NHTC2001-20124

PULVERIZED COAL COMBUSTION AND ITS
INTERACTION WITH MOISTURE

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ABSTRACT

A mathematical model for combustion of wet pulverized coal in fluidized bed was developed. The equations for species concentration, energy, devolatilization, ash release to the gaseous ambient, burning of carbon and drying of the particles are solved numerically. The rate of mass consumption is kinetically controlled and simultaneous devolatilization and char combustion was considered. All chemical formulae were established for all species present in the reacting flow. Several tests were performed taken into account the reciprocal influence between wet sub-bituminous coal particles and gaseous phase. The influence of moisture in coal combustion was also analyzed. A slight reduction in combustion time was found with the increasing of the wetness in the particle and a catalytic effect of the water was detected in the conversion of CO to CO_2. Concerning the gas phase (CO), it was observed that the presence of moisture causes the displacement of the combustion zone. It was found good agreement with the experimental data available in the literature.

Keywords: Coal combustion, moisture, mathematical model.

NOMENCLATURE

A Area (m^2), frequency factor (s^{-1})
C Specific heat ($J\,kg^{-1}\,K^{-1}$), concentration ($gmol\,cm^{-3}$)
D Diffusivity ($m^2\,s^{-1}$)
d_p Particle diameter (m)
E Activation energy ($kJ\,mol^{-1}$)

G_{air} Air consumption per unit area ($kg\,m^{-2}\,s^{-1}$)
G_p Particle consumption per unit area ($kg\,m^{-2}\,s^{-1}$)
G_Σ Total consumption per unit area ($kg\,m^{-2}\,s^{-1}$)
$\overline{G_s}$ Relative consumption ($Y_s G_p / G_\Sigma$)
$\overline{h}$ Equivalent heat transfer coefficient ($J\,m^{-2}\,s^{-1}\,K^{-1}$)
H_g Gas enthalpy ($J\,kg^{-1}$)
H_Σ Bulk flow enthalpy (constant) ($J\,kg^{-1}\,m^{-2}$)
k_j Reaction rate of the reaction "j" (Arrhenius equation).
L Latent heat of vaporization ($J\,kg^{-1}$)
m Mass (kg)
N_p Number of coal particles per unit volume
P Pressure (Pa)
r_i Molar fraction of the specie "i"
R Ideal gas constant ($cal\,gmol^{-1}\,K^{-1}$)
R_o Ideal gas constant ($J\,kmol^{-1}\,K^{-1}$)
t Time (s)
T Temperature (K)
W Flow velocity ($m\,s^{-1}$)
x Position in the channel (m)
Y Mass fraction
α_{ox} Coefficient of oxidizer excess
δ^* Thickness of boundary layer (equal $d_p/2$)
ε Emissivity
φ Ratio of CO to CO_2 formed in coal combustion
μ_i Molecular mass of the specie "i" ($kg\,kmol^{-1}$)
μ_g Average molecular mass of gaseous phase ($kg\,kmol^{-1}$)

ρ Density (kg m^{-3})

σ Stefan – Boltzmann constant (W m^{-2} K^{-4})

Subscripts and Superscripts

a water
C carbon
ef effective
g gas
o initial
ox oxidizer
p Particle
R Ashes
s Particle constitute
sat Saturated
V Volatile
w Wall

INTRODUCTION

The mathematical modeling of the pulverized coal combustion presents numerous difficulties due to the complex links between the physicochemical processes involved. There are many research works dealing with coal combustion in fluidized beds, but only a few are dedicated to study the influence of the moisture contained in the coal particles (Agarwal et al., 1986; Hobbs et al., 1992, Smoot, 1998). A numerical model for coupling drying and devolatilization for large particles in fluidized bed coal combustion was developed by Agarwal et al. (1986). They admit that devolatilization and drying can happen simultaneously, but with different time scales, without chemical reactions among the volatile material and the moisture leaving the particle. In a first stage, it takes place simultaneous drying and devolatilization and, in a second moment, only devolatilization will occur. It is assumed that there is no coal combustion after devolatilization.

In order to illustrate the importance of drying in coal combustion, Hobbs et al. (1992) presented a one-dimensional countercurrent model for fixed-bed coal gasification. Besides other processes, the steady-state model considers coupled coal drying and devolatilization, oxidation of char and different gas and solid temperatures. They concluded that moisture, in typical operational conditions, influences the combustion process in less than 5%, for large particles. However, the influence of moisture considering small particles is not addressed.

Smoot (1998) reports that the combustion of low-rank coal (moisture contents in the range of 2 kg of H_2O/kg of dry coal) is a difficult process, which requires a deeper understanding of the phenomenon. Research activities in this area will contribute for the development of commercially viable power plants.

In the present work a mathematical model which couples drying and devolatilization in coal combustion was developed. This model, without considering the moisture content, was previously presented by Krioukov and Costa (1998). The aim of this study, besides improving the model by including the coal drying process, is to evaluate the influence of the moisture

in the coal combustion. The numerical results obtained in this study are compared with available experimental data.

