NUMERICAL SIMULATION OF A CERAMIC KILN USED IN FRITS PRODUCTION

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Abstract. The present paper describes a methodology of study and modeling the thermal energy transport in ceramic frits melting kilns with oxy-firing combustion process through the development of a numerical simulation in Fortran language coupled with a simulation in a CFD software. The domain of analysis consists of a rectangular refractory kiln, working in a mean inside temperature of 1400 °C. The aim of this work is to generate technical subsidies in order to reduce energy consumption in this particular kind of kiln, without a production reduction. The thermal problem is composed by three distinct forms of heat transfer: diffusion, advection and radiation. The numerical procedure is based on the method of finite volumes. The entire numerical domain is modeled using a Fortran language algorithm. In the radiation analysis, the Gebhart method of radiosity was applied to the radiation heat transfer inside the kiln. The cited algorithm is used in association with commercial CFD software, necessary to solve the field of fluid flow inside the kiln. In such a case the k- ε model of turbulence was selected. Numerical predictions from the model can be used in order to find a more adequate configuration to the kiln, specially the kiln camera where the raw material is processed.

Keywords: Numerical Simulation, Thermal analysis, Ceramic kiln, Ceramic Frits.

1. INTRODUCTION

In ceramic industry most of kilns work in a high temperature level, required to burn the raw ceramic material. Inside the field of ceramic, frits kilns are responsible for the melting process of the refractory material of frits that serves as a main component for coating diverse types of ceramics. These kilns operate with internal temperature around 1, 400 °C and a predominantly turbulent flow. For the past decades, the Brazilian ceramic industry has been replacing oil for natural gas as fuel for combustion kilns, with no further adjustments with respect to the furnace, reducing its energetic efficiency. There are several recent works in the literature dedicated to energetic analysis of different combustion kilns. Kawaguti *et al.* (2004) conducted a numerical analysis of an intermittent furnace in CFD, achieving satisfactory results for flow velocity field. An experimental and numerical analysis of a tunnel kiln was presented in Nicolau *et al.* (2002), by mean of a FORTRAN code, developed with basis in finite volumes method, with good agreement between numerical and experimental results. In Nieckele *et al.* (2005), a numerical modeling of a industrial aluminum melting furnace was performed with the commercial software FLUENT, presenting results with regard of oil and gas combustion.

Many studies with commercial CFD software assistance, however, are limited to the analysis of kiln internal processes, idealizing its structure as insulated and excluding it from further analysis. A more complete numerical modeling is presented in this work, including an internal numerical modeling plus a numerical modeling of the structure in order to provide data to predict the impact of the process in the whole kiln. This is accomplished through the modeling of a real frits kiln, with a 100% oxy-firing natural gas combustion, separated into two parts and solved in two different environments: a FORTRAN code based on the finite volume method and the commercial CFD software Ansys CFX. The numerical modeling of the two simulation's components and the coupling are presented and discussed.

The internal flow in the kiln cavity is solved by Ansys CFX, giving as results the velocity field of the combustion products, thermodynamic properties of the same flow and wall heat transfer coefficients. These results are then inserted in a FORTRAN code, which uses these results to solve the heat transfer in the kiln's structure, the external heat transfer and the phase change of the frits mass.

2. NOMENCLATURE TABLE

Symbol	Description	Symbol	Description			
V	velocity vector	μ_{t}	turbulent viscosity			
ρ	density	k	turbulence kinetics energy			
$\frac{\partial p}{\partial x_i}$	specific force due to the pressure acting in the system boundaries	ε	turbulent dissipation			
C_p	specific heat at constant pressure	C_{μ}	$k - \boldsymbol{\mathcal{E}}$ turbulence model constant			
β	coefficient of thermal expansion	Da	Damkohler number			
k_c	thermal conductibility	l	turbulence characteristic length			
Т	temperature	U_L	flame's laminar velocity of propagation			
q"	rate of internal heat generation	δ_{L}	front flame thickness			
μ	absolute viscosity	$k_{bimolec}$	bimolecular reaction rate coefficient			
Φ	viscous dissipation function	A_p	pre-exponential factor			
C_i	specie concentration	b	exponential factor from Arrhenius			
\boldsymbol{j}_i	diffusion flux	Ε	activation energy			
<i>m</i> ''' _i	volumetric rate of constituent i generation	R	universal gas constant			
σ_{k}	turbulence model constant for the k equation	q_{rv}	spectral radiative heat flux			
$\sigma_{_{\! arepsilon}}$	$k-oldsymbol{arepsilon}$ turbulence model constant	K _{av}	absorption coefficient			
P_k	shear production of turbulence	K _{sv}	scattering coefficient			
C_{ε^1}	$k-oldsymbol{arepsilon}$ turbulence model constant	Α	linear anisotropy coefficient			
C_{ε^2}	$k-oldsymbol{arepsilon}$ turbulence model constant	G_{v}	spectral incident radiation			
$\mu_{\scriptscriptstyle e\!f\!f}$	effective viscosity					

