NUMERICAL STUDY ON THE TRANSIENT IGNITION OF SINGLE COAL PARTICLE WITH THE CMVC-CPDNLG MODEL

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Abstract. *This paper deals with a parametric study on the transient ignition of single particle coal combustion. Simulation were carried out using the CMVC (Continuous Model for Volatile Combustion) in which a comprehensive devolatilization sub-model was implemented. Devolatilization has important effects on the ignition, as well as on the remaining steps of coal combustion. Therefore, accurate predictions for the pyrolysis phase claim devolatilization models which are more phenomenological in nature. In this paper, the CPDNLG (Chemical Percolation Devolatilization Model- Nitrogen and Light Gases) devolatilization model was used to estimate pyrolysis rates as well as volatile gas composition. The parametric study showed that ignition might be homogeneous, heterogeneous, or hetero-homogeneous depending on heating rate, particle size, coal rank, gas temperature, and oxygen concentration. In the analysis, for the majority of the cases, hetero-homogeneous ignition prevailed.*

Keywords: Coal ignition, CMVC-CPDNLG model, pulverized solid combustion

1. INTRODUCTION

Coal is the most abundant fossil fuel in the world, accounting for about 34% of all the electricity generated (Williams et al., 2001). Pulverized coal combustion is the option for the conversion due to the relatively high combustion intensity. Pulverized fuels (50 to 500 μm) burn, in general, by three different processes. Heating, drying and pyrolysis (i) that sustains homogeneous combustion of volatiles - gas flame (ii), and, lastly, heterogeneous char oxidation (iii) at particle surface and in the porous structure. These processes are not necessarily sequential; some overlapping is observed in most of the cases. Either, gas phase combustion or coal heterogeneous oxidation must be preceded by ignition. It is generally accepted that, depending on a combination of different factors, ignition may take place at the particle surface, due to heterogeneous reaction, or in the gas phase, due to volatile combustion. Which mechanism prevails is still a subject of recent research. Large particles, at low heating rates are more prone to ignite homogeneously (volatiles combustion) while small particle heated rapidly, in general, ignite by direct attack of oxygen on the whole coal (surface and porous structure) as pointed by Essenhigh *et al.*, (1989). Annamalai and Durbetaki (1977), claimed a transition of the ignition phase in the burning of coal particle. Howard and Essenhigh (1967, 1967a) claimed that small bituminous coal particle ignites most probably at the surface. Annamalai and Durbetaki (1977) showed that a seam bituminous particle which size is below 350 μm might not undergo gas phase ignition. A comparative study of the ignition behavior of wood, peat and coal was presented by McLean (1982). Couturier *et al.* (1996) have discussed the ignition and flame stability of pulverized wood flames. Solomon and co-workers (1990) performed experiments in coal combustion. Photographs of several ignited coal particles were carefully observed. They concluded that the injected particles first ignite and appear to burn at the surface of the particle, indicated by the fact that the width of the luminosity is roughly that of the particle diameter. The second ignition phenomenon takes place after the particles have burned for a short time. The calculated dimension of this second luminous zone is about three times the original dimension. This implies a radiant gas flame (CO oxidation) at about two particle radii far from the surface of the particle. More than 80% of Rosebud sub-bituminous coal particles (53-75 μm diameter) surrounded by a dry ambient airflow (850 °C, 1 atm) that exhibited the first ignition has also exhibited the second ignition phenomenon. Chen et al (1993) presented a novel experiment to study the ignition of pulverized coal. The coal samples were about 136 μm, in average, ranking from sub bituminous to anthracite. In their experiments, video images revealed that ignition of the bituminous and sub bituminous coals apparently occurred heterogeneously. Mühlen and Sowa (1995) conducted experiments in a pressurized heated-grid apparatus, concluding that the temperatures of homogeneous and heterogeneous ignition are strongly influenced by oxygen partial pressure and heating rate as well as coal rank and maceral composition.

Fuertes *et al.* (1993) use captive technique for direct measurement of ignition temperatures of coal and char particles. The measured temperatures were in the range from 685 °C, for a high-volatile bituminous coal, to 1090 °C for the metallurgical coke. Ignition of coal, char and carbon particles has been also under investigation (Fu and Zhang, 1992, Lee *et al.*, 1995).

