COMPUTATIONAL SIMULATION OF FLUIDIZED BED COAL COMBUSTOR BY A 3D FLUID DYNAMICS TRANSIENT MODEL[1]

Anderson Willian de Souza Baltazar[2]
José Adilson de Castro[3]
Alexandre José da Silva[3]

Abstract

Fluidized bed processes are well known since 1920 and are extremely used in chemical and oil industries. Although to combustion systems this equipment only started to be recognized in the 80-90's ages, after the interest of electric generation. Fluidized bed makes possible the use of various types of fuels, which normally are rejected in industrial process. Among them can be cited coals with high ash and sulfur contents, biomasses and some residues of industrial and agricultural segments. The fluidized bed technique is not spread out in Brazil yet, but worries about energetic matrix has been opened the discussion about another electric energy sources. Thermal generation is one of this options that can use fluidized bed combustor. The Brazilian coals are characterized by their high ash and sulfur content fact that make impossible to use them directly in conventional thermoelectric facilities. Therefore, the use of fluidized bed to produce hot gas for power generation is a promising technique to overcome the use of impure raw materials with high combustion efficiency and energy savings. Mathematical models have shown like an efficient tool to investigate operational conditions reproducing virtually industrial processes. The objective of this work is to simulate the gas-solid fluid dynamic in a transient, 3D model evaluating the reactor heating process to start the coal feeding to burn. The model uses the multiphase concept simulating the flow in a 3D fluidized bed reactor. Transport equations of mass, momentum and energy are solved by the finite volume method for non-orthogonal system implemented in a complex computational code written in Fortran 90/95. The phases are modeled using continuum mechanics principles where collection of particles is considered identical having a representative diameter and density. The results have been shown very close agreement with results previously consulted.

Key words: Multiphase flow; Mathematical modeling; 3D; Transient; Computational simulation.

SIMULAÇÃO COMPUTACIONAL DE COMBUSTOR DE LEITO FLUIDIZADO POR UM MODELO FLUIDODINÂMICO TRANSIENTE EM 3D

Resumo

Processos em leito fluidizado são bem conhecidos desde 1920 e são extremamente usados em indústrias químicas e de petróleo. No entanto para sistemas de combustão este equipamento somente começou a ser reconhecido nas décadas de 80 e 90, depois do interesse para geração elétrica. Leito fluidizado torna possível o uso de vários tipos de combustíveis, os quais normalmente são rejeitados nos processos industriais. Dentre estes podem ser citados carvões com alto teor de cinzas e enxofre, biomassas e alguns resíduos industriais e agrícolas. A técnica de leito fluidizado não está muito difundida ainda, mas a preocupação com a matriz energética tem aberto a discussão sobre outras fontes de energia. A geração térmica é uma dessas opções que pode usar leito fluidizado. Os carvões brasileiros são caracterizados por seus altos teores de cinzas e enxofre fato que impossibilita seu uso diretamente in indústrias termelétricas convencionais. Porém, o uso de leito fluidizado para produzir calor para geração de energia é uma técnica promissora que possibilita o uso de matérias-primas impuras com alta eficiência de combustão e energia. Os modelos matemáticos têm se mostrado como uma ferramenta eficiente para investigar condições operacionais reproduzindo virtualmente processos industriais. O objetivo deste trabalho é simular a fluidodinâmica gás-sólido em um modelo transiente 3D avaliando o processo de aquecimento do reator para o início da alimentação de carvão para a queima. O modelo utiliza o conceito de multi fases para simular o escoamento em um reator de leito fluidizado em 3D. As equações de transporte de massa, energia e momentum são resolvidas pelo método de volumes finitos para um sistema não ortogonal implementado em Fortran 90/95. As fases são modeladas usando principio de mecânica do contínuo, onde um uma coleção de partículas são consideradas idênticas tendo um diâmetro e densidade representativa. Os resultados têm mostrado muito boa concordância com resultados previamente consultados.

Palavras-chave: Escoamento multi-fásico; Modelagem matemática; Transiente; 3D; Simulação computacional.

