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MODELING GASIFICATION OF BRAZILIAN COALS AND BIOMASS IN A BUBBLING BED REACTOR

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Abstract: *In this investigation a bubbling bed reactor is proposed as a key equipment for gasification of coal with high ash content, typical of Brazilian coals combined with biomass to produce gas for thermoelectric applications. The process variables are modeled based on transport equations of momentum, energy and chemical species of 4 phases, where 3 phases are pulverized one and the other phase is gas. In order to discretise and solve the transport equations with appropriate initial and boundary conditions, the finite volume discretisation procedure is used. The SIMPLE algorithm is applied for coupling the velocity and pressure fields. The solution of the discrete algebraic equations is carried out with the alternate direction iteration algorithm combined with tridiagonal matrix solution. The concept of granular temperature is used to account for the solid to solid interactions. Rate equations for momentum, energy and chemical species exchanges are proposed to model the interphase interactions. The model is tested to investigate the combustion of biomasses and high ash Brazilian coals. A dessulfurising bed is used to control the gas product and keep thermal stability of the reactor. Numerical and experimental results from a pilot scale reactor indicated that is possible to produce gas with quality compatible with the requirements of those for thermal generation with high combustion rates, although complex flow pattern is developed within the reactor. The model indicated that that up to 25% of biomass and 75% of coal with high ash (< 30 %) is possible with stable operation. This ratio also has been obtained in the pilot plant with coals and biomasses with up to 35% of volatile matter, as the volatile matter increases the process stability is deteriorated.*

Keywords: *Transport Equation, Heat and Mass Transfer, Mathematical Modeling, coal gasification*.

1. INTRODUCTION

Technologies based on fluidized beds have been successfully developed for several kinds of industrial applications. The advantage of these technologies is the high conversion rates attained due to high efficiency of heat and mass transfer allowed by excellent gas and fine particles contact. On the other hand, process stability and fluidization conditions are difficult to be attained and controlled under industrial scale. In addition, bed stratification and particle agglomeration are usually observed with consequent inner deterioration of reaction conditions. Particularly on the field of coal gasification, the fluidized bed reactor is attractive due to high rates of gasification and the possibility to handle low quality of pulverized coals. In this paper, a model able to investigate internal conditions of coal and biomasses gasification within a fluidized bed reactor is proposed based on the multi-fluid theory and applied to model a pilot scale reactor operating with high ash coal blended with biomasses. A pilot flame is used to preheat the bed while air is continuously blown in the lower part of the reactor. The pulverized coal and biomasses are fed through the upper part and a counter flow is established with the gas. At the first stage of contact with the gas the coal particles volatile and the final combustion is carried out in the bubbling bed, then the temperature of the bed is elevated and the pilot flame can be stopped. The results of the outlet gas are compatible with thermoelectric generation of middle power. A schematic view of the concept is shown in Fig. (1). Exhaust gas are used for feed a turbine which uses pressurized oxygen and burners with auxiliary fuel composed of natural gas or ethanol.