MATHEMATICAL MODEL

In this work the coal particles composition is obtained from proximate analysis and are constituted by: a) moisture with mass fraction Y_a; b) volatile matter with mass fraction Y_V, where volatiles yield is a result of coal pyrolysis, producing gas mixture described by its chemical formula and respective mass fractions Y_{V_i}; c) char with mass fraction Y_C. All char is considered fixed carbon; d) ash with mass fraction Y_R, constituted by solid species which don't experience chemical change while released to the gaseous ambient. Each species of the ash is characterized by its chemical formula and respective mass fractions Y_{R_i}. This approach is important since the model was developed based on detailed chemical kinetics of the gaseous phase, which require an exact knowledge of the chemical formula of the each substance and its rate releases in the reacting flow. This approach allows, in the energetic characterization of the substances, to use the enthalpy concept, irrespective if it is coal, gaseous mixture or individual species, obtained from well known database (JANAF or IVTANTERMO).

Basically, the model considers a one-dimensional two-phase flow comprising the pulverized coal and hot air, assuming that the gas and the particles possesses the same momentum; the rate of mass consumption is kinetically controlled; the gas leaving the particles spreads out instantly in the channel section; gaseous diffusion along the channel is neglected; the particles are spherical and all with the same diameter; the thermal conductivity of the particle is very high; there is no interaction among particles and the pressure is constant. The following quantities,

$$G_\Sigma = G_{air} + G_p, \quad G_p = N_p W m_p, \quad G_s = Y_s G_p / G_\Sigma,$$

where $s \in (a, V, C, R)$, are required for the model description. Following, each phenomenon involved is described separately showing the respective equation.

Moisture vaporization

Frank-Kamenetski, (1989) established that rate of drop water vaporization depends on the drop temperature and can be written by

$$\frac{dm_a}{dt} = \frac{D_{ef} A_a P \mu_{H_2O}}{\delta * R_o T_p} \ln(1 - \frac{P_{sat}(T_p)}{P}) \tag{1}$$

This equation can be used to simulate the moisture vaporization from coal particles. After some algebraic manipulation, Eq. (1) becomes

$$\frac{d\overline{G}_a}{dx} = \frac{N_p W}{G_\Sigma} \frac{D_{ef} A_a P \mu_{H_2O}}{\delta^* R_o T_p} \ln\left(1 - \frac{P_{sat}(T_p)}{P}\right) \equiv f_a \qquad (2)$$

where A_a is the partial area of particle occupied by moisture.

Volatile Combustion

In the present work the yield of the volatiles is represented by a part of Kobayashi's model taking into account $Y_{V,o}$ and $Y_{C,o}$, known by proximate analysis. Therefore, the concept of "undecomposed mass" becomes only auxiliary in the resolution of the equation for mass consumption, given by

$$\frac{dm_V}{dt} = -m_{VC}(0.4K_1 + 0.8K_2) \qquad (3)$$

where m_{VC} is the initial mass coal on d.a.f..Eq. (3) needs to be integrated in time until Y_V becomes zero. This assumption is possible because it is known that the volatile yield increases with temperature in the absence of an oxidizer (Kobayashi et al., 1976). However, when the temperature level surpass 1800 K, in the oxidizing atmosphere, heterogeneous reactions in the particle surface are dominants. For this reason heavy volatiles (for example, $C_{10}H_5$) burn with the char, decreasing the volatiles yields quickly. Therefore, we can write Eq. (3) in form

$$\frac{d\overline{G}_V}{dx} = -\frac{\overline{G}_{VC}}{W}(0.4K_1 + 0.8K_2) \equiv f_V \qquad (4)$$

where $K_1 = B_1 \exp(-E_1/R_o T_p)$, $K_2 = B_2 \exp(-E_2/R_o T_p)$ and B_1, B_2, E_1, E_2 are kinetic parameters determined by Kobayashi et al. (1976).

Burning of Carbon

Monson et al. (1995) proposed a global model for char combustion in the external particle surface, given by

$$\frac{dm_C}{dt} = -A_k \exp\left(-\frac{E_k}{R_o T_p}\right) P_{O_2}^{0.5} A_{p,C} \qquad (5)$$

where P_{O_2} is the partial pressure of oxygen and A_k, E_k are kinetic parameters determined by Monson et al. (1995). After some algebraic manipulation, one obtains

$$\frac{d\overline{G}_C}{dx} = -\frac{4.836}{W} P_{O_2}^{0.5} A_k \left[\exp\left(\frac{-E_k}{R_o T_p}\right)\right] \cdot \left(\frac{N_p W}{G_\Sigma}\right)^{\frac{1}{3}} \times$$
$$\times \left(\frac{\overline{G}_C}{\rho_C}\right) \Big/ \left(\sum_s \frac{\overline{G}_s}{\rho_s}\right)^{\frac{1}{3}} \equiv f_C \qquad (6)$$

