EVALUATION AND OTIMIZATION OF EQUIPMENTS EMPLOYING NATURAL GAS OR LIQUID FUEL[1]

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Abstract

The choice of the type of fuel used as energy source for the aluminum melting can be of extreme importance for a better performance as well as for a greater preservation of the equipments. The option of a liquid or gaseous fuel can significantly alter the combustion aspects inside the furnace, such as the shape of the flame and the distribution of temperature and heat flux. In the present work, numerical simulations were carried out using the commercial package FLUENT, analyzing different cases with two types of fuel: a spray of liquid pentane and a natural gas jet, both reacting with pure oxygen. The results showed the possible damages caused by the process if long or too intense and concentrated flames are present, increasing very much the wall temperatures and compromising the heat flux on the aluminum surface.

Keywords: liquid fuel, natural gas, combustion, industrial furnaces

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1. Introduction

In order to evaluate the flow and heat transfer inside industrial equipment like furnaces or incinerators, and to perform a design optimization, the numerical simulation of the combustion process may prove to be a good alternative. Due to the complexity of the problem and great number of variables involved, a reliable analysis can only be possible with powerful software. The abundance of natural gas and the political need for developing a market in Brazil for this fuel, which can also very well meet the growing environmental restrictions, can motivate the substitution of fuel oil. It is, however, of fundamental importance to know if the operating characteristics of the equipments are maintained or even improved.

There are several works in the literature dedicated to the numerical investigation of combustion processes with different models. The Eddy Dissipation Concept (EDC) and the Probability Density Function (PDF) models were studied in the works of Gran and Magnussen (1996), Gran et al. (1997), Ma et al. (1999), and Magel et al. (1996). Desjardin and Frankel (1996) presented a numerical simulation using the Linear Eddy Model, and compared it with the results of two other models: (1) the Stationary Laminar Flamelet Model, and (2) the Conditional Moment Closure Method. Gomes et al. (1997) compared numerical results carried out with the generalized finite rate method with experimental data, obtaining a good qualitative agreement. Goldin and Menon (1998) showed a comparison between various PDF turbulent combustion models in non-premixed turbulent jet flames. They investigated the performance of a conventional PDF model against a proposed model, in which the solution of the chemical kinetics was decoupled from the solution of the momentum equation. Eaton et al. (1999) provided an overview of the combustion modeling technology applied to fossil-fuel combustion, and showed some comparisons between numerical results and experimental data. Nieckele et al (1998, 1999, 2004) analyzed the flow field inside aluminum furnaces with different types of burners and operating conditions. Brewster et al (2001) investigated numerically and experimentally an industrial aluminum melting furnace with oxygen enriched combustion. The model over estimated the turbulent mixing and, on the other hand, the CO (carbon monoxide) concentrations were under estimated near the burner region, probably because the kinetic effects were neglected. Mukhopadhyay et al (2001) showed that the flame height grows with the fuel velocity for a given air-fuel ratio, and with the reduction of the air velocity, for a given fuel velocity. Nieckele et al (2002) simulated a turbulent natural gas flame in a cilindrical furnace, using finite rate models. The results showed a good agreement with the experimental data found in the literature.

With respect to the numerical modeling of the spray flow of liquid fuels, Jones et al (2000) proposed a stochastic modeling for the turbulent dispersion of the spray droplets. Reveillon et al (2000) modeled numerically the vaporization of liquid fuel sprays in a turbulent non-premixed flame, proposing a single model that predicted the source terms for the mean mixture fraction and its variance. Demoulin et al (2002) investigated numerically the turbulent combustion of a liquid fuel spray, and utilizing probability density functions for each fluctuating variable in the liquid and gas phases, showed that a correct description of the temperature fluctuations caused by the presence of the droplets in the flow field is crucial for a better estimation of the reaction rates.

The purpose of the present work is the comparison of the combustion process inside an aluminum melting furnace, using two different types of fuel with similar heating power: natural gas and liquid pentane.

The turbulent flow and heat transfer analyses were carried out using the commercial software FLUENT, V6.1. The governing conservation equations for mass, momentum, energy and n-1 species were solved via a finite volume formulation. To simulate the combustion process the generalized finite rate model was employed, with a combined Arrhenius-Magnussen reaction rate expression. High temperatures due to the combustion reactions require the modeling of a radiation source term for the energy equation. For the turbulence phenomena, the two differential equation $\kappa-\varepsilon$ model was chosen. An additional model is necessary to describe the coupling between the continuous and discrete phases (pentane droplets) of the liquid fuel.