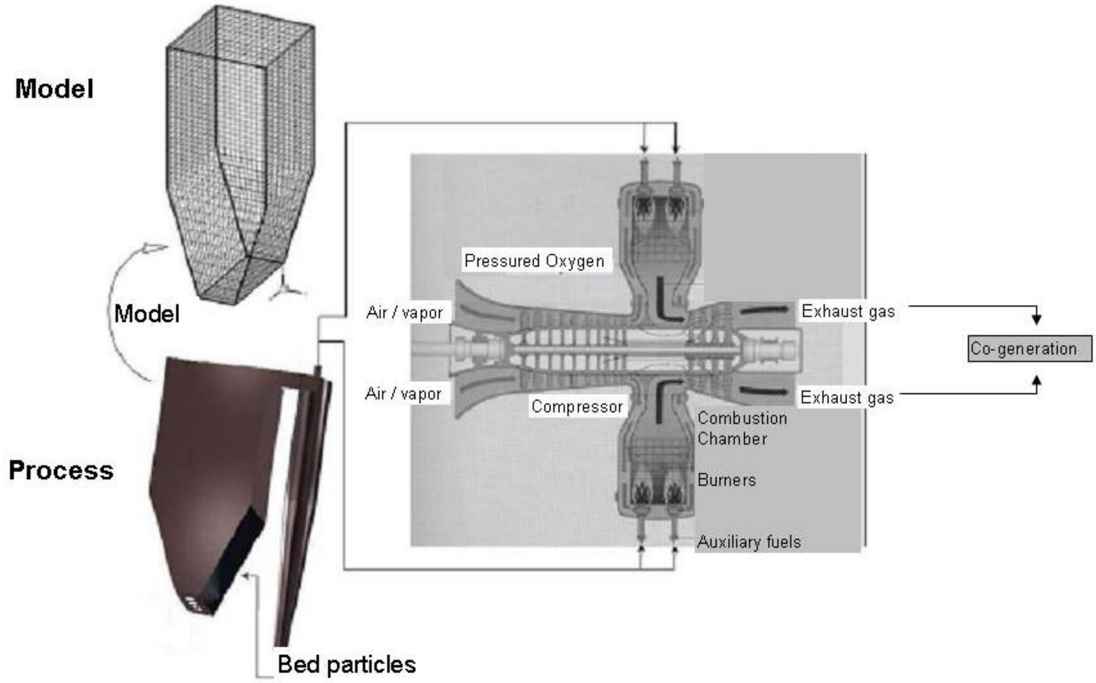


Figure 1 schematic view of gasification process based on bubbling bed reactor

This combination gives rise high efficiency of the thermal process and the inner temperature can be controlled by air and water vapour addition. In addition, it is possible to use co-generation process for recovering thermal energy of the turbine exit gas. Although the integrated process is important to evaluate the whole efficiency, this investigation will focus only on the fluidized bed gasification phenomena. The relevance of the investigation is due to the gasification process plays an important role for the operation stability of the whole system. This system has been experimentally tested and has proved the feasibility, although long term operation of the pilot plant has not been carried out yet. Fluidized bed reactors are widely used in the chemical industries and the basic principles are commonly discussed in the literature (Karppanen, 2000; Kunni and Levenspiel, 1991 and Taghipour, et al., 2005). The model approaches are usually based on continuum theory (Taghipour, et al., 2005) or discrete particles models (Tsuji, et al., 1993). Continuum theories, although neglects some particle-particle interactions phenomena treats the control volumes as a representative macroscopic behaviour, while, on the other hand, discrete formulations can handle particular particles interaction. However, for practical applications the number of particles necessary to represent the reactor behaviour is prohibitive even for supercomputers. On the other side, the continuum approaches can handle representative number of particles and models based on empirical correlations has been successfully used to investigate several inner phenomena (Taghipour, et al., 2005; Tsuji, et al., 1993; Van Wachen, et al., 2001 and Zhong, et al., 2007) . In this investigation the continuum approach is selected and empirical correlations is used to account for averaged particle-gas-particle interactions. Simulations are carried out in order to compare the internal response of the reactor gasification of pulverized coal and biomasses injections. The model is based on the multi-phase theory (Austin, et al. 1997; Castro, et al, 2000; Nemtsov, and Zabaniotou, 2008; Castro, et al, 2002 and Castro, et al, 2005) and considers explicitly four phases (gas, pulverized coal, pulverized biomasses and dessulfurizing bed). Each phase has its own composition and properties, and reactions involving all phases are considered.

2. METHODOLOGY

The methodology used in this paper to investigate the bubbling bed reactor for gasification of coal and biomasses is focused on the formulation of a mathematical model based on the continuum theory and applied to a multiphase system.

2.1 Model formulation

In this section, major features of the mathematical model are presented. The mathematical model consists of a set of strongly coupled transport equations to describe the motion, energy, chemical species and phase transformations. In this model four phases are considered. The gas phase is composed of the blast injection through a gas distributor at the bottom of the bed and the gas generated by chemical reactions, namely, combustion and gasification of coal and biomasses, including volatile matters evolution, water shift and adsorption reactions taking place at the dessulfurizing bed. The pulverized coal and biomasses are charged by lateral injection and drop down by gravity forces, on the other hand, the gas acts on the particles promoting bed fluctuation and chemical reactions takes place until all volatile matters and carbon being consumed. The temperature is controlled aiming at avoiding liquid phases formations. The model is constructed with basis on the multiphase principle where each phase interacts with one another exchanging momentum energy and mass due to chemical reactions and phase transformations. For each control volume four phases coexists and the space is completely filled with gas and particles. The rates of momentum, energy and mass transfer are modeled by semi empirical relations and can be found elsewhere (Austin, et al. 1997; Castro, et al, 2000 and Castro, et al, 2002). In this model the chemical species are considered explicitly for each phase, as listed in Tab. (1), and mass transfer rates are determined from relations presented in the literature.

Momentum equations for the gas phase:

$$\frac{\partial\left(\rho_g \varepsilon_g u_j\right)}{\partial t} + \frac{\partial}{\partial x_k}\left(\rho_g \varepsilon_g u_k u_j\right) = \frac{\partial}{\partial x_k}\left(\varepsilon_g \mu_g \frac{\partial}{\partial x_j}\left(u_j\right)\right) - \frac{\partial}{\partial x_j}\left(\varepsilon_g P_g\right) - \sum F_g \tag{1}$$

Momentum equations for pulverized coal biomasses and dessulfurizing bed:

$$\frac{\partial\left(\rho_i \varepsilon_i u_j\right)}{\partial t} + \frac{\partial}{\partial x_k}\left(\rho_i \varepsilon_i u_k u_j\right) = \frac{\partial}{\partial x_k}\left(\mu_{eff} \frac{\partial\left(u_j\right)}{\partial x_j}\right) + \rho_i \varepsilon_i g_j - \sum F_i \tag{2}$$

