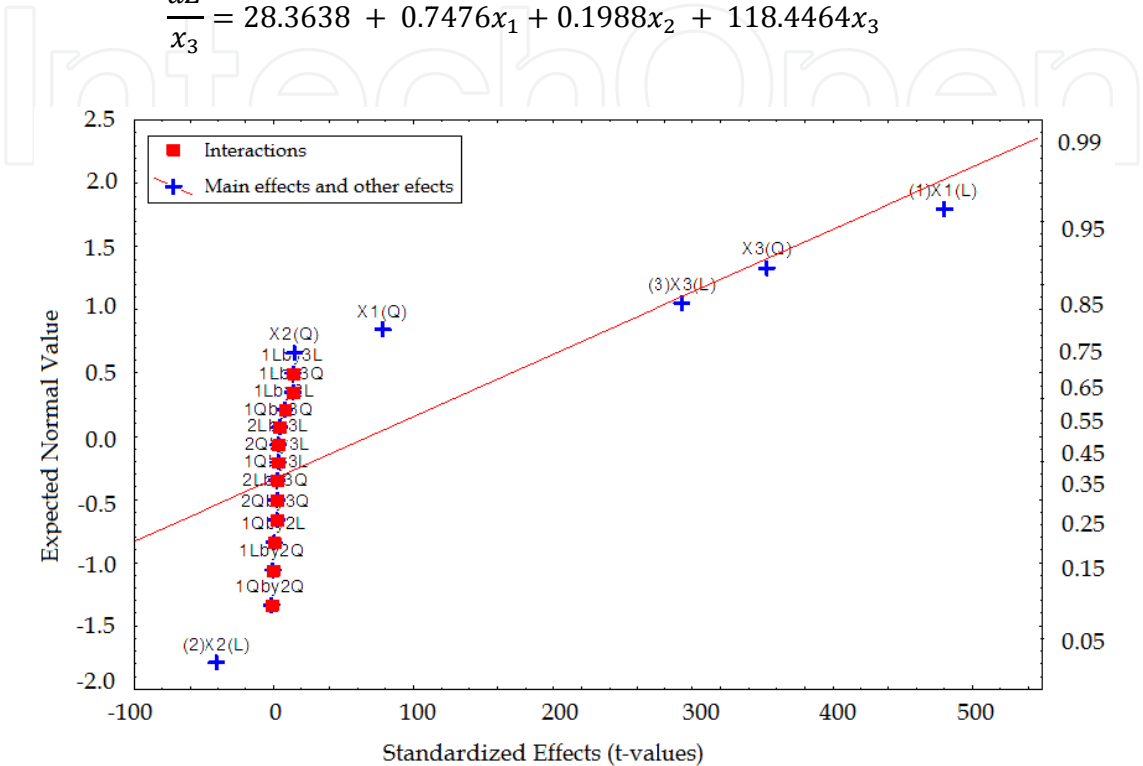


Fig. 8. Curve of standardized effects of the factorial design

The critical point in the surface response are found by solving these equation systems for the condition of  $\frac{dZ}{dx_1} = 0$ ,  $\frac{dZ}{dx_2} = 0$  and  $\frac{dZ}{dx_3} = 0$ . This criterion of solution was based on the recommendations of the authors Martendal et al. (Martendal et al., 2007) and the calculated values for the critical point are:  $x_1=-1.7850$  K,  $x_2= 0.9306$  W/m<sup>2</sup>.K,  $x_3=-0.2298$  mathematical model.

Analyzing this result, we know that the variables  $x_1$ ,  $x_2$  and  $x_3$  must take values -1 or 0 or +1, according to the criteria adopted in factorial design. Because the calculated values should approach to these values adopted, but it can be observed that some solutions of  $x_1$ ,  $x_2$  and  $x_3$  are a bit different of these values adopted, this is possible by simplifying considered in equation (13). Then according to these considerations, the approximations must be in such form, where  $x_1 = -1.7850 \approx -1$  (mold temperature, in environment),  $x_2 = 0.9306 \approx +1$  (latent heat release, 150 W/m<sup>2</sup>.K) and  $x_3 = -0.2298 \approx 0$  (mathematic model, Scheil relationship).