Table 01 – Nomenclature table for equations (1) - (12).

3. PROBLEM SET UP

The kiln's solid structure consists of refractory material. Its geometry was idealized in this work, as rectangular shaped and main dimensions of 2.7 m wide, 1.95 m high and 4.55 m long. All walls have a constant thickness of 0.45 m. Raw mass of frits is pushed, in steady regime, into the kiln's internal cavity by an endless screw through the back of the kiln. That frit's mass accumulates in the back plane of the cavity and flows to the bottom plane as it melts. It flows through the bottom plane till the front plane, where exits the kiln by an opening situated below the burner. This process is continuous, with a frit's mass flow out of the internal cavity. Figure 1 illustrates the kiln geometry, while Fig. 2 identifies the cited planes.



Figure 1. Kiln geometry.

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The internal geometry of the kiln is approximated to rectangular shape with a frontal burner and a lateral chimney exit. Its main dimensions are 1.8 m wide, 1.05 high and 3.65 m long. Raw frit's mass melts inside the cavity and flows out of the kiln in a steady regime. The combustion is 100% oxy-firing natural gas. The idealized geometry of the cavity is shown in Fig. 2.



Figure 2. Cavity geometry.

The burner was simplified as two round openings, positioned at the center line of the front plane of the cavity. They are distanced by 145 mm of height. In the top opening, fuel is admitted with a part of the pure oxygen. In the bottom entry is injected the remaining pure oxygen. The opening's diameters are 30 and 60 mm for the top and bottom opening respectively. The bottom opening center is located at 610 mm from the bottom plane, while the top opening is at 755 mm from the same. The combustion products outlet is rectangular with dimensions of 100 x 150 mm, and is located in the cavity's left plane.

The bottom and the back plane of the cavity are modeled as the frit's bath. An energy sink is prescribed in both of them to simulate the sensible and latent heat of the bath.

The modeled domain in the commercial software Ansys CFX is the kiln's internal cavity, i. e., the problem's fluid domain. Within this domain is solved the combustion of natural gas, the combustion products flow with turbulence and internal media radiation.

The independent FORTRAN code models the solid domains given by the kiln's structure and the internal frit's mass. The coupling between the two models treats the solid-fluid interface inside de kiln.

4. CFX MODEL DESCRIPTION

4.1. Conservation equations

The physical phenomenon is governed by the conservation equations of mass, linear momentum, energy and chemical species.

The following hypotheses were admitted: all fluids were assumed Newtonian, mixture properties were considered to depend on the properties of each species weight by its mass fraction, dynamic viscosity, thermal conductivity and molecular diffusion coefficient were considered only temperature dependent and density of the mixture followed ideal gas law.

The general formulation of the conservation equations is presented in Eq. (1) to (4).

$$\frac{\partial \rho}{\partial t} + div(\rho \mathbf{V}) = 0$$

$$\frac{\partial(\rho \cdot \mathbf{V})}{\partial t} + \nabla \bullet \Big[\rho \cdot \mathbf{V} \otimes \mathbf{V} - \mu \Big(\nabla \mathbf{V} + \nabla \mathbf{V}^{\mathrm{T}} \Big) \Big] = \frac{\partial p}{\partial x_{i}} + S_{M}$$
(2)

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$$\rho c_{p} \frac{DT}{Dt} = \nabla \bullet (k_{c} \nabla T) + q'' + \beta T \frac{DP}{Dt} + \mu \Phi$$
(3)

$$\frac{DC_i}{Dt} = -\nabla \bullet \boldsymbol{j}_i + m^{"'}_i \tag{4}$$

The global model is separated in two parts: commercial CFD model and FORTRAN code model. Both are briefly described as it follows.