Ash release

The ash release is proportional to the char combustion in according to the volumetric consumption hypothesis. Therefore, we can write the ash consumption rate as

$$\frac{d\overline{G}_R}{dx} = f_C \frac{\overline{G}_R}{\overline{G}_C} \frac{\rho_c}{\rho_R} \equiv f_R \qquad (7)$$

Species conservation

The species conservation is described by a set of non-linear differential equations that determines the concentration of the substances in the gas phase. Consider a set of reversible reactions given by

$$\sum_i v'_{ij} A_i \rightleftharpoons \sum_i v''_{ij} A_i, \quad i = 1...n \quad j = 1....m \qquad (8)$$

where, A_i is the "i" substance, v'_{ij}, v''_{ij} are stoichiometric coefficients, n is the reacting species number and m is the reversible reactions number. Let's assume a set of irreversible reactions as

$$\sum_i v'_{is} A_i \rightarrow \sum_i v''_{is} A_i, \quad s = (m+1),...,(m+r) \qquad (9)$$

where r is the irreversible reactions number. The reverse reactions in reactions given by Eq. (8) are handled like forward reactions. So, the stoichiometric coefficients are given by

$$v_{ij} = v''_{is} - v'_{is}; \quad n_{ij} = v'_{is}; \quad j = s; \qquad s = 1,...,m$$
$$v_{ij} = v'_{is} - v''_{is}; \quad n_{ij} = v''_{is}; \quad j = s+m; \quad s = 1,...,m$$
$$v_{ij} = v''_{is} - v'_{is}; \quad n_{ij} = v'_{is}; \quad j = s+m \quad s = (m+1),...,(m+r)$$

Therefore, the forward reactions have the numbers $j = 1,...,m$, the reverse reactions $j=(m+1),...,2m$ and irreversible reactions $j=(2m+1),...,(2m+r)$, taking into account the appearance or exclusion of species in the reacting flow. Then, the molar number (n_i) of the "i" substance in a volume (V) is given by

$$\frac{1}{V}\frac{dn_i}{dt} = \sum_j v_{ij} k_j \left(\prod_q C_q^{n_{qj}}\right) C^{m_j} \quad j = 1...(2m+r); i,q = 1..n \qquad (10)$$

where C_q is the molar concentration of the "q" substance, m_j is the participation index of the M catalytic substance in the "j" reaction ($m_j =1$ or $m_j =0$). Knowing that

$$r_i = \frac{n_i}{N}, \quad N = \sum_i n_i, \quad C_i = \frac{r_i P}{R_o T}, \quad C = \frac{N}{V}$$

one can write

$$\frac{dr_i}{dt} = \sum_j \nu_{ij} k_j \left(\frac{P}{RT}\right)^{\overline{m}_j} \prod_q r_q^{n_{qj}} - r_i \sum_q \sum_j \nu_{qj} k_j \left(\frac{P}{RT}\right)^{\overline{m}_j} \prod_q r_q^{n_{qj}}$$

When very small values of concentrations are involved convergence problems arise. To by-pass this problem, the variable r_i is replaced by $\gamma_i = -\ln r_i$ making the chemical kinetics equations in exponential form, given by (Krioukov, 1995)

$$\frac{d\gamma_i}{dx} = \frac{1}{W}\left(-e^{\gamma_i}\sum_j \nu_{ij}\Omega_j + \sum_q \sum_j \nu_{ij}\Omega_j\right) \qquad (11)$$

where

$$\Omega_j = k_j \left(\frac{P}{RT_g}\right)^{\overline{m}_j} \exp\left(-\sum_q n_{qj}\gamma_q\right), \qquad \overline{m}_j = m_j - 1 + \sum_q n_{qj}$$

$$j = 1,\ldots,(2m+r), \qquad\qquad i, q = 1,\ldots,n$$

Gas energy

The gas energy equation couples gas temperature, species concentration and gas enthalpy (Alemassov et al., 1971), and is given by

$$H_g - \frac{\sum H_i r_i}{\sum r_i \mu_i} = 0 \qquad (12)$$

where $H_i = f_i(T_g)$ is the molar enthalpy of the "i" substance.

Mass conservation for the whole mixture

Making $G_\Sigma = G_p + G_g = const$, one can write

$$\sum_s \overline{G}_s + \frac{P\mu_g}{R_o T_g}\frac{W}{G_\Sigma} - \frac{P\mu_g}{R_o T_g}\cdot\sum_s \frac{\overline{G}_s}{\rho_s} - 1 = 0 \qquad (13)$$

Energy equation for the bulk flow

Making $\sum H_s G_s + H_g G_g = H_\Sigma = const$, the energy equation is settled by

$$\sum_s H_s \overline{G}_s + H_g \rho_g W (1 - A_{kp})/G_\Sigma - H_\Sigma/G_\Sigma - Q_w = 0 \qquad (14)$$

where A_{kp} is the area of the channel occupied by the particles; Q_w is the heat transfer flux through the wall channel; $H_\Sigma = H_g^o G_g^o + H_p^o G_p^o$ is the enthalpy per unit area (J m^{-2} s^{-1}), which is constant. Recall that H_g and H_p are not constant.