The values of  $x_1 = -1$ ,  $x_2 = +1$  and  $x_3 = 0$  in Table 1 corresponds to the line 8, that means Z - temperature after 1.5h of solidification that is 767.562 K, justly this value corresponds to the minimum temperature of factorial design. This solution proved the validity of the modeling for the optimization process of the casting by factorial design, despite that this prove of the modeling represents a proof trivial. Also this result is to agree with the result obtained by finite elements, see Figure 6.



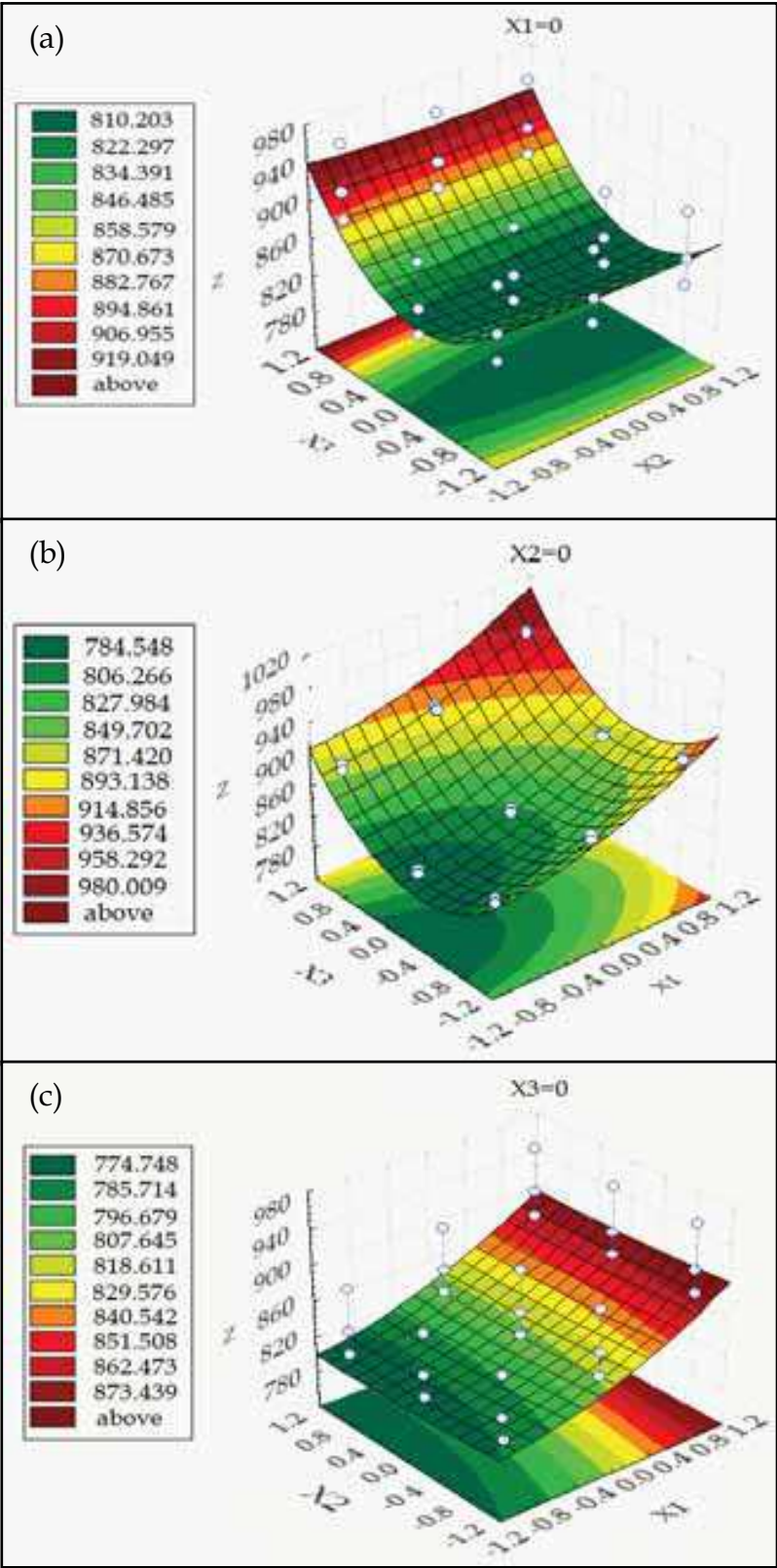


Fig. 9. Response surface plots showing the effect of the (a)  $x_2$  and  $x_3$  factors,  $x_1$  was held at zero level, (b)  $x_1$  e  $x_3$  factors,  $x_2$  was held at zero level and (c)  $x_1$  and  $x_2$  factors,  $x_3$  was held at zero level