4.2. Cavity model

The software Ansys CFX is based on the finite volume method. This model's objective is to solve the combustion gases flow inside the kiln.

4.2.1. Advection and turbulence model

The High Resolution scheme (Ansys, 2006) was used to solve the transport of properties inside the cavity. It computes a locally weight factor between first and second order approximation. For turbulence, the model $k - \varepsilon$ was adopted, for it's has been largely tested and its results published in the scientific literature for turbulent flows, as presenting a good relation between computational effort and numerical accuracy. Its mathematical inclusion in the problem is represented by two more variables in the linear system. This model is based in the eddy viscosity concept, that associate effective viscosity μ_{eff} with

turbulent viscosity μ_t (Ansys, 2006) by:

$$\mu_{\rm eff} = \mu + \mu_t \tag{5}$$

Turbulent viscosity is defined as:

$$\mu_{t} = C_{\mu} \rho \frac{k^{2}}{\varepsilon} \tag{6}$$

The variables kinetics energy k and turbulent dissipation ε are computed from the transport equations for kinetics energy, Eq. (7), and turbulent dissipation, Eq. (8).

$$\frac{\partial(\rho k)}{\partial t} + \nabla \bullet (\rho \nabla k) = \nabla \bullet \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho \varepsilon$$
(7)

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla \bullet(\rho \nabla \varepsilon) = \nabla \bullet \left[\left(\mu + \frac{\mu_{t}}{\sigma_{\varepsilon}} \right) \nabla \varepsilon \right] + \frac{\varepsilon}{k} \left(C_{\varepsilon 1} P_{k} - C_{\varepsilon 2} \rho \varepsilon \right)$$
(8)

4.2.2. Combustion model

The Eddy Dissipation Model, EDM, was used to solve the combustion inside the kiln. This model was applied when the chemical reaction rate is fast relative to the transport processes in the flow.

According to Stephen (2000), an important dimensionless parameter in combustion is the Damkohler number, Da. The fundamental meaning of the Damkohler number is that it represents the ratio of a characteristic flow or mixing time to a characteristic chemical time, thus

$$Da = \frac{t_{flow}}{t_{chem}} = \frac{lU_L}{\delta_L k^{1/2}}$$
(9)

Where k is the turbulence kinetics energy, l the turbulence characteristic length, U_L the flame's laminar velocity of propagation and δ_L front flame thickness.

For high Da numbers, i.e. $Da \gg 1$, it can be considered that the chemical reaction rate is fast if compared to flow species transport. In the presented work, Da number was estimated of order 1000.

Natural gas was modeled as a 100% methane mixture and its combustion as a single step reaction, Eq. (10). The bimolecular coefficient rate $k_{bimolec}$ was based in the Arrhenius model, Eq. (11).

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \tag{10}$$

$$k_{binolec} = A_p T^b \exp\left(\frac{-E}{RT}\right)$$
(11)

In Eq. (11) T is temperature.

The EDM model considers stoichiometric reaction and does not account for sub-reactions dissociations in the reaction. As an endothermic process, this limitation promotes overestimated temperatures in the combustion's products.

4.2.3. Radiation model

To solve the radiation within the kiln, the differential approximation model, P1, was adopted. The Differential Approximation is a simplification of the Radiation Transport Equation, which assumes that the radiation intensity is isotropic or direction independent at a given location in space. The P1 model is valid for an optical thickness greater than 1. The spectral radiative heat flux for an emitting, absorbing and linearly scattering medium is computed as:

$$q_{rv} = -\frac{1}{3(K_{av} - K_{sv}) - AK_{sv}} \nabla G_v$$
⁽¹²⁾

Although differential approximation model P3 is more accurate than P1 for most applications, it raises the numerical complexity. In the problem solved, the P1 model was chosen over P3 as numerical complexity is already high, for having to solve combustion in a 3D fluid flow.

4.2.4. Mesh and convergence



Hexahedral mesh properties						
Number of nodes	304,832					
Number of elements	291,238					
Number of faces	2676					

Figure 3. Cavity mesh

A non-uniform hexahedral mesh was generated for the cavity, as illustrated in Fig. 3. A mesh refinement was made in the inlet and outlet regions, counting 291,283 control volumes with a minimum orthogonality angle of 38.6 °. Mesh details are available in Fig. 3.