Du and Annamalai (1994) presented a transient model for ignition of coal particle. The model was continuous and the kinetics of oxidation of volatiles was that of the oxidation of methane. Coal particle temperatures were time dependent but spatially uniform. For devolatilization, they used the kinetic parameters of two competing reactions given by Ubhayakar *et al.* (1976). They claimed that the transition of ignition phase (TIP), from heterogeneous to homogenous ignition mode occur at particle size of about 400 microns. Particles, smaller than the size for TIP, ignite heterogeneously at first, while those larger than that experiment volatiles gas phase ignition. Their theoretical investigations concerned a gas at 1500 K containing 23% O_2 (mass fraction).

Du et al. (1995) presented a model for group combustion of a cylindrical stream of coal particles (64 μm). They found that homogeneous ignition occurs for a dense cloud, while heterogeneous ignition occurs for a dilute cloud.

Chen et al. (1996) studied the ignition of coal particles by thermogravimetry and differential thermal analysis. Experiments were carried out at low heating rate, particle sizes in the range of 37 to 4000 μm. The main conclusion were: (i) increasing coal quality, from lignite through bituminous to anthracite, the type of ignition change from homogeneous ignition through hetero-homogeneous ignition to heterogeneous ignition and (ii) with increasing coal particle size, the type of ignition for the bituminous coal change from hetero-homogeneous to homogeneous ignition.

Sun and Zhang (1998) performed a detailed experimental study of the ignition of coal particles at high pressures in a thermogravimetric analyzer. A possible shift in the mechanism of ignition, from homogeneous to heterogeneous, was suggested at high pressure. Grotkjær et al. (2002) conducted an experimental study on the ignition of biomass particles. They proposed that the ignition process is initiated by oxidation reactions on the straw surface. The higher particle surface temperature promotes the ignition of the surrounding volatiles that may form a diffusion flame away from the particle.

This ample review shows that, most of the research was concentrated on experimental work. Theoretical study is still modest and the models presented were based on different level of assumptions. Basically, particles were treated as isothermal, devolatilization models were not phenomenological and gas phase reactions mechanisms were quite simplified.

In this work, we present a transient ignition study of coal particles, based on the CMVC model in which a phenomenological pyrolysis sub-model (CPDNLG) was implemented. Up to now, the authors are not aware of any publication in the field in which such tools were employed.

2. NUMERICAL MODEL

In this work, we used the CMVC model ("Continuous Model for Volatiles Combustion") to analyze the transient ignition mode. The model was primarily used to investigate the burning of coal and char particles under pressurized conditions (Gurgel Veras *et al.*, 1999). It was further improved to allow the analysis of NO formation in the devolatilization phase of a burning coal particle (Gurgel Veras *et al.* 1998). More recently, the CMVC model was extended to analyze pulverized biomass combustion. Here, a description of the main characteristics of the CMVC model is provided.

The model was designed to calculate the dynamic chemically reacting flow around an isolated solid fuel particle in one-dimensional geometry. In this continuous model, the width of reaction zone in the gas phase is not infinitesimal, as assumed in the flame sheet model, but rather established by the local concentration of the reactants and the gas temperature.

Particle temperature distribution is possible along with the transient effects. If heating rates are high, there will be a temperature gradient inside the solid matrix. Devolatilization rates predicted by models that assume coal and biomass particle temperature as spatially uniform far exceed those that take into account the distribution of the temperature in the solid matrix.

Specific heat and thermal conductivity for coal and biomass are function of temperature and the local level of thermal degradation. Char is modeled as carbon with the specific heat calculated with the parameters given by the NASA SP-273 computer code (Gordon and McBride, 1971).

Devolatilization rates and volatiles composition were calculated with the CPDNLG (Chemical Percolation Devolatilization Model, Nitrogen and Light Gases) model. Gas phase reactions are calculated in two steps, physical properties also varies as a function of local gas concentration, pressure and temperature.