And the continuity equation holds for all phases:

$$\frac{\partial\left(\rho_i \varepsilon_i\right)}{\partial t} + \frac{\partial}{\partial x_k}\left(\rho_i \varepsilon_i u_k u_j\right) = \sum_{n=1}^{nreacts} R_n \tag{3}$$

The phase energy conservation reads:

$$\frac{\partial\left(\rho_i \varepsilon_i h_i\right)}{\partial t} + \frac{\partial}{\partial x_k}\left(\rho_i \varepsilon_i u_k h_i\right) = \frac{\partial}{\partial x_k}\left(\varepsilon_i \frac{K_i}{Cp_i} \frac{\partial}{\partial x_j}\left(h_i\right)\right) + \sum_i \dot{E} + \sum R_n^i \Delta h_n^i \tag{4}$$

And the chemical species conservation for each phase is given by:

$$\frac{\partial\left(\rho_i \varepsilon_i \phi_l^i\right)}{\partial t} + \frac{\partial}{\partial x_k}\left(\rho_i \varepsilon_i u_k \phi_l^i\right) = \frac{\partial}{\partial x_k}\left(\varepsilon_i D_{\phi_l}^i \frac{\partial}{\partial x_j}\left(\phi_l^i\right)\right) + \sum M_{\phi_l} R_{\phi_l}^i \tag{5}$$

In the above equations, indexes i represents phases, j is velocity components and n are chemical reactions. D is effective diffusions coefficient, ρ and ε are phase density and volume fractions, respectively. The complete meaning of the variables appeared in above equations are presented in Tab. (1). The phases and chemical species considered in this model are presented in Tab. (2).

Table 2. Phases and chemical species modeled.

Phases	Chemical Species ()
Gas	N_2, O_2,CO,CO_2, H_2, H_2O, SiO, NO, NO_2,SO,SO_2
Pulverized coal/charcoal	C, volatile, SiO_2, Al_2O_3, MgO, CaO, gangue, SiC, K(K_2O), P(P_2O_5), S, FeS, N, O
Dessulfurizing bed	CaO, $CaCO_3$, $MgCO_3$, SiO_2, Al_2O_3, MgO, CaO, gangue, P_2O_5, CaS, SiS

2.1 Boundary and initial conditions

The boundary conditions assumed to the velocity field at the wall surfaces is no slip conditions. At the gas inlet in the bottom feeders mass flow and pressure are specified. At the outlet, fully developed flows are assumed. For the particulate phases inlet inflow is specified and at the outlet no velocity gradient is assumed. For the surfaces wall heat transfer is considered both, convective heat coefficient and radiation heat flux. Inlet gas temperature is specified while inlet pulverized phases are set as room temperature. An initial condition for the dessulfurizing bed is specified as initial bed height without motion while zero volume fraction for the pulverized coal is assumed.

2.3 Numerical features

The partial differential equations are solved with the help of finite volume method and a general non-orthogonal system is provided for each control volume. For coupling velocity and pressure fields of the gas phase the well known SIMPLE (Patankar, 1980) algorithm is used while for pulverized coals the continuity equation coupled with momentum equations was used to calculate the velocity and phase fraction fiels. The solutions of the particulate phases are obtained using simultaneously the momentum and continuity equations and the effective viscosity is calculated by solving the granular temperature equations of each phase with respective equations relating granular temperature and flowing parameters. Details of the granular temperature formulation and model parameters can be found in Taghipour et al. (Taghipour, et al., 2005), Zhong et al (Zhong, et al., 2007) and Nemtsov and Zabaniotou (Nemtsov, and Zabaniotou, 2008). The main chemical reactions used in this model are coal gasification, combustion and water shift. The rate equations for these reactions were adapted from similar applications previously modeled by Austin et al (Austin, et al. 1997), and Castro et al (Castro et al, 2000, 2002 and 2005). The numerical grid used in these simulation were determined by mesh tests with fixed time step of 0.01s. The final grid assumed presented comparative error less then 2% for the same time step. Final calculations were done with a 25x25x60 mesh.

3. RESULTS AND DISCUSSIONS

The model was used to predict transient 3D operation of the pilot scale fluidized bed reactor operating with blending of biomass and coal. The blending ratio was determined by considering outlet gas composition and temperature. Before starting to predict the pilot plant conditions it was compared the results obtained for a small reactor in laboratory scale those predicted by other researchers. Figure 2 shows pressure drop and bed expansion for the experimental setup. As can be observed the present model predicted average pressure drop when compared with Syamlal and Gidaspow results while for expansion ratio it predicted slightly lower expansion. However, all models under predicted the expansion ratio in comparison with experimental results. This discrepancy may be attributed mainly to uncertainty of the drag coefficients correlations.