The convergence was obtained with basis in two distinct parameters: residual error below than 1.10^{-4} for all transport equations, and variables balance with less than 1% error.

4.2.5. Boundary conditions

There are two mass inlets and one outlet. The mass flow rates are 0.02 kg/s for natural gas and 0.08 kg/s for oxygen. In the gas burner inlet is injected all the gas mass and 0.02 kg/s of oxygen mass, 25% of the total of oxygen. In the oxygen burner inlet is injected all the oxygen that's left, 0.06 kg/s. The inlet temperatures of gas and oxygen were set as 300 K and a medium turbulence was considered, 5%. The outlet condition was set as prescribed mass flow of 0.1 kg/s of combustion products. With these conditions the kiln has a nominal thermal power of 1 MW.

All refractory walls were considered as insulated. The posterior and inferior surfaces represented the frits mass and bath, respectively, where an energy sink of 60 kW/m² was prescribed in order to represent both the energy necessary to elevate the raw frits mass temperature till the fusion range and to melt it. The total energy sink is 507.6 kW (50% of the total).

5. FORTRAN MODEL DESCRIPTION

Six arrays variables are imported from CFX results as known variables for the FORTRAN code: (a-b-c) velocity component in the i-direction, (d) combustion products density, (e) combustion products specific heat at constant pressure, (f) wall heat transfer coefficient.

The FORTRAN model is limited to the treatment of the kiln solid domain. It is based in the method of finite volumes and in the concept that the inside flow of the kiln is known as is the properties derived of the flow. As the numerical algorithm it uses the Gauss-Seidel method to solve the algebraic equations system derived from the discretization of the conservation equations, Eq. (1) to (3).

In this model are solved heat diffusion in the walls, internal and external convective heat exchange and radiative exchanges in both interfaces, internal and external. The bath frits are also modeled in this section.

5.1. Mesh

The mesh generated for the structure in FORTRAN is composed only for hexahedral and orthogonal elements. In the solid-fluid interfaces an infinitesimal surface is used to treat the radiation term. This is essential to solve the radiation term in the equations as for elevated temperatures this term grows important. A transversal section cut of the mesh is shown in Fig. 4. The blue elements represent the solid domain, kiln walls, while the green elements are the fluid domain inside the kiln. The orange elements are the infinitesimal surfaces.

				_								
	139	140	141		142				143	144	145	
126	127	128	129	130	131 132 133			134	135	136	137	138
113	114	115	116	117	118 119 120			121	122	123	124	125
100	101	102	103	104	105 106 107			108	109	110	111	112
	93	94	95		96				97	98	99	
80	81	82	83	84	85	85 86 87			89	90	91	92
67	68	69	70	71	72	73	74	75	76	77	78	79
-54	55	56	57	58	59	60	61	62	63	64	65	66
	47	48	49		50				51	52	53	
- 34	35	36	37	38	39 40 41			42	43	44	45	46
21	22	23	24	25	26 27 28			29	30	31	32	33
8	9	10	11	12	13 14 15		16	17	18	19	20	
	1	2	3		4				5	6	7	

Figure 4. Solid domain mesh.

5.2. Heat diffusion and advection model

First order approximations are used to represent the derivatives in the energy equation for the heat diffusion. It's applied in the kiln walls and raw frits mass. As advection scheme, the upwind scheme is used. This is applied in the flow inside the kiln and in the frits mass flow through the kiln.

5.3. Combustion model

A combustion model was developed to calculate the combustion energy inside the kiln. This energy is distributed in the combustion products flow through heated mass volumes at the adiabatic flame temperature. The number and choice of

volumes is based on the flame size from CFD and the nominal total energy of combustion. This combustion model considers the reaction dissociations, obtaining temperatures more realistic than the EDM model used on CFX.

5.4. Radiation model

The wall radiation exchange is based in the Gebhart method (Siegel and Howell, 1992). It was applied as nonparticipating media. This method takes into account the multiples reflexions that occurs inside the kiln. Form factors are calculated by the algebraic technique of form factors. The analytics equations for form factors can be found in Incropera and Dewitt (2003).