1 *Technical contribution to the 3rd International Meeting on Ironmaking, September 22 – 26, 2008, São Luís City – Maranhão State – Brazil*

2 *Student in Graduate Program in Metallurgical Engineering EEIMVR/UFF Pólo Universitário de Volta Redonda. anderson@metal.eeimvr.uff.br*

3 *Professor in Graduate Program in Metallurgical Engineering EEIMVR/UFF Pólo Universitário de Volta Redonda.*

1 INTRODUCTION

Reactional processes that use fluidized bed are Known since 1920, but started to be famous only in 1970, despite was used in many process in the chemical an oil industry.[1] The fluidized bed, however, only started to be recognized in the 80's and 90's with increase of the interest in the installations for energy generation. Mainly because the process opened the options of fuels used and researches concluded that positives environmental influences can be obtained with this equipment. The fuels used in the fluidized bed processes can present low quality, such as, low rank coals, mine residues, trash and diverse types of biomasses[1]. The models of fluidized bed combustors are scarce yet mainly due to the complex mathematical modeling and the instable character of numerous equations that must be solved to determine the process.[2] Problems with energetic matrix has been opened the discussion about the use of new processes to electric generation in Brazil. The thermal generation is one of this options that makes possible the fluidized bed reactor use to burn coals and biomasses. The Brazilian coals presents high ash and sulfur content which is impossible to directly use in conventional thermoelectric facilities. Therefore, the use of fluidized bed to produce hot gas for power generation is a promising technique to overcome the use of impure raw materials with high combustion efficiency and energy savings. Mathematical models have proved their efficiency to investigate optimum operational conditions and reproduce virtually the industrial processes. The objective of this work is to develop a computational model that simulates the fluidized bed phenomena considering two phases. The model uses the multiphase concept to simulate the flow in a 3D fluidized bed reactor. Transport equations of mass, momentum and energy are solved by the finite volume method for non-orthogonal system implemented in a complex computational code written in FORTRAN 90/95. The phases in this model are modeled using continuum mechanics principles where collection of particles is considered identical having a representative diameter and density. The solid phase momentum equation is modified by addiction of one term to account momentum exchange due to particle-particle collisions, this term including the kinetic theory model.[3] The granular temperature, Θ, is defined to represent the specific kinetic energy of velocity fluctuations or the translational fluctuation energy resulting from the particle velocity fluctuations.[4] In granular flow, particle velocity fluctuations about the mean are assumed to result in collisions between particles being swept along together by the mean flow. The granular particle temperature equation can be expressed in terms of production of fluctuations by shear, dissipation by kinetic and collisional heat flow, dissipation due to inelastic collisions, production due to fluid turbulence or due to collisions with molecules, and dissipation due to interaction with the fluid.[3] Despite of the development of models to simulate fluidized beds have been achieved maturity, the results validation with experimental measurements must be done, mainly because some correlations used in the models are empirical or semi-empirical. This work considers a transient 3D model fluidized bed, where three phases are considered gas and two solid phases: one sand that is initial material in the bed and other coal that start to be fed after sand temperature reach 450ºC. The fluid dynamics considering the motion three phases in a semi-industrial fluidized bed reactor is analyzed. Therefore, the main objective of this work is to show the heating behavior of reactor to start feeding the coal to burn.

2 MATHEMATICAL MODEL

2.1 Transport Equation

The present model consists of describing the phenomena that occur in the interior of a semi-industrial fluidized bed reactor as a system of three phases that interact between it transferring mass, momentum and energy. The mathematical formulation follows hypothesis of the continuous media and as such can be formulated through transport equations. The phenomena of transference of mass, momentum and energy in the interior of a fluidized bed reactor are represented by the general transport equation (equation 1). Where the index i represent the considered phase. The effective diffusion coefficient (Γ_ϕ) assumes different meanings and models in agreements of equation to be solved, for example if the momentum equation is the equation to be solved the effective diffusion coefficient assumes the dynamic viscosity. The source term (S_ϕ) represents generation or consumption of mass, momentum and energy. In the source term are considered for example the phenomena of interaction among phases, mechanics interactions resulting in the coupling between the equations of conservation of mass, momentum and energy. The models of momentum and energy were obtained of literature and are detailed in another works for different studies like fluidized bed.[4]

$$\frac{\partial(\varepsilon_i \rho_i \phi_i)}{\partial t} + div\ (\varepsilon_i U_i \phi_i) = div\ (\varepsilon_i \Gamma_{\phi_i}\, grad\ \ \phi_i) + S_{\phi_i} \quad (1)$$

The equation to consider the fluctuations energy of solid particles was introduced in the model and can be described by equation 2 [4].