Energy equation for the particle

The energy balance on a single coal particle is given by (Tang and Ohtake, 1988)

$$\frac{dT_p}{dt} = \frac{A_p \overline{h}(T_g - T_p) - A_p \sigma\varepsilon(T_p^4 - T_w^4) + \frac{dm_v}{dt}L_V}{C_\Sigma \sum m_s} +$$
$$\frac{-(1-\varphi)\frac{dm_C}{dt}\frac{\Delta H_{CO}^+}{\mu_C} - \varphi\frac{dm_C}{dt}\frac{\Delta H_{CO_2}^+}{\mu_C}}{C_\Sigma \sum m_s} \qquad (15)$$

which takes into account that the particle is heated by convection, radiation and heat generated throughout vaporization of volatile matter and heterogeneous reaction in its surface. In the present simulation a more complete form of the energy equation is used, as

$$\frac{dT_p}{dx} = \frac{\frac{4.836}{W}\left(\frac{N_p W}{G_\Sigma}\right)^{\frac{1}{3}}\left(\sum_s \frac{\overline{G}_s}{\rho_s}\right)^{\frac{2}{3}}\left[\overline{h}(T_g - T_p) - \sigma\varepsilon(T_p^4 - T_w^4)\right]}{C_\Sigma \sum_s \overline{G}_s} +$$
$$+ \frac{+ f_V L_V + f_a L_a + (T_g - T_p)\left[\sum_s f_s C_s^g - f_C\left(\frac{1+\varphi}{2}\right)\frac{C_{O_2}\mu_{O_2}}{\mu_C}\right]}{C_\Sigma \sum_s \overline{G}_s} -$$
$$- \frac{f_C\left[(1-\varphi)\frac{\Delta H_{CO}^+}{\mu_C} + \varphi\frac{\Delta H_{CO_2}^+}{\mu_C}\right]}{C_\Sigma \sum_s \overline{G}_s} \qquad (16)$$

where $f_V L_V$ represents the energy spent in the pyrolysis of the volatiles and $f_a L_a$ the energy spent in the water vaporization. The term following the $f_a L_a$ in Eq. (16) represents the energy spent in heating the volatiles and ashes up to the gas temperature; $C_\Sigma = \sum(\overline{G}_s C_s)/\sum \overline{G}_s$ is the average heat capacity of the particle (J kg^{-1} K^{-1}); ΔH_{CO}^+, $\Delta H_{CO_2}^+$ are the heat formation of the CO and CO_2 (J kmol^{-1}); C_s^g are the average heat capacity calculated in the film temperature for all species that leaves the particle and C_{O_2} is the heat capacity of oxygen.

Ratio of CO and CO_2 formation

The heterogeneous reaction in the particle surface produces CO and CO_2 as a function of its temperature (Monson et al., 1995). The reaction is described by

$$C + \frac{1+\varphi}{2} \Rightarrow \varphi CO_2 + (1-\varphi)CO \qquad (17)$$
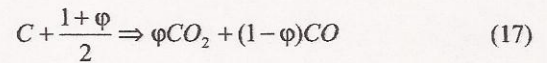
where the ratio of CO to CO_2 formed is related by

$$\frac{1-\varphi}{\varphi} - A_c \exp(-E_c/R_o T_p) = 0 \qquad (18)$$

where A_c and E_c are kinetic parameters established by Monson et al. (1995). The reaction $C+CO_2 \rightarrow 2CO$ also takes part of the reaction mechanism.

Reaction constants in coal combustion

The thermal decomposition of coal particles is assumed to consist of a series of chemical reactions with reaction constants k_i. These constants are determined for each particular reaction. With this assumption, the emission of volatile is described in the model by a zero order reaction: $\rightarrow V_i$, with $i=1..n_V$, where n_V is the number of the volatiles species, and its reaction rate is given by

$$k_{V_i} = -0.001 \frac{Y_{V_i}}{\mu_{V_i}} \frac{G_\Sigma f_V}{1 - \sum \overline{G}_s} \qquad (19)$$

where f_V is given by Eq. (4).

Note that the devolatilization happens proportional to initial mass of each volatile species (d.a.f.) and the volatile composition in the two competing reaction is the same. In spite of having other devolatilization models in the literature, the model used here shows good overall agreement with the available experimental data.