While a quantitative analysis of equation (14) was made, will soon be made a qualitative analysis of equation (13) by means of graphic representation of this equation and this discussion will be confronted with factorial design of the solidification process parameters (Table 1) and Figure 8. Figure 9 presents the response surface plots (Aslan, 2007; Paterakis et al., 2002), obtained from equation (13), that describe the influence of the factors on the overall desirability, Figure 9(a) shows the 3D response surface relationship 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 897.176, 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 color band. 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 the same characteristic as previously mentioned.

Figure 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  $Z$  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 of 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. Note that, for a given value of  $x_1$ , as the  $x_3$  increases and the  $Z$  increases reaching the highest value of 953.026, as can be seen in Table 1.

Figure 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 9(b).

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 Figures 7 and 8. Note that, for a given value of  $x_1$ , as the  $x_2$  increases and the  $Z$  increases reaching the highest value of 868.171, as can be seen in Table 1.

Three level Box-Behnken design referred to Table 1 showed as results Pareto's diagram of Figure 7 and curve of standardized effect of the factorial design of Figure 8. According to these results was estimated a mathematic model for  $Z$  (represents the result of the temperature after 1.5 h of solidification) based in equation (9) and through the process of maximizing and minimizing of this model was found the optimal values of  $x_1$ ,  $x_2$  and  $x_3$ . It was also shown the graphical interpretation of equation (13) so qualitatively and this interpretation this related to factorial design of the solidification process parameters (Table 1). Consequently it was shown that three level Box-Behnken is a very powerful tool to optimize and predict results in quantitative and qualitative way. This tool can be used in research, optimization and prediction of industrial processes, saving manpower, material and time in order to improve cost and quality of the product.

This work has done the numerical simulation by finite element method to the copper alloy solidification in sand mold and also this simulation was accompanied with the process of optimization of solidification parameters. This type of study accompanied with the cellular automata or cellular automaton can help minimize the defects generated during solidification. One microstructural feature that can affect the final properties of copper alloy shape castings is microporosity, formed due to the combined effects of volumetric shrinkage upon solidification. Porosity in castings is a defect that results from the interaction of a number of processes: volume change, nucleation and growth of the solid phase, diffusion of dissolved species, and the interaction of interphase surfaces. Although some of these individual processes may be treated analytically, combining the processes into a predictive tool requires the numerical calculation power that has only become available over the last few decades due to the development of digital computers.

#### 4. Conclusion

In this study, a three-level Box-Behnken factorial design in qualitative form and combining with a response surface methodology was employed for modeling and optimizing three operations parameters of the casting process. According to this study, it was observed when the parameters of the solidification process are in the following state, such as, mold temperature in the environment, convection phenomenon in its fullest expression and the latent heat release to the model Sheil shows a minimum temperature after 1.5 h of solidification. Also this result was verified by finite element method. 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. Also this optimization tool can be used in other research areas, optimizing and predicting industrial processes, saving manpower, material and time in order to improve cost and quality of the product.

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The convection and conduction heat transfer, thermal conductivity, and phase transformations are significant issues in a design of wide range of industrial processes and devices. This book includes 18 advanced and revised contributions, and it covers mainly (1) heat convection, (2) heat conduction, and (3) heat transfer analysis. The first section introduces mixed convection studies on inclined channels, double diffusive coupling, and on lid driven trapezoidal cavity, forced natural convection through a roof, convection on non-isothermal jet oscillations, unsteady pulsed flow, and hydromagnetic flow with thermal radiation. The second section covers heat conduction in capillary porous bodies and in structures made of functionally graded materials, integral transforms for heat conduction problems, non-linear radiative-conductive heat transfer, thermal conductivity of gas diffusion layers and multi-component natural systems, thermal behavior of the ink, primer and paint, heating in biothermal systems, and RBF finite difference approach in heat conduction. The third section includes heat transfer analysis of reinforced concrete beam, modeling of heat transfer and phase transformations, boundary conditions-surface heat flux and temperature, simulation of phase change materials, and finite element methods of factorial design. The advanced idea and information described here will be fruitful for the readers to find a sustainable solution in an industrialized society.

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