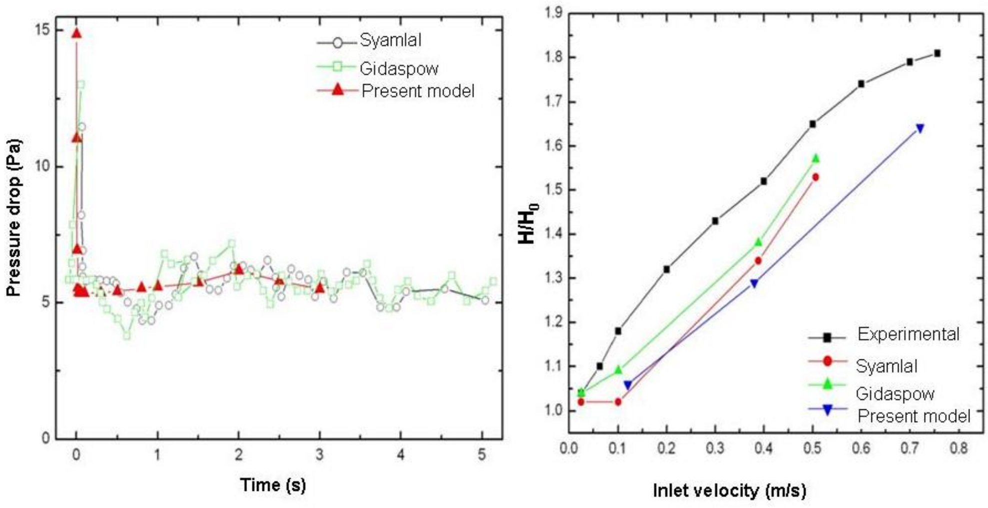
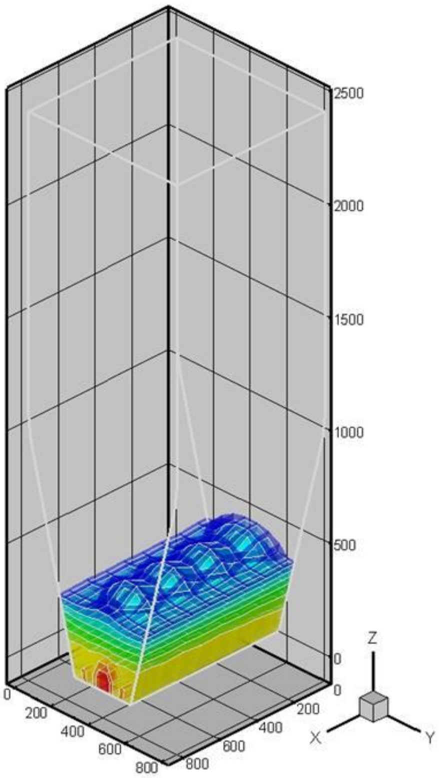
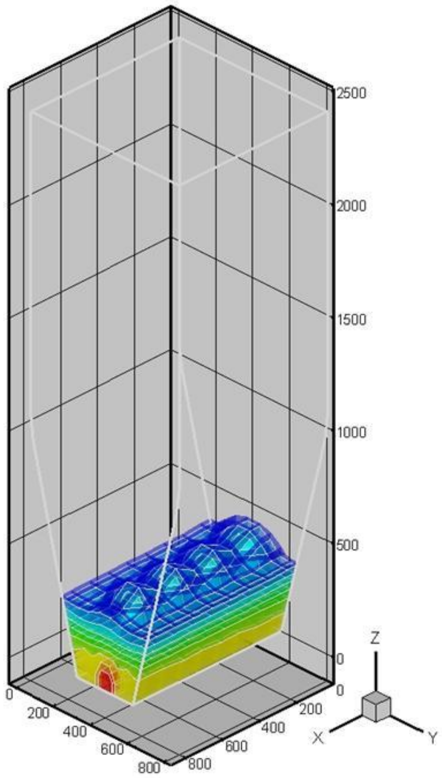


Figure 2. Model parameters compared with previous work

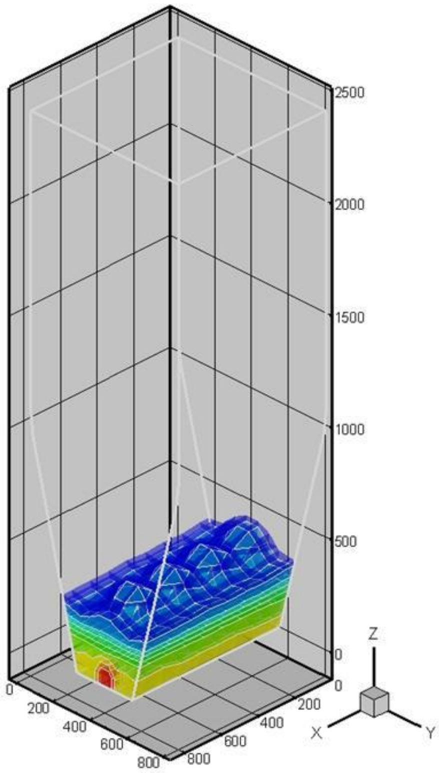
Figure 3 shows dessulfurizing bed evolution. As the process evolutes the bed experiences expansions and contraction cycles while ashes of the unburned coal and biomasses are incorporated into the bed.