2. Problem set-up

The geometry corresponds to that of a simplified furnace, which was represented as a rectangular prism of 4.0m length, 1.5m wide and 2.0m height. A schematic diagram of the geometry with the coordinate system is presented in Fig. 1, while Fig. 2 illustrates details of the frontal plane, and different view of the inlet configuration.

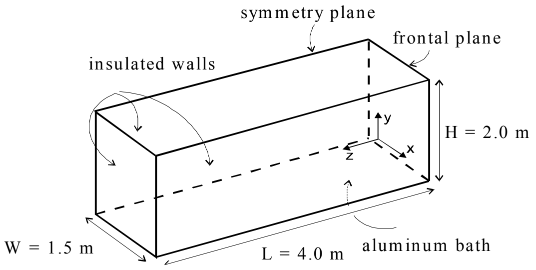


Figure 1– Schematic of the furnace

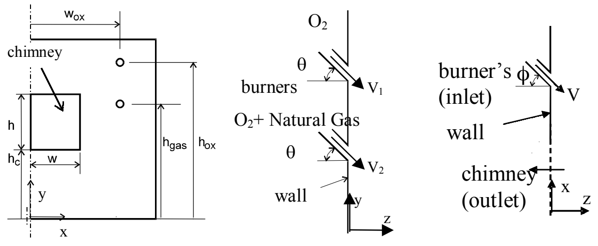


Figure 2– Injection and chimney geometry

The lower limit of the furnace was considered to be the liquid aluminum surface with a small aluminum oxide layer of 5 mm above it. The aluminum oxide layer was considered to describe the oxidization of the aluminum surface by the water that results from the combustion, which can act as an isolator and can compromise the quality of the product.

The vertical symmetry plane passes through the center of the chimney between the two pairs of oxygen and fuel injectors. The inlets of oxygen and fuel as well as the outlet of the combustion products are located at the same wall (Fig. 2). The center of the burner is located 0.65m above the aluminum oxide layer and 0.80m away from the symmetry plane, with an internal diameter of 0.0192m (fuel injection) and external radius of 0.0096m (oxygen injection through the annular gap, surrounding the fuel jet). The oxygen injector is located 0.20m above the burner, with the same dimensions. So that the jets are directed away from the refractory walls, angles of 15° in the vertical plane and 10° in the horizontal plane were set. The height of the center of the rectangular chimney coincides with that for center of the burner, its half width measures 0.50m and its height measures 0.60m.

The furnace has a nominal thermal power of 1.25 MW per burner (2.5 MW total). Considering a typical aluminum load of 16 tons (which corresponds to a volume of $6m^3$ and a latent heat of 397.4 kJ/kg) and an approximate process time of 1 hour, a negative heat sink of 1.77 MW (71% of the total) was prescribed, in order to represent both the energy necessary to melt the entire load of aluminum and the possible heat losses inherent in the process.

Two cases were analyzed (half furnace, due to the geometry symmetry), concerning the gas and liquid fuels: the first one with a 1.25 MW natural gas (h_{ci} = 44800 kJ/kg) flame, and the second one with a 1.25 MW pentane (h_{ci} = 38345 kJ/kg) flame. The mass flow rates were, therefore, for the gas and liquid fuel, 3.47×10^{-2} kg/s and 2.97×10^{-2} kg/s. Considering the specific mass of the pentane and natural gas as 620 kg/m^3 and 0.795 kg/m^3 (at 1 atm and 25 C) respectively, and an inlet cross section of 2.89 × 10^{-8} m^2 (central orifice), the magnitude of the inlet fuel velocities were 159 m/s and 0.175 m/s,. The oxygen-fuel ratio was stoichiometrically defined for both cases. The total oxygen mass flow rate was equally divided into each inlet. Considering its specific mass of 1.3 kg/m^3 and the natural gas composition, oxygen was injected at 260 Nm^3/h for the first case, and for the pentane case at 0.106 kg/s.