Similarly, the emission of moisture in gaseous ambient is described by the zero order reaction: $\rightarrow H_2O$ with the reaction rate given by

$$k_{H_2O} = -\frac{0.001 Y_{H_2O} G_\Sigma f_a}{\mu_{H_2O} \left(1 - \sum_s \overline{G}_s\right)} \qquad (20)$$

Similarly, for carbon combustion, based on the reaction described by Eq. (17), we have

$$k_{CO_2} = 2\varphi k_C \quad \text{and} \quad k_{CO} = (1 - \varphi)k_C$$

where

$$k_C = 9.06\,10^{-3} \frac{A_r}{\mu_C} A_k T_g^{0,5} \exp\left(\frac{-E_k}{R_o T_p}\right) \qquad (21)$$

where A_r is the partial area occupied by carbon in the particle, and φ is obtained by Eq.(18). For the ash, the reaction constants are given by

$$k_{R_i} = k_C Y_{R_i} \left(\frac{\mu_C}{\mu_{R_i}} \frac{\overline{G}_R}{\overline{G}_C} \frac{\rho_C}{\rho_R}\right) \qquad (22)$$

The resulting mathematical model has (n + 9) algebraic differential equations with the unknowns γ_i, $\overline{G}_a$, $\overline{G}_V$, $\overline{G}_C$, $\overline{G}_R$, T_p, T_g, W, H_g and φ. Its solution is numerically feasible only using special methods for treating the stiffness of the equation system. The method used here is described in Costa et al. (1999). The enthalpy and the entropy of the gaseous species are calculated by a seventh degree polynomial and of the solid species by a third degree polynomial, both with coefficients obtained from Alemassov et al. (1971). The specific heat is calculated by the derivative of the enthalpy with respect to temperature. The code was written in FORTRAN 90. The model is independent of the gas composition, that is, it can consider any mechanism of elementary reactions, rendering to the model generality.

RESULTS AND DISCUSSION

Comparison with other studies

The initial data used by the model are presented below. The gaseous phase is composed by air with two initial temperatures, 1410 K and 1900 K and pressure of 0.1 MPa. Both cases are studied. The fuel is sub-bituminous coal with the elemental formula $C_{7,032}H_{6,572}O_{0,438}Al_{0,0475}Si_{0,027}$. Table 01 presents a summary of coal properties used in the tests.

Coal particles of diameter 55 μm at 600 K enter the hot gas. The enthalpy of the coal was calculated by the scheme presented by Spilimbergo and Iskhakova (1996).

The mechanism of chemical reactions in the gaseous phase includes 48 substances and 136 elementary reactions (Westbrook and Dryer, 1981, Calcote and Keil, 1988). The kinetic coefficients of Eq. (6) were determined empirically fitting the experimental data of Jost et al. (1984), and their values are $A = 16$ kg m^{-2} s^{-1} atm$^{-0,5}$ and $E = 32.21\,10^6$ J kmol^{-1}. This fitting was necessary because their original values were established in the absence of the volatile matter, which is known to affect the consumption rates.

Table 01
Summary of coal properties

Coal type	Sub-Betuminous
Proximate analysis	
VM	46.54
Fixed carbon	49.41
Ashes	4.05
Volatile Matter (%)	
CH_4	43.75
C_6H_6	41.25
O_2	3.75
CO	7.50
CO_2	3.75
Ashes (%)	
Al_2O_3	60.00
SiO_2	40.00
Heat of combustion (coal)	30.59 MJ kg^{-1}

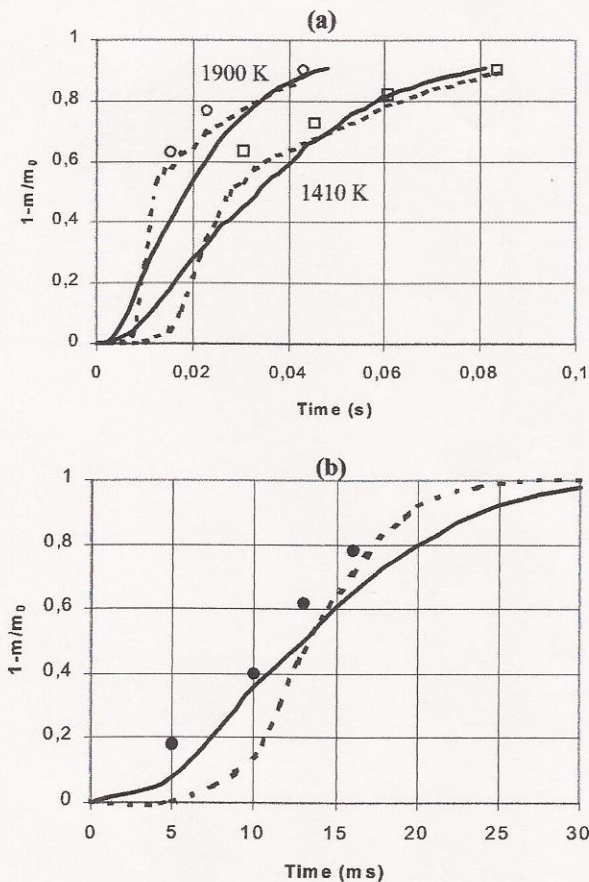Fig. 1 Comparison of the results predicted by the model (——) with (a) experimental data of Jost et al. (o , □) and numerical data of Veras et al (·····) for 1410 K and 1900 K. (b) with the consumption of volatile for 1900 K with experimental data (●) and numerical (······) of Visona and Stanmore.