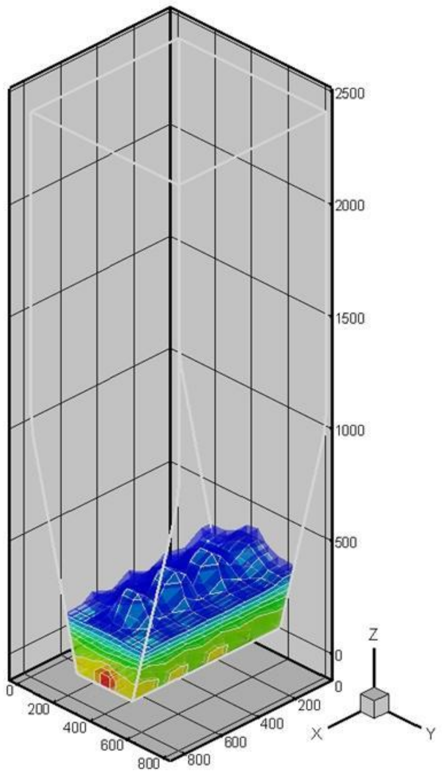




a) time = 10 minutes

b) time = 20 minutes



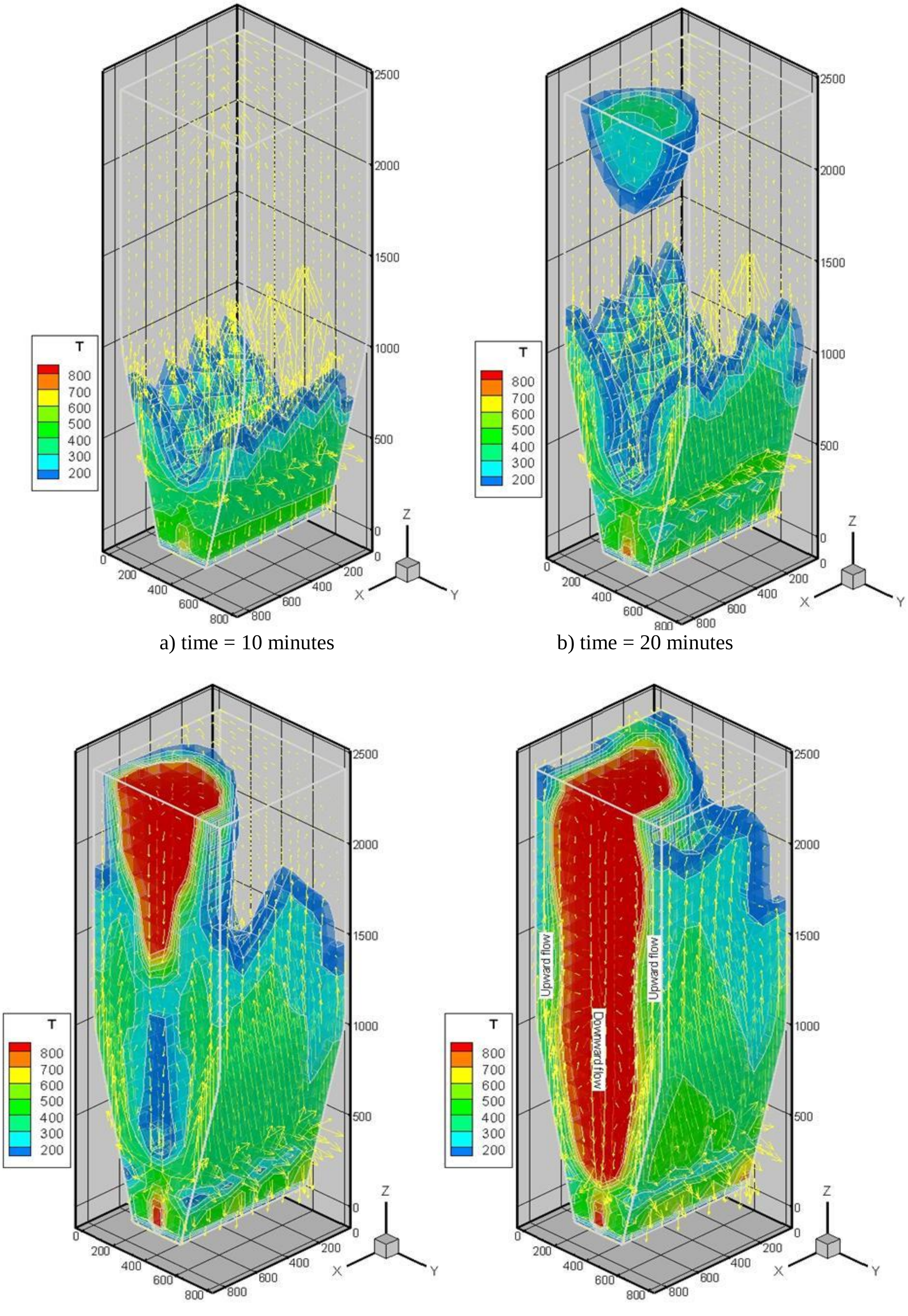


c) time = 40 minutes

d) time = 60 minutes

Figure 3. Bubbling bed expansion and contraction for 50% of Brazilian coal and 50% of biomass (charcoal)

Figure 4 shows representative results of pulverized coal/biomass and the gas phase temperature evolution for 1 h of continuous operation. In the first stage, Fig. (4a), the gas is heated up by burning auxiliary fuel and then the region of dessulfurizing bed increase the temperature. In the second stage, coal is fed from the upper part of the reactor and the ascendant high temperature gas promotes the devolatization and gasification of pulverized coal. The temperature of the gas increases as the reactions proceeds. At this moment, the auxiliary flame is stopped and the reactions is thermally self-sufficient. As the reaction