The composition considered for the natural gas, the molecular weight of the species, M_i, the formation enthalpy h_i^o (reference temperature of 298 K) and the specific heat cp_i are presented in the table below (Van Wylen, 1976, and Kuo, 1986):

Table 1 – Natural gas properties

Species	**% m_i**	**M_i**	**h_i^o [kJ/kg]**	**cp_i [J/(kg K)]**
CH_4	70.3	16	-74 895	2 222
C_2H_6	17.8	30	-83 863	1 731
C_3H_8	0.69	44	-103 860	1 549
CO	0.00	28	-110 530	1 043
CO_2	6.93	44	-39 353	840
N_2	4.28	28	0.0	1 041
H_2O	0.00	18	-241 830	2 014
O_2	0.00	32	0.0	919

The following thermophysical properties were considered. The absolute viscosity and thermal conductivity were set equal to μ= 1.72 × 10^{-5} Pa s. and k= 0.0241 W/(m K). The diffusion coefficient of all species in the mixture was equal to the N_2 diffusion coefficient, 2.88 × 10^{-5} m^2/s. The species' specific heat at constant pressure were obtained as a function of temperature, and the mixture specific heat was obtained by a weighted mass fraction average.

To model the pentane spray concerning the liquid fuel problem, 15 inlet points were uniformly distributed into the fuel inlet region. The droplets flow is defined from initial conditions related to the injection points of the discrete phase in the gaseous mixture. These conditions will be used as the start point for the integration of the droplets equation of motion and calculation of their trajectories. Since the surface combustion of the particle is not being modeled, the droplets must vaporize to react with the gaseous phase. Therefore, the inlet temperature of the droplets influences the point where the combustion reaction will start. The vaporization temperature was defined as the same temperature at which the droplets enter the domain (303 K), indicating that vaporization starts immediately after they are inside the furnace, that is, no inert heating occurs. Unless the particle temperature has reached the boiling point, the vaporization is controlled by the fuel vapor pressure (defined as 8.2 × 10^4 Pa) and by the droplets diffusion coefficient (6.1 × 10^{-6} m^2/s). If the boiling temperature is reached, the boiling rate equation (eq. (23)) is used to predict the convective boiling of a discrete phase droplet. In that case, the rate of phase change of the liquid fuel is extremely dependent on its latent heat (3.63 × 10^5 J/kg).

2. Model description

For simulating the turbulent flow within the furnace, the time average forms of the continuity and linear momentum equations were solved via the finite volume technique, with the commercial code FLUENT, version 6.1. The Boussinesq's hypothesis was adopted, leading to an effective viscosity $\mu_{ef} = \mu + \mu_t$, where μ and μ_t are the absolute viscosity and turbulent viscosity, respectively. The turbulent viscosity

μ_t was obtained by the $\kappa-\varepsilon$ turbulence model, which has been extensively employed along the years in the simulation of turbulent flow.

The continuity, momentum and energy equations were solved simultaneously with the equations of turbulence model equations, providing the solution for the turbulent flow problem. The density of the gaseous mixture was calculated using the ideal gas law, $\rho = p_{op} / [R.T\ \Sigma_i\ (m_i/M_i)]$, where p_{op}=1 atm is the average operation pressure inside the furnace, T is the temperature, m_i and M_i are the mass fraction and molecular weight of the species, and R is the universal gas constant..

For all dependent variables, wall functions were employed for setting up the conditions close to the solid boundaries, following the procedure described in Patankar and Spalding (1967) and in Launder and Spalding (1974).

Due to the high temperatures found inside the furnace, it is necessary to account for the radiation heat transfer, and the Discrete Transfer Radiation Model (DTRM) was selected. In this model, the change in the radiant intensity is integrated over all wavelengths, along a path *S* (Siegel and Howell, 1981). The radiant intensity is obtained by the integration along several directions starting from each control volume on the domain surfaces. The source for enthalpy due to radiation heat transfer is calculated locally by summing the changes in intensity for all the rays crossing the control volume. The Weighted Sum of Gray Gases Model (WSGGM) was used for the calculation of the absorption coefficient, (Fluent User's Guide, 1995; Smith *et al*., 1982).

To model the combustion process, the generalized finite rate model with three different reaction rates was employed. In this model, the chemical species distributions are determined through the solution of their transport conservation equations. The gas phase transport was calculated solving a set of *n-1* conservation equations for chemical species, where *n* represents the number of species. The rates in the combustion reactions were calculated by using three models: the Arrhenius model, the Magnussen model and the combined Arrhenius-Magnussen model (Fluent, 1995).

The prediction of the trajectory of a discrete phase droplet is performed by integrating the force balance on the droplet, which is written in a Lagrangian reference frame. As the trajectory of a particle is computed, the droplet stream variation of heat, momentum and mass are incorporated in the subsequent continuous phase calculations. By doing so, the interphase exchange is alternately computed, considering the droplets trajectories and the conservation equation for the gaseous mixture, until the solutions in both phases stop to change.