Fig. 2. (a) Relative mass fraction for char and volatiles for 0%, 20% and 40% of moisture. (b) Gas temperature for 0%, 20% and 40% of moisture.

As this model admits the gas temperature variation as the chemical reactions rate increases, it was used a very high value for the air excess coefficient (α_{ox}=30, for example) to simulate a constant temperature in the gaseous environment.

For each run, the particle temperature never increased more than 600 K above the gas temperature, what is in agreement with the extensive experimental data of Pomerantsev et al. (1986).

The results obtained by the model for the total mass consumption of the particles were compared with the experimental data of Jost et al. (1984) and the numerical results of Veras et al. (1999). As shown in Fig.1 the agreement is good. The results obtained for the consumption of the volatile matter were compared with the experimental results of Visona and Stanmore (1996), again demonstrating good agreement. However, inspecting Fig. 1, one can see that it is necessary
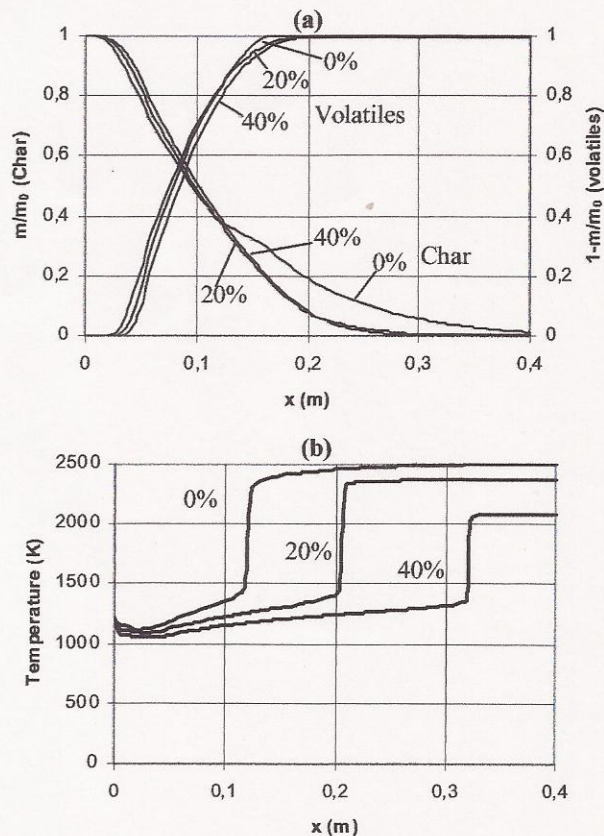
to improve the mathematical model for better results for the initial stage of the process.

As it can be observed, the mass and volatile consumption predicted by the model are a little slower than the experimental data. This is due, partly, to the formulation of the model which considers the combustion process being only kineticaly controlled.

Influence of Moisture

This test is conducted with the same initial conditions already reported, changing only the enthalpy of the coal to take into account the presence of the moisture. One should observe that with the increment of the wetness (U_m) the reacting flow becomes poorer, since G_{ox} and G_p are constant.

When $U_m = 0\%$ one has the stoichiometric conditions, that is, $\alpha_{ox} = 1$.

In the following figures it is presented the results obtained for $U_m = 0\%$, 20% and 40%. The combustion conditions of the sub-betuminous dry coal are preserved for the wet coal.
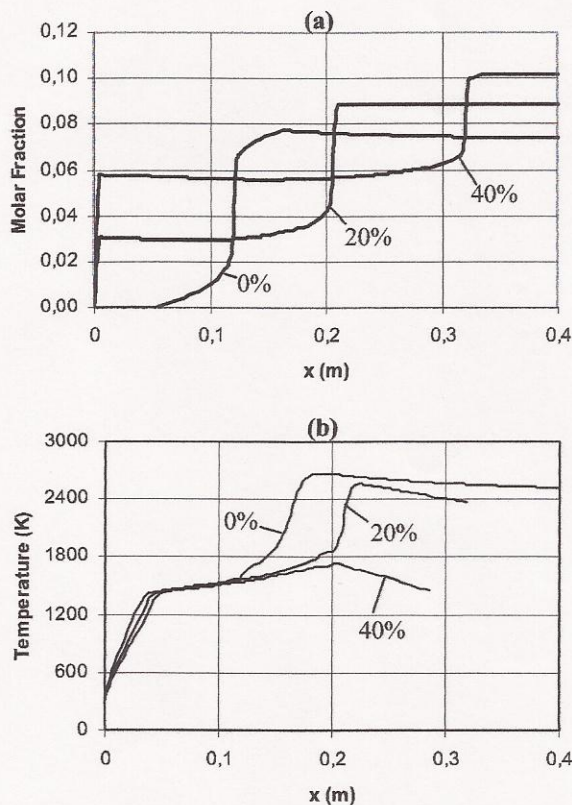
Fig. 3. (a) Molar fraction of the H_2O and (b) Particle temperature for 0%, 20% and 40% of moisture.