rates increases the temperature of the whole reactor increase and the process reaches stable operation, as show in Fig. (4c) and (4d).



a) time = 10 minutes

b) time = 20 minutes

c) time = 40 minutes

d) time = 60 minutes

Figure 4. Temperature and flowing conditions evolution of the bubbling bed for 50% of Brazilian coal and 50% of biomass (charcoal) - temperature unit: ^oC.

Figure 5 shows the pulverized coal trajectories fed from the upper part of the reactor and the composition of volatile matter and ashes of coal. As observed the coal particles experiences downward motion while reaction takes place. The volatile matter is consumed in the upper part of the reactor and the ashes are incorporated into the dessulfurizing bed.

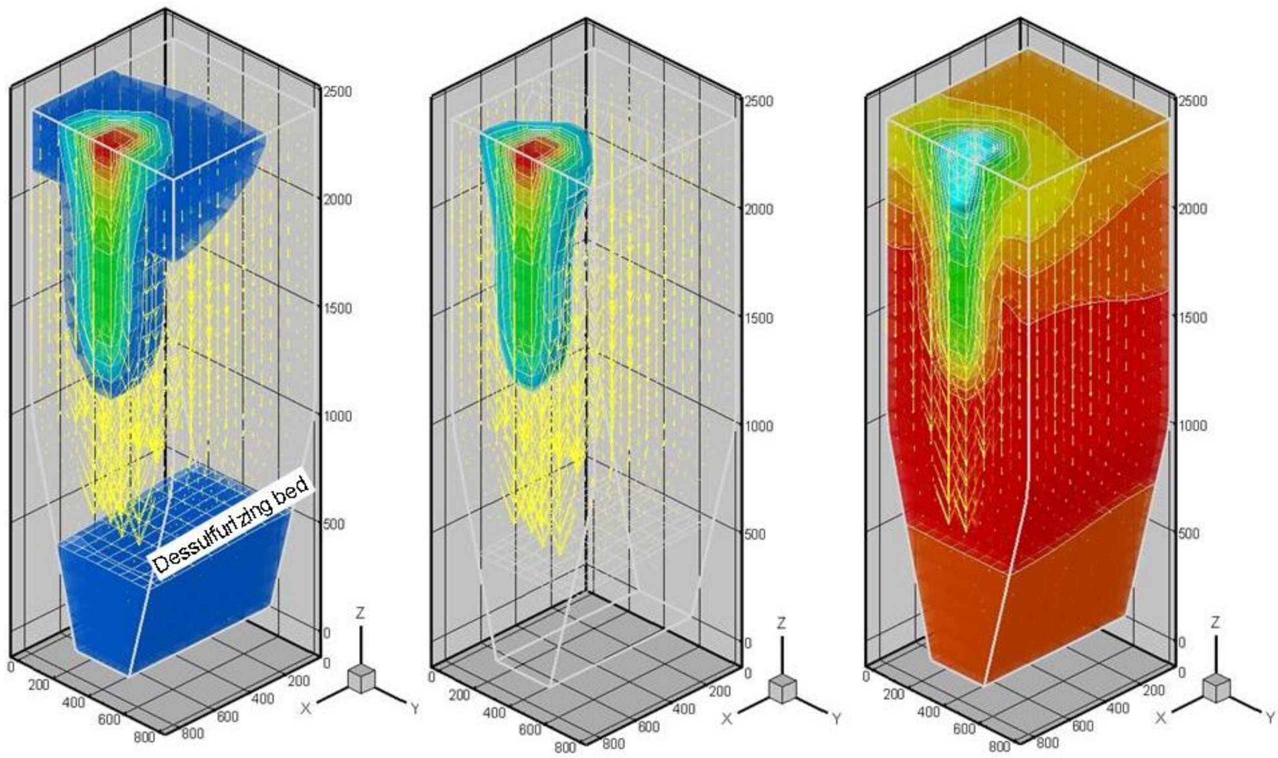


Figure 5. pulverized coal particle trajectories and coal composition evolution after 60 minutes of uninterrupted operation