There are basically two mechanisms that control the droplets evaporation, depending on its temperature level, T_p. If the temperature is higher then T_{bp} (boiling point) the boiling process is convective, and no longer controlled by the diffusion of molecules on the droplets surface to the continuous phase and the fuel vapor pressure. The coupling between the discrete and continuous phases appears as source terms in the momentum, energy and mass equations for the continuous phase. The drag force acting on the droplet in axial direction depends on the mass flow rate of the droplet. The mass transfer to the continuous phase is calculated by examining the mass change of the droplet as it passes through each control volume:

Two cases were considered. Natural case was employed as fuel for the first case, while for the second case, the simulation was carried on with pentane as the liquid fuel. A five step mechanism was selected for case 1, and a simple mechanism of one step was implemented for case 2, as shown in Table 2.

The stoichiometric coefficients for each reaction must be specified in accordance to equations in Table 2. The Magnussen reaction rate expression does not require any additional information. The parameters for Arrhenius and Arrhenius-Magnussen models are shown in Tables 3 and 4, where β_k was set as zero for all reactions.

Table 2 – Reactions

Case 1 – Natural Gas	**Case 2 – Liquid Fuel**
$CH_4 + 3/2\ O_2 \rightarrow CO + 2\ H_2O$	$C_5H_{12} + 8\ O_2 \rightarrow 5\ CO_2 + 6\ H_2O$
$CO + 1/2\ O_2 \rightarrow CO_2$	
$C_2H_6 + 5/2\ O_2 \rightarrow 2\ CO + 3\ H_2O$	
$C_3H_8 + 7/2\ O_2 \rightarrow 3\ CO + 4\ H_2O$	

Table 3 – Arrhenius reaction rate parameters – Case 1

Reaction	A_k (m^3/s)/kmol	E_k J/kmol	γ_{CH4}	γ_{C2H6}	γ_{C3H8}	γ_{O2}	γ_{CO2}	γ_{CO}	γ_{H2O}
1	5.01×10^{11}	2.00×10^8	0.7	-	-	0.8	-	0	0
2	6.19×10^9	1.26×10^8	-	0.1	-	1.65	0	-	0
3	5.62×10^9	1.26×10^8	-	-	0.1	1.65	-	0	0
4	2.24×10^{12}	1.70×10^8	-	-	-	0.25	0	-	-

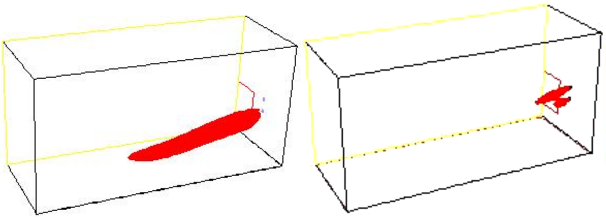
Table 4 – Arrhenius reaction rate parameters – Case 2

Reaction	A_k(m^3/s)/kmol	E_k J/kmol	β_k	γ_{C2H5}	γ_{O2}	γ_{CO2}	γ_{H2O}
31	3.60×10^9	1.26×10^8	0	0.25	1.5	0	0

3. Results

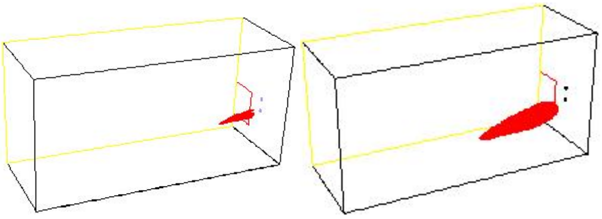
The flow field inside the furnace was numerically obtained with FLUENT for the two types of fuel. The solution was considered converged when the sum of the normalised residuals of all equations was less than 10^{-4} and the normalised enthalpy residual was less than 10^{-6}. After a mesh test, an approximately uniform mesh of 371250 (55×82×90) control volumes was generated with the FLUENT auxiliary tool GAMBIT (Fluent, 2002).