Fig. 4 (a) Molar fraction of CH_4 (——) and C_6H_6 (——) along of the channel and (b) Molar fraction of CO for distinctive moisture levels.

With the increment of the moisture, the releasing time of the volatile matter increases. For this reason the T_g level is reduced with the increase of the moisture content (Fig 2(b)). The char burning time, by its turn, is slightly reduced (Fig. 2(a)). This fact was observed experimentally by Jung and Stanmore (1980). In the model, this fact can be explained when we observe that for dry coal, the stoichiometric condition (α_{ox}=1) applies. With the increase in the moisture, the initial mass of carbon is relatively reduced, which provides α_{ox} >1, what causes a larger initial concentration of the O_2 in the gaseous phase. Therefore, char combustion rate is faster. Figures 2(b) and 3(b) presents the behavior of the temperatures T_g and T_p along the combustion channel for different moisture levels.

It was verified that with the increasing of moisture level, the temperature gradient of the gas in the zone of gaseous combustion is reduced and moved along the channel (Fig. 2(b)). This happens because the gas releases energy to H_2O with the consequent reduction of the reaction rate in the gaseous phase. The influence of the moisture in the particle temperature is less significant (Fig. 3(b)). The energy loss from the particle 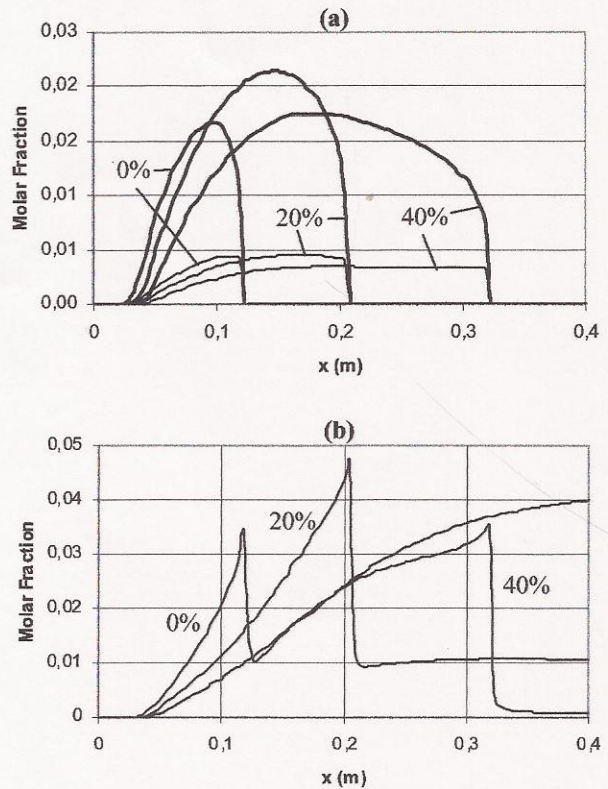to the gas, due to the moisture, is compensated by a larger concentration of O_2 in the gaseous phase, increasing the heterogeneous reactions during the whole process.

In this aspect, one can observe interesting effects for U_m=40%. The particle of the coal is entirely consumed before the ignition of the volatile material. This can be seen in Fig. 4(a), where the evolution of the CH_4 and C_6H_6 present in the gaseous phase is reported. It is evident that with the increase in U_m the place in which the concentration decreases moves along the channel. These findings require a deeper analysis in order to be fully confirmed.

Clearly, a larger rate of U_m corresponds to a larger molar fraction of the H_2O at the end of the process (Fig. 3(a)). It can also be seen that for 0.12 m < x < 0.2 m one has r_{H_2O} (U_m = 0%) > r_{H_2O} (U_m = 40%). The reason for this is that the combustion of the volatile happens earlier for $U_m = 0$.

The role played by the intermediary substance CO (Fig. 4(b)) is interesting. This figure shows that CO presents a peak in the combustion zone, an indication of its accumulation and burning in the combustion zone. Its monotonic growth at the end of the channel is due to the combustion of the remaining char, generating small concentrations of CO (T_p > 1800 K).

CONCLUDING REMARKS

The mathematical model developed in this work for pulverized coal combustion demonstrated good behavior when the main physical phenomena are considered, namely, the combustion in the gaseous phase, combustion of the char, release of residues and simultaneous drying and devolatilization.