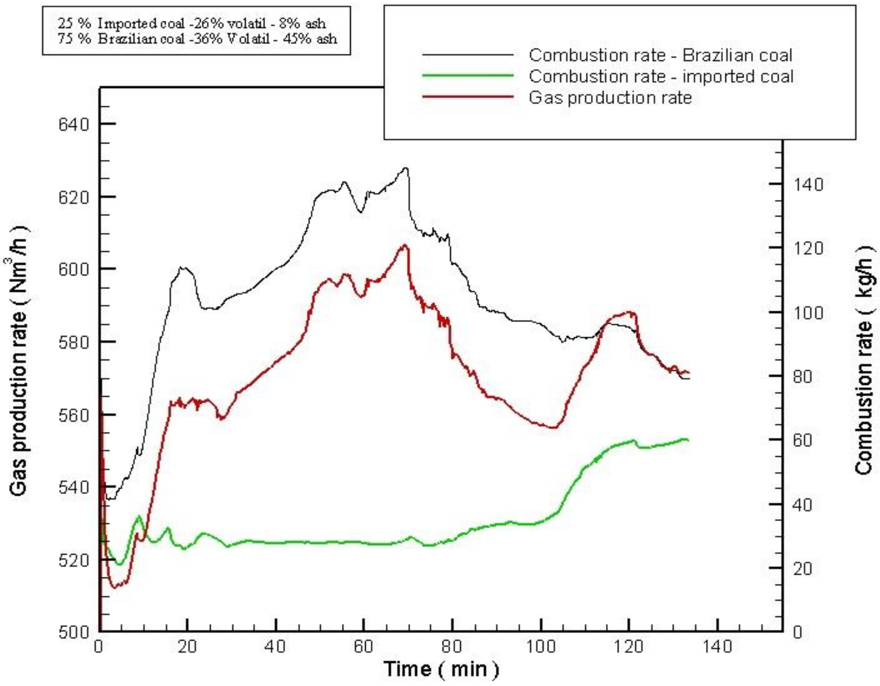


Figure 6. Gas production and combustion rates for Blend of Brazilian and imported coals

Figure 6 shows the gas production of the reactor as a function of time for 25% of imported and Brazilian coals. Regarding to the composition of the coals mainly the differences are the amount of volatile matter and ash content. At the beginning of the process the gas production start to increase and the decreases to finally became oscillating around an average value of the production target. The amount of gas and temperature targets are defined by the reactivity of the coals and the amount of oxygen blown into the feeders located at the bottom of the reactor. Figure 7 shows the averaged gas and temperature evolution. Due to process instability, the composition and temperature oscillates around the targets.