5.5. Frits mass model

The frits mass flow inside the kiln is modeled as a moving solid. The mass flow through each finite volume of the mesh is prescribed in the model and only the heat energy diffusion and advection is solved. A heat energy sink was prescribed in this model in order to represent the energy consumption by the material.

6. RESULTS

6.1. CFX results

All results presented below are for steady state solution. The CFX velocity field is inserted in the FORTRAN code in order to create the flow of gases inside the kiln. This flow is used to transport the thermal energy of the FORTRAN combustion routine. The temperature field obtained with the CFX combustion is only used to estimate the flow field and properties. Figures 5 to 8 present the results from the flow field inside the kiln that were numerically obtained with the Ansys CFX and imported to the FORTRAN code. Although the final temperature field inside the kiln is solved through the FORTRAN code, the properties estimated with the CFX play an important part in the final results. The purpose of presenting these results is to show that they suffer a great numerical variation through the kiln internal cavity.

Density and specific heat at constant pressure are the internal flow's thermodynamic properties more significant to this work. They have a high temperature dependency. In Fig. 5 are presented the CFX results for density in the longitudinal midplane of the cavity and specific heat in three longitudinal plans.

Figure 6 illustrates an isosurface of 2650K and the velocity field through a x-z plane passing by the burner, at y = 0.61 m. The wall heat transfer coefficient and wall convective heat flux in the left, top and right internal walls are shown in Fig. 7. These variables are solved by the CFX through scalable walls functions, using empirical correlations for the wall heat transfer and then calculating the wall heat transfer coefficient from the former. Figure 8 compares experimental data from the external left wall temperature distribution with the one numerically obtained to the inside left wall.



Figure 5. Inside flow density (a) and specific heat at constant pressure (b).

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The effects of the flame on the flow field and properties can be appreciated in Fig. 5 and 7. Density and specific heat undergo a wide variation in the flame region, while numerical values for heat transfer coefficient and heat flux increase significantly in the same zone.

An estimation of the flame size brings accuracy to the FORTRAN combustion model. This estimation can be obtained by an isothermal surface at a determined temperature estimated with basis in the theoretically released energy of combustion. An isothermal surface at 2750 K is shown in Fig. 6.

The flame shape is slightly inclined to the left plane of the cavity because of the outlet located in that plane. The temperature level inside the kiln is approximately 2600K.



Figure 6. (a) Isosurface of T = 2750 K; (b) Velocity field at mid-plane.

To solve the internal convective heat exchange in the FORTRAN code, the wall heat transfer coefficient obtained with the CFX is inserted as a known property in the first fluid volumes next to the interface solid-fluid, the kiln internal wall. Three walls are represented in the Fig. 7. The first is the left side of the internal kiln wall, where the outlet is situated. The middle one is the roof and the third one is the right side of the internal kiln wall. The z axis stars at the front of the kiln cavity, where the burners are situated and increase till 3.65 m, where the back of the kiln cavity is located. The zero from the y axis is located at the internal bottom of the kiln, and increase till the internal roof at 1.05 m. The x axis goes from the left internal wall, where the outlet is, till the right internal wall.



Figure 7. (a) Wall heat transfer coefficient; (b) convective heat flux.

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As expected from the non-symmetry forced by the cavity outlet being in the bottom left side of the kiln while the burners are located in the front center, the wall heat transfer and the wall heat transfer coefficient are not symmetric.

The dependency between the heat coefficient and the heat flux in (a) and (b) is most remarkable at the internal roof. Negative values of convective heat flux represent heat going from the flow to the wall. Positive values represent heat going from the wall to the flow. This happens at the corners in the back of the cavity, where the regions of cooler flow are concentrated and the while the walls are heated by radiation.

The wall heat transfer coefficient relation with the flow field velocity is presented in Fig. 6 (b), where the velocity in the longitudinal mid-plane is shown. The region of higher velocity value coincides with the region of higher wall heat transfer coefficient.

The temperature distribution in the external left wall of the real kiln obtained with a infrared camera is presented in Fig. 8 (b). It present a large fillet through all the z coordinate at y=0.3 m as result of a external metal beam used for the kiln structure, contrasting with the refractory walls. The temperature distribution for this fillet is neglected as the infrared camera was set to refractory material emissivity. Figure 8 (b) is compared with the temperature distribution on the same wall but in the internal face solved with CFX. The temperature scales are local for each case. The z axis starts at the back of the cavity and ends in the front plane, so the burner is located in z = 3.55 m. The y axis starts at the bottom plane.