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s \rho_s \Theta_s) + grad\ (\varepsilon_s \rho_s \Theta_s \vec{v}_s)\right] = (-p_s \bar{I} + \bar{\tau}_s) : grad\, \vec{v}_s + grad\ (k_{\Theta_s} \cdot grad\, \Theta_s) - \gamma_{\Theta_s} \quad (2)$$

Where, (Θ_s) is the granular temperature, (I) is the admensional stress tensor, ($\bar{\tau}_s$) is the stress tensor, p_s is the solid pressure, (γ_{Θ_s}) is the collision energy dissipation.

2.2 Computational Simulation

The simulation of fluidized bed consists to solve the governing equations of mass, momentum and energy in a semi-industrial fluidized bed reactor. The kinetic theory of granular flow is used to consider the conservation of solid fluctuation energy; it was used to closure of the solid stress terms.[4] The momentum exchange coefficients can be calculated by specifying drag functions. In this study the drag function used is the equation modified by Richardson and Zaki, which was modified to know the neighbors particles.[7] The drag function and drag coefficient are showed in the equations 3 and 4 respectively.

$$F_m = -C_{d_{g-s}}\left[\frac{3\varepsilon_s \rho_s}{4 d_s \varphi_s}\right]\left|\vec{U}_g - \vec{U}_s\right|\left(\vec{U}_g - \vec{U}_s\right) \quad (3)$$

$$C_{d_{g-s}} = \left[\frac{24}{\mathrm{Re}_{g-s}} \left(1 + a\,\mathrm{Re}_{g-s}^{\,b}\right) + \frac{c}{1 + \dfrac{d}{\mathrm{Re}_{g-s}}} \right] \left(\frac{\varepsilon_g}{\varepsilon_g - \varepsilon_s} \right)^{-4,65} \quad (4)$$

The terms a, b, c and d in the drag coefficient equation are functions of shape factor of solid (φ).[(7)]To the set of differential equations represented by equation 1 must be imposed initial and boundaries conditions that represents the process to be simulated. The simulation parameters can be seeing in table 1, while the pulverized coal properties in table 2. The coal diameter 4.2 mm and density is 1250 kg/m^3 and is fed with a rate of 0.11 kg/s on the top of reactor.

Table 1. Fluidized bed reactor simulation parameters.

Description	**Value**	**Comment**
Particle density, ρ_p	2600 kg/m^3	sand
Gás density, ρ_g	1.225kg/m^3	Air
Particle diameter, d_p	2.5mm	Uniform distribution
Restitution coeficient, e_{ss}	0.90	Literature value
Initial fraction on the bed, ε_{s0}	0.60	Fixed value
Gas superficial velocity, U	0.0857m/s	U_{mf}
Pressure of entry	1atm	Fixed value
Bed heigth	0.30m	Fixed value
Entry condition	Velocity	Gas velocity
Out conditions	Flow	Developed
Time steps	1s	Especified
Convergency criterion	10^{-6}	Especified

Table 2: Coal properties

Immediate analysis (% dry)	Ash	39.56
	Volatiles	44.06
	Fix carbon	55.94
Fuel rate (kg/s)		0.11
Element Analysis (% dry mass, ash free)	C	45.50
	H	3.07
	N	9.90
Ash (% mass as oxides)	SiO_2	24.88
	AL_2O_3	10.98
	Fe_2O_3	1.35
	MgO	0.13
	CaO	0.85