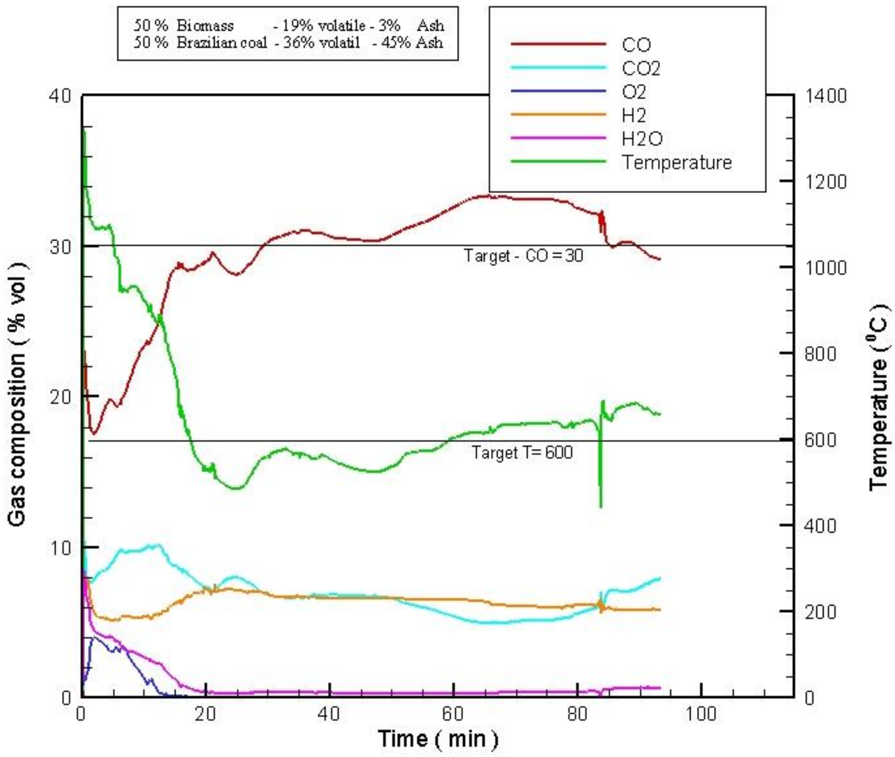


Figure 7. Outlet gas composition and temperature as a function of time for 50% of Brazilian coal and 50% of biomass (charcoal)

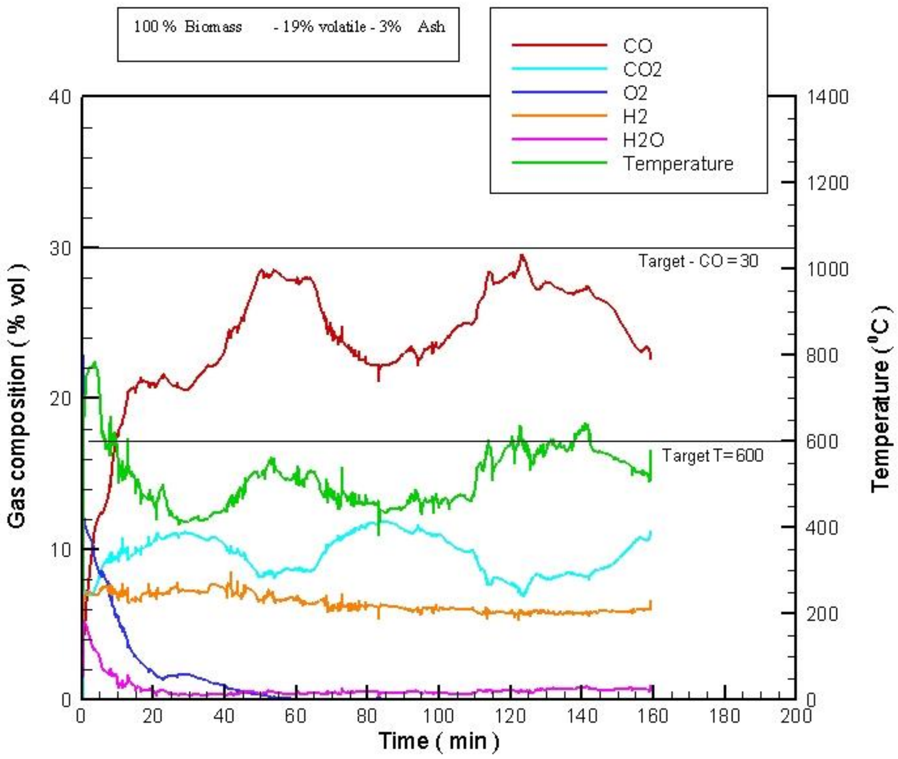


Figure 8. Outlet gas composition and temperature as a function of time for 100% of biomass (charcoal)

Figure 8 shows similar results for pulverized charcoal with same trend. When 100% of biomass is fed the gas composition and total amount burned out charcoal changes in order to attain the temperature target.

As the amount of ash of the charcoal is very low, the undesirable effect of dessulfurizing bed deterioration is minimized. Similar trend was observed for different ratios of charcoal and Brazilian coal with adjustment of oxygen enrichment and gas production. Stable operation can be achieved for all configurations of charcoal and coal proportion, however as the high ash content is increased the blubbling dessulfurizing bed must be increased and renewed.

4. CONCLUSIONS

In this paper the gasification of Brazilian blended with imported coals and biomass was investigated. Firstly an experimental laboratory scale cold non reactive experiment was predicted in order to address the bubbling conditions of the bed. Then, the model was improved to account for reaction rates and the simulations were carried out to a pilot plant reactor for gasification of coals. Based on the simulations results of the pilot plant for the gasification of biomass and coal reactor the following conclusions were pointed out: a) The bubbling fluidized bed reactor is able to produce gas for thermoelectric facilities using coal and biomass blends; b) The model was capable of reproducing the bubbling and flowing conditions of gas and pulverized phases; c) this investigation indicated that up to 25% of biomass and 75% of coal with high ash (< 30 %) is possible with stable operation. This ratio also has been obtained in the pilot plant with coals and biomasses with up to 35% of volatile matter. It was observed that as the volatile matter increases the process stability is deteriorated (evidenced by numerical prediction of instability of the bed). Therefore strict operational conditions are necessary to avoid particles stratifications and deterioration of dessulfurizing bed.

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