Figures 3 and 4 present isosurfaces of temperature both fuel. Figure 3 corresponds to T= 2000K, while at Fig. 4, T=3000 K. Both flames follow the direction of the inlet jets, away from the refractory walls and downward into the load's surface. At Fig. 3a, a long isosurface can be seen for Case 1, while a very small isosurface of T=3000K can be seen in Fig. 4a. For Case 1, the combustion starts near the entrance, where very high values are then obtained, and rapidly the temperature level drops to 2000K. For Case 1, the temperature level inside the furnace is approximately 1500K. The same behavior is not seen for the pentane. At Fig. 3b, two small isosurface equal to T=2000 K can be seen near the burner. At Fig. 4b, a larger region around them, corresponding to a warmer isosurface, T=3000K, can be seen. The pentane flame appears to be displaced from the inlet, which can be explained by the fact that the droplets must first vaporize and to be absorbed by the gaseous



(a) natural gas (b) pentane

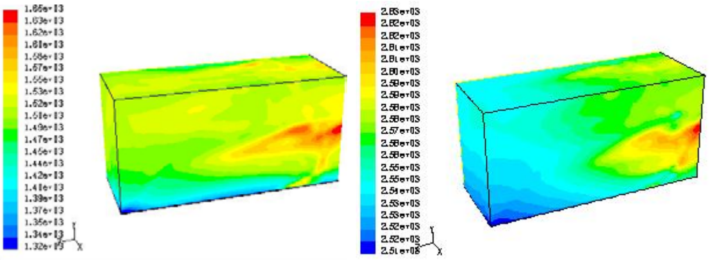
Figure 3– Isosurfaces: T=2000K



(a) natural gas (b) pentane

Figure 4– Isosurfaces: T=3000K

mixture to react with the oxygen. For Case 2, the temperature level inside the furnace is much higher, approximately 2500K.



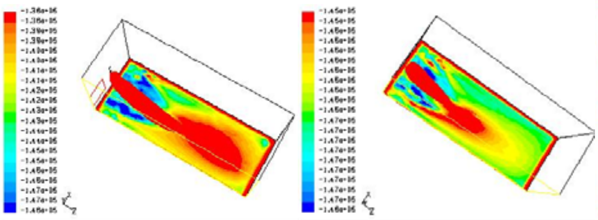
(a) natural gas (b) pentane

Figure 5 – Temperature at the refractory walls.

The purpose of the comparison is to show different shapes of the flame associated to different types of fuel and its combustion aspects. While the gas flame extends itself through the furnace, the pentane flame is more intense and concentrated in the first third of the domain. That leads to a less uniform temperature distribution on the refractory walls (shown in Fig. 5) and could also compromise the uniformity of the heat flux on the aluminum surface. At Figure 5, the influence of the flame at the refractory wall is clearly seen in both cases, by the warm spots at the side wall. These warm spots can damage the refractory wall, increasing the cost of the project. Although qualitatively the temperature distribution is similar for both cases, the temperature level inside the furnace is much higher with the pentane than with natural gas, as already mentioned.

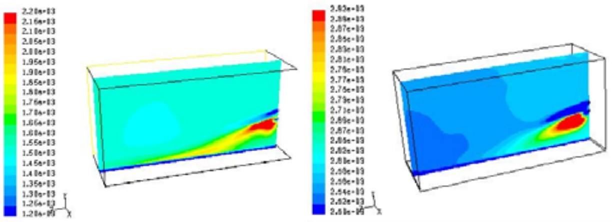
The radiation heat flux on the aluminum surface is presented at Fig. 6. At this figure the isosurface representing the flame is also shown. Due to the high temperature flame, the radiation heat flux is dominant. It can be seen large values of the radiation heat flux under the flame for both cases. Since the pentane flame was much more concentrated, a less uniform heat flux was obtained in this case.

Figure 7 shows the temperature distribution on a plane that passes through the injectors (x = 0.80m). In both cases, it can be seen the cold oxygen jet over the pentane spray and natural gas jet, close to the inlet region. Due to the combustion, a substantial temperature raise can be observed in both cases. The high temperature region can be interpreted as the flame region. Thus, it can be seen, that the flame region is closer to the entrance for the natural gas case than it is for the pentane case. It is also observed that the temperature level inside the furnace is higher for the liquid fuel than for the natural gas combustion.