The energy sources that are results of chemical reactions, phase transformations and sensitive heat exchange due mass exchange, the energy source due convective heat is calculated by equation 5 and the heat exchange coefficient is calculated by Ranz Marshall equation 6.[(5)]

$$\dot{E}_i^j = h_{i-j} A_{i-j} \left[T_i - T_j \right] \tag{5}$$

$$h_{g-i} = \frac{K_g}{d_i} \left[2{,}0 + 0{,}6 \left(Re_{g-i} \right)^{0{,}5} \left(Pr_g \right)^{1/3} \right] \tag{6}$$

2.3 Results and Discussion

The results presented in this section were obtained by computational simulation with developed model. The Figure 1 shows a schematic figure of semi-industrial fluidized bed reactor and dimensions used as simulation parameters, while Figure 2 shows the mesh generated by transport equations discretization using the finite volume method. The heating of reactor is done through alcohol combust with gas excess to produce hot gas at temperature of 850ºC. This fact is considered and used in the model. The heating is an important phase of process, because the coal only can be fed after the bed temperature material (sand) reach 450ºC, after this the coal start to be feed to burn. Although the gas continues to be heated with alcohol until the temperature into de fluidized bed achieves to reach 850ºC. Then the alcohol combust is gradually down until the combustion process has sustainable continues alone, or the combustion process have energy sufficient to keep for the process. Figure 3 shows the temperature curve of sand particles, which reach 450ºC in approximately four hours after fluidization process starting.

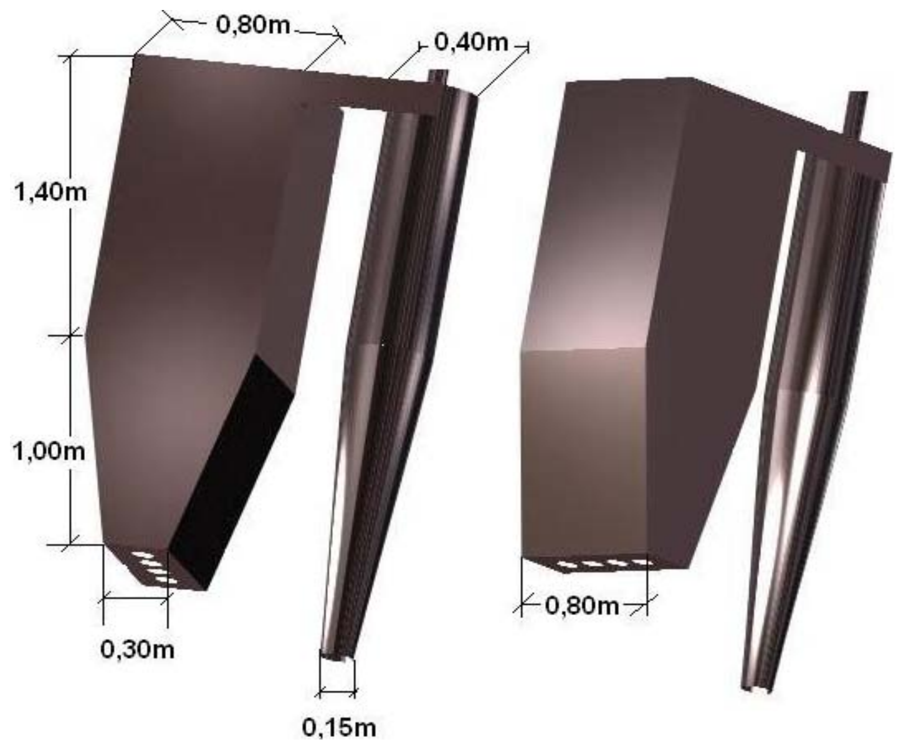

Figure 1. Schematic figure of fluidized bed reactor.