Figure 8. Left wall temperature distribution (a) CFX results (b) experimental data.

6.2. FORTRAN results

A fictitious flow was inserted in the FORTRAN code in order to test it. It is a uniform flow starting in the front plane, going through the kiln cavity until it reaches the back plane, descending to the last layer of finite volumes, next to the bottom plane, returning then to the front plane and finally exiting the kiln cavity by the outlet in the left plane.



Figure 9. (a) Solid front wall temperature distribution, (b) solid left wall temperature distribution.

The combustion was assumed to occur in the first layer of volumes, next to the front plane, in the XY plane. The combustion was solved for the methane-oxygen stoichiometric reaction. Fig. 9 presents the temperature distribution obtained for that case in the front wall at a distance of 0.075 m from the internal solid-fluid interface (a). The temperature distribution at the same distance on the left wall is also presented (b). The y axis stars at the external bottom wall of the kiln. The zero in the x axis is located at the external left wall and the z axis goes from the external front wall to the external back wall. The temperature is given in Kelvin

	Experimental data		CFX nume	erical results	FORTRAN numerical results		
	Energy [kW]	Fraction [%]	Energy [kW]	Fraction [%]	Energy [kW]	Fraction [%]	
INLETS							
Oxygen	0	-	0	-	0	-	
Fuel	0	-	0	-	0	-	
Raw frits mass	0	-	0	-	0	-	
Theoretical combustion energy	1125	-	1002.9	-	1012	-	
OUTLETS							
Flow outlet	446	39.6	441.0	43.97	429	42.39	
Frits mass flow outlet	389	34.6	507.6	50.61	368	36.36	
External heat rate losses by walls	246	21.9	0	0	204	20.16	
Total energy outlet	1081	96.1	948.6	94.58	1001	98.91	
Theoretical total energy outlet	1125	100	1002.9	100	1012	100	
Theoretical-results difference	44	3.9	54.3	5.42	11	1.09	

Table 02 - Experimental data and CFX results comparison.

Table 2 brings a comparison between experimental data from the real kiln and the numerical results obtained with CFX and FORTRAN. The numerical values for the FORTRAN results are not accurate, since a fictitious flow was prescribed instead of the CFX flow solved. The energy transferred to the frits mass flow in the CFX numerical results is prescribed in the model, based on estimated properties of the frits. The value estimated for this case was 507.6 kW, but can fluctuate from 400 to 500 kW depending on the frits composition. The experimental data brings a value of 389 kW. The combustion products flow exiting the kiln's cavity represent almost 40% of the input energy for the experimental data and 44% for the CFX results. The flow's temperature however differs from an order of 1000K, going from 1300K on the experimental data to 2600K on the numerical results. The elevate temperature in the CFX model is caused by the idealization of the kiln as insulated and the overestimation of temperatures in the combustion model EDM. By examining the experimental data in Tab. 2 it can be seen that the insulated condition is not a good approximation since over 20% of the input energy losses occurs by the walls to the external environment. Comparing numerical results from CFX and FORTRAN, is possible to see that the FORTRAN code provides important results not presented in CFX results such as that external heat rate losses by walls, essential for predicting the impact of the inside kiln process in the kiln structure.

7. CONCLUSIONS

The numerical simulation of the process inside a ceramic frits kiln with CFD and a global FORTRAN code proved to be a helpful tool in two main aspects. The first one is to provide good values estimation for different variables, with the CFD, for the global case in the FORTRAN code, allowing the easy investigation of the influence of several variables in the process as burner position, fuel and oxidizing type and kiln geometry. The second is to provide data for a more complete approach of the problem involving also the structure of the kiln, not idealizing it. This can contribute to improve several aspects of industrial interest as reduction of material cost on maintenance of the refractory walls, increase of the efficiency of the fusion process, improve productivity and optimization of burner position and kiln geometry.

The comparison of the CFD results with experimental data proved that the mathematical models used in the numerical simulation are consistent with the real phenomena. Further comparison with global results from the FORTRAN code is expected to have even better accuracy with experimental values.

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