Theoretical investigation of coal combustion necessarily claims modeling of coal devolatilization. Since the process of coal pyrolysis is quite complex, it is expected that the results from the CMVC model are dependent on the applicability of the pyrolysis model (sub-model) for the case under investigation. Applications of such models, usually, are restricted to the experimental conditions in which the rate parameters were collected. The rate parameters are dependent on the kind of coal, heating rate, devolatilization temperatures and pressures, to mention few. Generally, pyrolysis sub-models are based on single and double competing reactions with fixed Arrhenius parameters. Three pyrolysis model based on two first order competing reactions given by, Kobayashi et al. (1976), Ubhayakar et al. (1976) and Gat et al. (1983) have been used extensively. Volatiles evolved can be taken as (i) light gases (H_2, CO, CH_4) and (ii) tar, in the CMVC model. The rates of light gases and tar should then be linked to the two rate equations, respectively. The composition of light gases and tar evolved can be taken as an input data. However, in order to track more specifically the evolution of a large number of species, it is required a model based on a multiple independent parallel reactions. Such model is known as Distributed Activation Energy Model – DAEM. Donskoi and McElwain (2000) have criticized this model, regarding computational efforts. Predictions of pyrolysis rates in cases where the instantaneous temperature varies require integration for every time step and point in space.

Specifically, in the CMVC model, particle is treated as non-isothermal and the model is transient. Therefore, every control volume has its temperature and devolatilization histories that determine the instantaneous mass release. The computational effort, however, is plenty justified if the predictions are quantitatively more accurate for a broad range of burning conditions. Detailed models for coal pyrolysis should, then, replace models based on single or double reactions. Such sub-models, of course, are not commonly applied in comprehensive codes for coal combustion.

Currently, there are three network devolatilization models able to predict coal thermal decomposition under a broad range of temperature, heating rates and pressures. The models are: (i) Functional Group – Depolymerization, Vaporization Cross linking model (FG_DVC), Solomon et al. (1988); (ii) FLASHCHAIN (Niksa, 1991) and (iii) the

Chemical Percolation Devolatilization Model (CPD), Grant et al. (1989). In spite of the number of input data used in each of these models, they all have some features that are common: the coal is described with structural parameters obtained experimentally (i); tar release and bridge scission are described by means of statistical network model (ii); first order reaction rates with distributed activation energies are used for depolymerization, crosslinking and light gas formation (iii) and a correlation of vapor pressure with tar molecular weight to model the evaporation of tar (iv). The great advantage of such models relies on their phenomenological nature compared to the empirical approach observed in former ones. Some of these steps are shown in Figure (1) for a hypothetical coal molecule (Pittsburgh Seam bituminous).

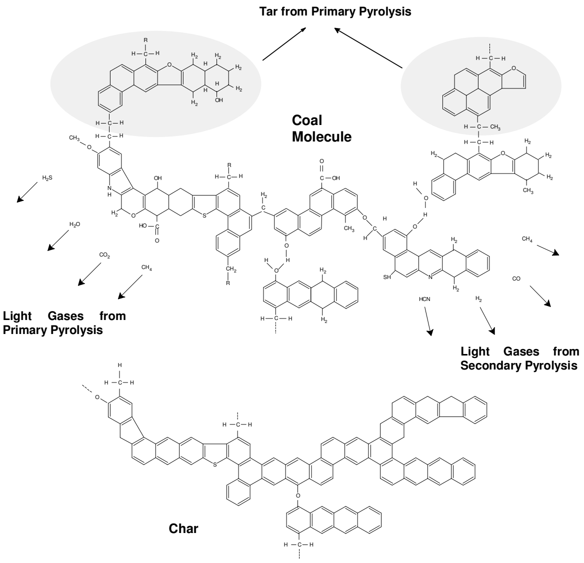

Figure 1: Hypothetical coal molecule under thermal degradation, (adapted from Solomon et al., 1988).

The CPDNLG model has the capability of predicting the fractions of coal mass released in the form of CO, CO_2, CH_4, H_2O, and others. It also predicts the quantity and form of nitrogen released during devolatilization based on the chemical structure of the coal (Genetti, 1999). The dynamic release of light gases and tar as devolatilization progresses is important on the ignition and stabilization of coal flames. Knowledge of the amount and form of nitrogen that is released as volatiles as well as the mass that stays in the char is of great importance in predicting NO formation from homogeneous and heterogeneous reactions of coal particles. The CPDNLG model calculates the rate of volatiles evolution for coals which rank varies from lignite to anthracite. More recently, the CPD model was extended to predict the evolution of volatiles from biomass (Sheng and Azevedo, 2002). Also, the model can be applied for any heating rate, particle temperature and ambient pressure.