(a) natural gas (b) pentane

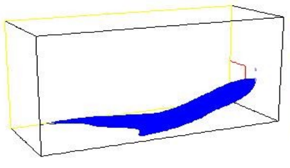
Figure 6– Radiation heat flux



(a) natural gas (b) pentane

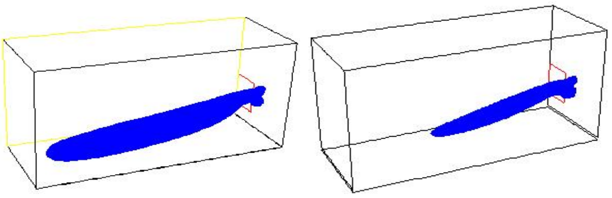
Figure 7 – Temperature. Plane y-z (x=0.8 m)

The methane (CH_4) is the most abundant component in the natural gas, representing 70% of its mass composition. Therefore, the analysis of this species gives a good idea of how the fuel is consumed inside the furnace. Comparison of the results for the pentane and methane are shown in Fig. 8. Figure 9 illustrates the isosurfaces of 3% of oxygen for both cases. Analyzing these figures, it is observed that the concentration surfaces of fuels and oxygen shows the same pattern observed for the temperature. These isosurfaces also give a good idea of how the flame distributes itself along the furnace. The flame region is understood to be the region where the highest consumption of fuel occurs, followed by a great heat



(a) natural gas (b) pentane

Figure 8 – Isosurfaces of 1% fuel

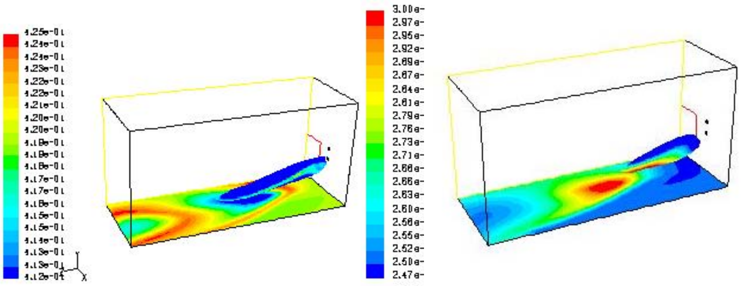


(a) natural gas (b) pentane

Figure 9 – Isosurfaces of 3% oxygen

release and temperature raise. Once again, it can be concluded that the combustion of pentane occurs faster, closer to the entrance.

Figure 10 shows the water distribution over the aluminum surface. High water concentration is not desirable because an aluminum oxide layer can be formed as water reacts with the surface of the load, which increases the thermal resistance and compromises the quality of the product. It is interesting to observe that the highest water concentration is under the flame for the pentane, but at the same region for the natural, one can find the lowest values. Note however, that the water distribution is almost uniform in both cases, with slightly higher value for the natural gas.



a) natural gas (b) pentane

Figure 10 – Water distribution over aluminum surface.

4. Conclusion

The numerical simulation of the process inside an aluminum melting furnace proved to be a helpful tool, which can contribute to improve several aspects of industrial interest, for example, reduction of material costs on maintenance of the refractory walls, increase of the efficiency of the fusion process, assurance of the quality of the product by the investigation of the deposition of water on the aluminum surface, better positioning of the burner and oxygen injectors, etc.

The numerical simulation also allows the easy investigation of the influence of several variables on the process; however, the mathematical models that will be used must be carefully chosen to maximize reliability on the results, not bringing unreal physical situations representing the phenomena.

The choice of the type of fuel used as energy source for the aluminum fusion can be crucial to achieve better efficiency on the process. In this way, the option for a liquid or gaseous fuel can significantly alter the combustion aspects inside the furnace, such as the formation of too long or too intense flames, leading to hot spots on the refractory walls and a non uniform heat flux distribution on the aluminum load.

The present analysis showed that it is possible to substitute the liquid fuel by natural gas. Although a longer flame was obtained for the natural, lower temperature level at the refractory walls is a positive factor for the substitution, as well as a more uniform heat flux at the aluminum surface.

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AVALIAÇÃO E OTIMIZAÇÃO DE EQUIPAMENTOS EMPREGANDO GÁS NATURAL OU COMBUSTÍVEL LÍQUIDO[1]

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Resumo

A escolha do tipo de combustível a ser usado como fonte de energia para a fusão de alumínio pode ser de extrema importância para o melhor desempenho, assim como maior preservação dos equipamentos. A opção entre combustível líquido ou gasoso pode alterar significativamente aspectos da combustão no interior do forno, como o formato da chama, distribuição de temperatura e fluxo de calor. No presente trabalho, simulações numéricas utilizando o software comercial FLUENT foram realizadas para analisar diferentes casos com dois tipos de combustível: pentano líquido pulverizado e um jato de gás natural, ambos reagindo com oxigênio puro. Os resultados mostraram os possíveis danos causados ao processo, se chamas longas ou muito intensas estiverem presentes, aumentando muitas as temperatures nas paredes e compromentendo o fluxo de calor na superfície do alumínio.

Palavras chave: combustível líquido, gás natural, fornos industriais.