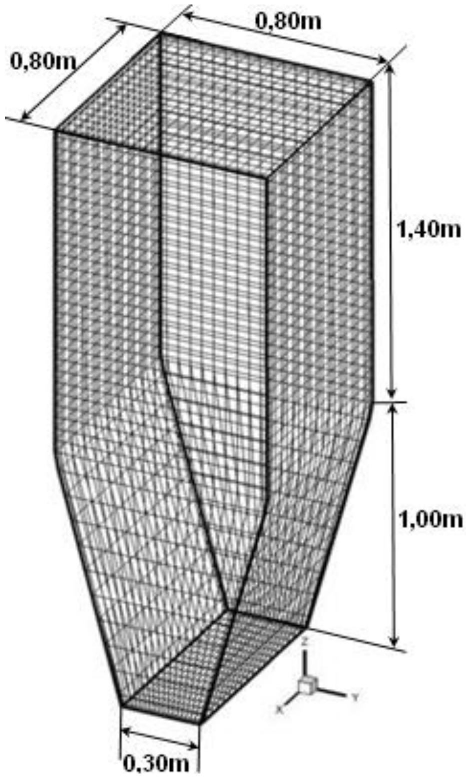

Figure 2. Mesh generated by volume finite method.

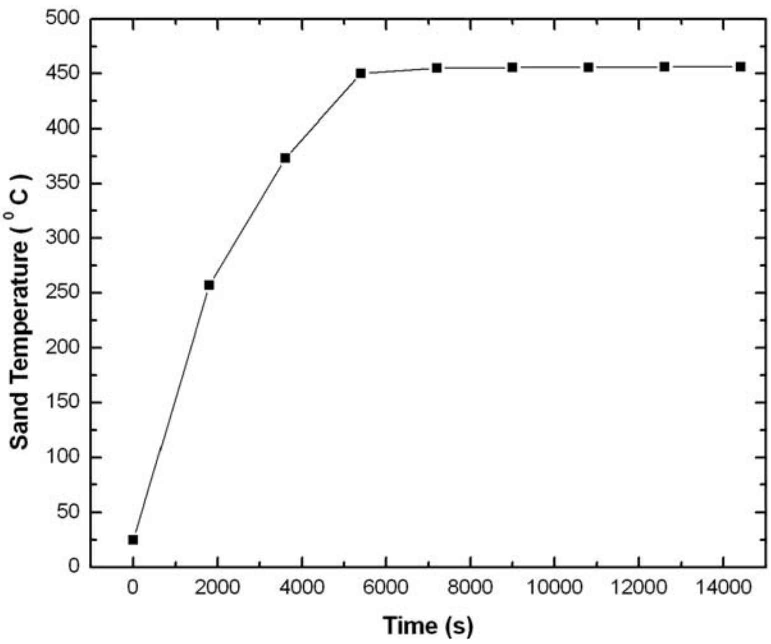

Figure 3. Curve of heating of fluidized bed reactor obtained by simulation.

The next figures show the behavior of combustion gases some seconds after the coal feeding starts the concentration of all figures is in percentage. In Figure 4 the behavior of O_2 shows that this gas has a higher concentration in the way of gas outlet, while in the bottom is short mainly in the corner where coal not reacted accumulate. Figure 5 the water steam that has the most concentration in the bottom of reactor justly where the coal accumulate. Figure 6 shows the behavior of CO_2 and

Figure 7 CO this reaction are competitors in the model then can be sight that CO_2 presents minor concentration in the corner while CO presents most concentration exactly in this point of exist accumulated coal.

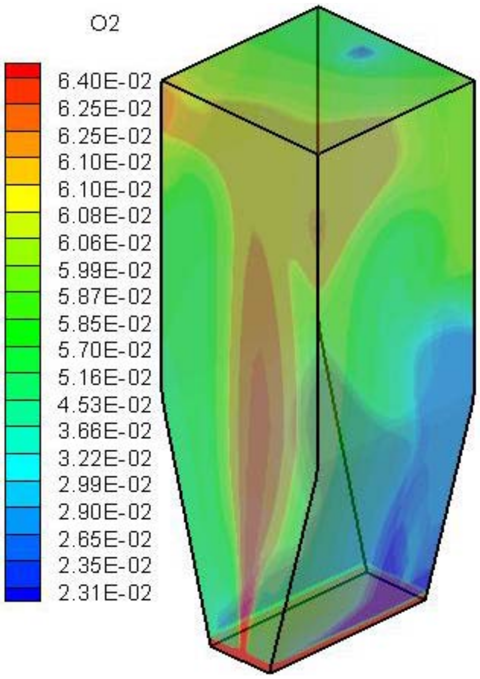

Figure 4. O_2 percentage distribution in fluidized bed reactor.