Figure (2) shows the dynamic evolution of CO and CH_4, under thermal degradation in an inert atmosphere (1200 K, 2 bar), for a 160 μm particle size for two coal types, lignite (**L**) and an anthracite (**A**) as predicted by the CPDNLG model.

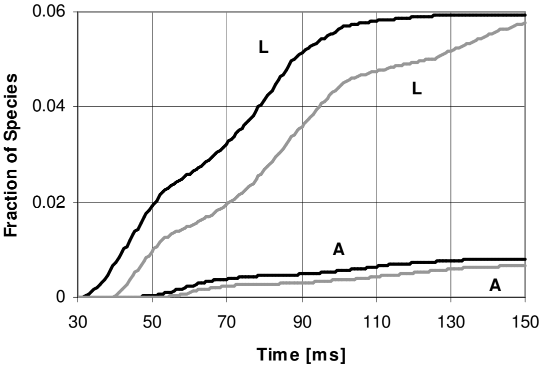

Figure 2: Dynamic evolution of CO (gray) and CH_4 (black) for lignite (L) and anthracite (A) coals.

As it shows, methane is evolved more rapidly and in higher amounts than CO for the lignite coal. These gases are almost insignificant for the anthracite. Carbon monoxide when reacting with oxygen liberates a great deal of energy, while the oxidation of CH_4 takes place in more successive steps. Water is an important source of radicals that accelerate the CO oxidation. Since water is evolved as a pyrolysis constituent, the conversion of CO to CO_2 is then facilitated. As it can be seen, this devolatilization model gives far more information about the evolution of volatiles through thermal degradation of different coals than simplified models. Predictions for 160 μm bituminous coal particle burning in an atmosphere of 10% by volume of oxygen, 0.4 MPa, 1170 K, were conducted with the CMVC-Kobayashi and CMVC-CPDNLG models. At 100 ms, the former model gave 1427 K for the particle temperature, while the temperature for the latter was 1665 K. Joutsenoja et al. (1999) measured particle temperature of 1719 K at 80 ms. Therefore, simplified models are not recommended for such mid gas temperatures. Also, the applicability of the CPDNLG model in pressures higher than atmospheric great extends the analysis of coal combustion in more advanced technologies. Several predictions were carried out and the results and discussion can be seen in the next section.

3. SOLID FUEL IGNITION

Ignition is a transient phenomenon in which complex chemical and physical processes are involved. For pulverized solid fuels that may undergo thermal degradation, ignition may take place at the surface of particle (heterogeneous ignition), in the gas phase (homogeneous ignition) due to volatiles oxidation and, also, simultaneously, called hetero-homogeneous, in which ignition is observed to occur simultaneously at the surface and in the combustible gas mixture surrounding the particle.

Direct application of the classical Semenov's thermal theory of ignition to solid fuel particles is not possible without some considerations. Particle ignition would be defined when the heat losses or its rate from the particle equals the heat generation or its rate. In other words ignition occurs when $dT_p/dt = 0$ where T_p is the temperature of the particle and t is time. In a real situation, however, this condition will not be attained if the ambient gas temperature is higher than the minimum ignition temperature. The particle, however, will certainly ignite at some point. This problem must then be overcome. By manipulating the particle's heat balance equation it is possible to get a more general ignition condition. This general criterion states that $dQ/dT = 0$ and $Q \geq 0$ at the time of ignition, where Q is the net heat supply rate to the particle from all possible sources. We are primarily concerned with ignition of solid particles in real combustors. Thus, we are discharging the condition for which the ambient gas temperature is lower than the critical ignition temperature for the solid fuel particle.