A characteristic of the mathematical model is that it requires the chemical formulae of the reacting species. Therefore, the model is independent of the gas composition. This means that it can consider any mechanism of elementary reactions and can deal with gaseous and solid species. Furthermore, thermochemical properties forms a database of the code, allowing to choose any coal composition in the simulation.

The comparison with experimental and numerical results showed good agreement when considering simulations for the global combustion rates of the particle and volatile matter. However, the coefficients for the combustion of char and volatile matter need to be better determined through experimental results.

The presence of moisture increases the char combustion rate, specially when it is considered the heterogeneous reactions between char and CO_2. Important catalytic effect is done by the water in the oxidation of CO, reducing its concentration, while the ratio CO_2/CO is increased.

The mathematical model can be improved including new species in database, including limestone in reacting flow and improving the devolatilization model to take into account light and heavy volatiles.

ACKNOWLEDGMENTS

REFERENCES

Agarwal, P. K., Genetti, W. E. and Lee, Y. Y., 1986, "Coupled drying and devolatilization of wet coal in fluidized beds." Chemical Engineering Science, Vol. 41, Nº 9, pp. 2373-2383.

Alemassov, V. E., Dregalin, A. F., Tishin, A. P., Khudiakov, V. A. and Kostin, V. I., 1971, "Thermodynamic and Thermophysical properties of the combustion products." Guia, Vol. I., VINITI. Moscou, URSS, (in Russian).

Calcote, H. F. and Keil, D. G., 1988, "Ion-molecule reactions in sooting acetylene-oxigen flames," Combustion and Flame, 74, pp. 131-146.

Costa, V. J., Krioukov, V. G. and Maliska, C. R., 1999, "Pulverized Coal Combustion: A Numerical Analysis of the Main Parameters," Proceedings of 15th Brazilian Congress of Mechanical Engineering, Águas de Lindóia, SP, Brazil.

Frank-Kamenetsky, D. A., 1989, "Difusion and heat transfer in Chemical Kinetics," Nauca, Moscou.

Hobbs, M. L., Radulovic, P. T. and Smoot, L. D., 1992, AIChE J., 38, 681

Jost, M. E., Leslie, I. and Kruger, C., 1984, 20º Symp. Inter. on Combustion/The Combustion Institute, pp.1531-1537.

Jung, K. and Stanmore, B. R., 1980, "Fluidized bed Combustion of wet brown coal," Fuel, 59, pp. 74-80

Kobayashi, H., Howard, J. B. and Sarofim, A. F., 1976, "Coal Devolatilization at High Temperatures," Proceedings 17º Inter. Symp. on Combustion/The Combustion Institute, p.411-425.

Krioukov, V. G., 1995, "Mathematical Modeling of Pollutants Emission," Proceedings of COBEM-CIDIM, Belo Horizonte – MG, Brazil.

Krioukov, V. G. and Costa, V. J., 1998, "Pulverized Coal Combustion in reacting flow: modeling of the main parameters", Proceedings of 7º Latcym, Salta, Argentina, pp. 81-86. (in Portuguese).

Monson, C. R., Germane, G. J., Blackham, A. U. and Smoot, L. D., 1995, "Char Oxidation at Elevated Pressures," Combustion and Flame, 100, pp. 669-683.

Pomerantsev, V. V., Arefhev, K. M., Akhmedov, D. B., Konovich, M. N., Korchunov, J. N., Rundiguin, J. A., Shagalova, S. L. and Shestakov, S. M., 1986, "Theoretical foundations in the practice of combustion," Leningrad, 2ª ed., Energoatomisdat. 312 p. (in Russian).

Smoot, L. D., 1998, "International research center's activities in coal combustion," Prog. Energy Combust. and Sci., Vol. 24, pp. 409 – 501

Spilimbergo, A. P. and Iskhakova, R. L., 1996, "Modeling of Reacting Flows in Nozzles," Brazilian Congress of Engineering and Thermal Sciences, Vol. 3, Florianópolis, SC, Brazil, pp. 1499. (in portuguese).

Tang, B. and Ohtake, K., 1988, "Computer Simulation and NO Formation in Pulverized-Coal Combustion," Coal Combustion Science and Technology of Industrial and Utility Applications, Ed. Hemisphere Publishing Corporation, pp. 199-206.

Veras, C. A. G., Saastamoinen, J., Carvalho Jr., J. A., and Aho, M., 1999, "Overlapping of the Devolatilization and Char Combustion Stages in the Burning of Coal Particles," Combustion and Flame, Vol. 116, pp. 567-579.

Visona, S. P. and Stanmore, B. R., 1996, "Modeling NO_x Release from a Single Coal Particle I. Formation of NO from Volatile Nitrogen," Combustion and Flame, 105: 92-103.

Westbrook, C. K. and Dryer, F. L., 1981, "Simplified reaction mechanisms for the oxidation of hydrocarbon fuels in flames," Combust. Sci. Technol., pp. 27, 31-43.