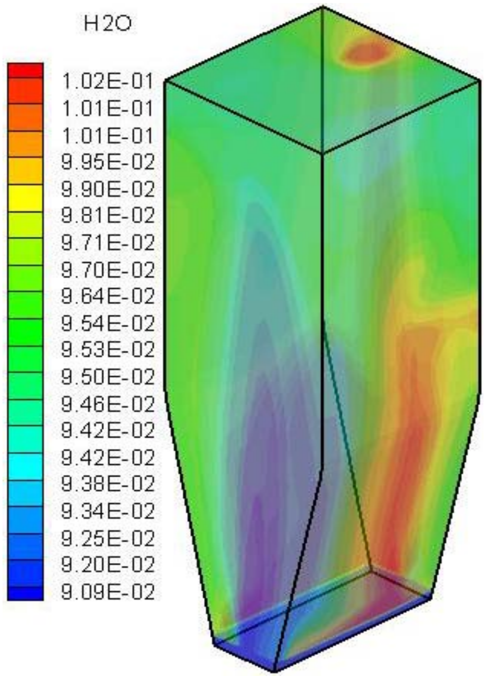

Figure 5. Percentage Distribution of water steam in fluidized bed reactor

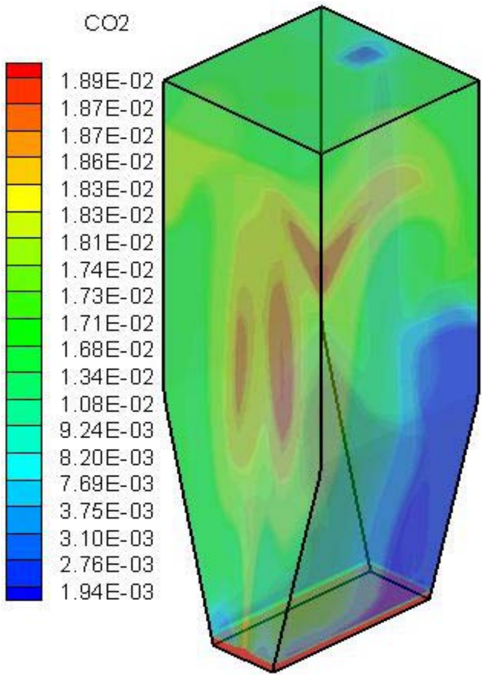

Figure 6. CO_2 percentage distribution in fluidized bed reactor.

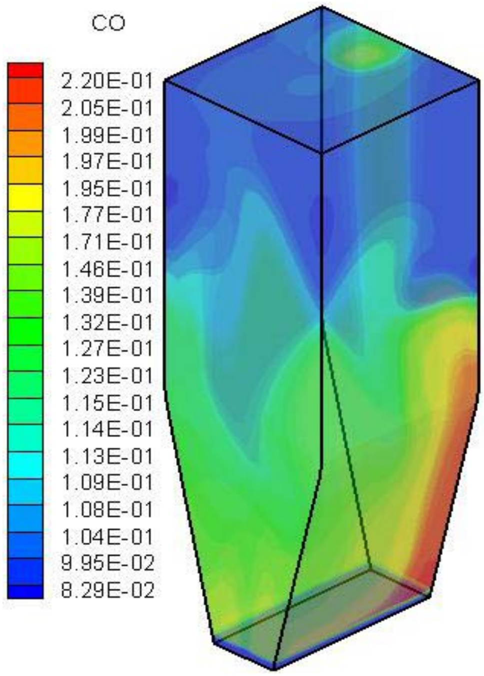

Figure 7. CO percentage distribution in fluidized bed reactor.

Figure 8 shows the graph with curves of combustion gases against time this results like anterior are preliminaries but represents the gas producing by the coal burning in the model. The O_2 gas decrease suddenly in the beginning of process While another gases increase with the time consuming O_2 and stabilize some seconds after combustion process starts. CO increase suddenly but after decrease probably by conversion in CO_2 that has the concentration increased and stabilize the behavior of water steam is so similar an increase in the beginning and stabilization after few seconds.

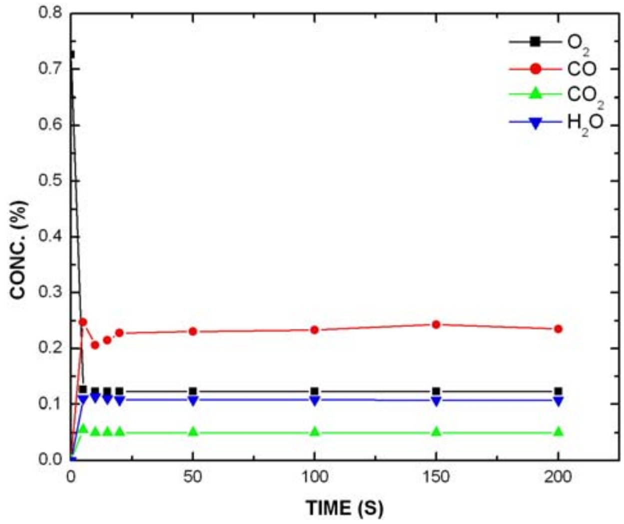

Figure 8. Graph showing the combustion gases curves against time.

Figure 9 shows the behavior of coal during combustion process. This fuel is fed by the reactor top and is arrested by the air stream, although a small part reaches the bottom and accumulates in the inferior corner generating a solid hold-up. This amount of coal not reacted yet, that react in this part of reactor doing that some concentration of combustion gases being greater in this fluidized bed section.

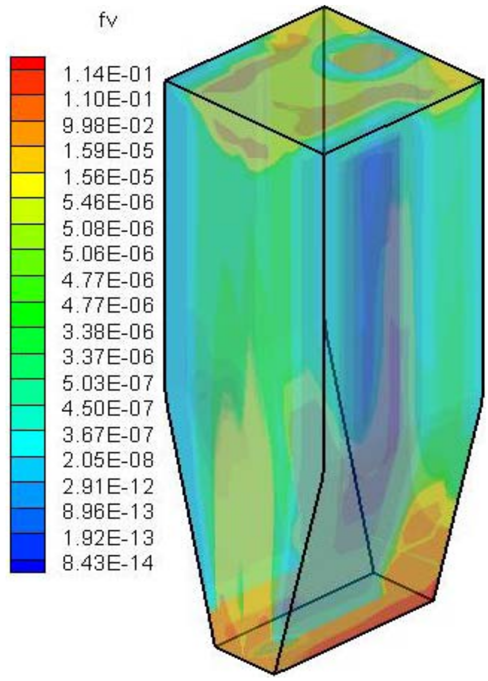

Figure 9. Coal behavior in the fluidized bed reactor.

4 CONCLUSIONS

A model to simulate the behavior coupled with reactional kinetics of coal substances have already developed. This model was developed with literature correlations both for fluid dynamic as for the kinetic of reactions, because this some adjusts could be done. Although the presented results showed very close agreements with searched results to this developing.

Acknowledgments

The author would like to express its thanks to CAPES and CNPQ by encourage and finance the research development, to professor Wolfgang Kalkreuth UFRGS coordinator of the project to which the development of this work is an integral part.

REFERENCES

1 BITTANTI, S. et al., 2000, A model of a bubbling fluidized bed combustor oriented to char mass estimation, IEEE Transactions on control systems technology, vol. 8, Nº 2, pp. 247-256.
2 Zhou, H. et al., 2004, DEM-LES of coal combustion in a bubbling fluidized bed part I: gas particle turbulent flow structure, Chemical engineering science, Nº 59, pp. 4193-4203.
3 GIDASPOW, D., 1994, Multiphase flow and fluidization: Continuum and kinetic theory descriptions, Academic press, San Diego.
4 TAGHIPOUR, F., ELLIS. N., WONG, C., Experimental and computational study of gas-solid fluidized bed hydrodynamics, Chemical Engineering Science, vol. 60, p. 6857-6867, 2005.
5 CASTRO, J.A., A multi-dimensional transient mathematical model of blast-furnace based on mult-fluid model, Institute for advanced material processing, Tohuku University, Japan, Doctored thesis, 2000.