Du and Annamalai (1994) have explored the ignition criterion mentioned above. They applied the inflection condition $dQ/dT_p = 0$ to the heterogeneous ignition for the transient model yielding a critical particle mass loss rate expression. When actual particle mass loss rate is greater than the mass loss rate at the inflection condition, the heterogeneous ignition (HIT) will occur at a specific particle temperature. In pulverized flames, ambient gas temperature is thought to be equal or higher than the minimum temperature for ignition. This approach has some simplified assumptions but has been used before. In this work, we choose different ignition criteria, for both heterogeneous and homogeneous ignition. The following equation was used in characterizing whole coal ignition (heterogeneous):

$$\frac{T_{oxid}(t) - T_{inert}(t)}{T_{oxid}(t)} \geq 1\% \tag{1}$$

In Eq. (1), T_{oxid} is the transient temperature of the particle surface when the surrounding gas has oxygen at some concentration, which means, surface and gas phase reactions are allowed to happen. T_{inert} is the transient temperature of the particle surface when heating is only due to energy transfer by diffusion and radiation from the surrounding gas and reactor's walls, respectively. Our model is able to predict the temperature distribution inside the particle, thereby allowing the transfer of heat to the center of the particle to be included in the surface ignition heat balance where heterogeneous reactions are, in fact, taking place.

The criterion for homogeneous ignition used by Du and Annamalai (1994) was also adopted here. The criterion states that the time any control volume has its temperature higher than the neighbors characterizes gas phase ignition (GIT). Since our model is also continuous, we are able, thus, to adopt the same approach. It is important to mention that direct attack of oxygen to the particle surface occurs simultaneously with volatiles combustion in the vicinity of the solid fuel. Furthermore, in the early moments of devolatilization, when volatile gases have not been released significantly, heterogeneous reactions may occur in the whole particle, rather than the char.

Figure (3) illustrates the criterion for heterogeneous ignition. The predictions were such that particle size was 200 μm, gas temperature was set 1300 K (1 bar) with oxygen mass fraction of 14% and the coal was bituminous. At this condition the average particle heating, before ignition, was less than 10000 K/s. This criterion separates particle heating calculated only from heat diffusion and radiation to that where combustion reactions take place (blue line). This criterion is based on the fact that self combustion is attained if ignition takes place (Kuo, 1996). This means that the particle would sustain combustion even if placed in a cold environment, provided oxygen is available.

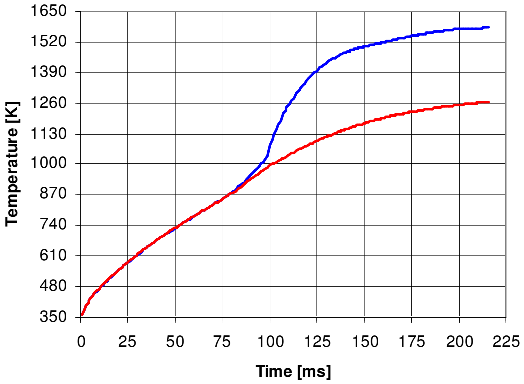

Figure 3: Particle surface temperature in oxidizing (blue) and inert (red) atmospheres.

In Fig. (3) heterogeneous ignition takes place at 86 ms, for which Eq. (1) is satisfied. At this time particle surface temperature is 924 K. The suddenly raise in particle surface temperature is first due to heterogeneous ignition, when the curves separate (≅ 924 K), and the second sharp increase, just after 100 ms, is by virtue of gas phase ignition (homogeneous ignition) that took place at about 89 ms, based on the criterion for this type of ignition. As it can be seen, the temperature of the surrounding gas (1300 K) is much higher than the expected ignition temperature (924 K), therefore, the particle experiments a continuous increasing in its temperature, though at different heating rates (red line). Rigorously, with a more conservative approach, it would be more precise to assume that the type of ignition was hetero-homogeneous, since the difference in time between the events was only 3 ms. This can be explained by the following. The particle surface works as a cold wall transferring heat from the reacting gas that surrounds the solid fuel. Heterogeneous reactions at the surface work as a heat source which transfer energy towards particle center. When the energy provided by these reactions is enough to compensate what is lost in heating the particle, less heat diffuses from gas to the solid, thus allowing homogeneous ignition to take place.

4. RESULTS AND DISCUSSION

At first, a high volatile bituminous (Polish hvb) coal, with 0 .741 Carbon (DAF), 0.043% H, 0.015% N, 0.1% O and 0.063% S was chosen for the predictions. Devolatilization rates were calculated by the CPDNLG model. Initial particle density was set to 1300 kg/m^3. The anthracite coal was a Niederberg Anthracite 0.830 Carbon (DAF), 0.051% H, 0.015% N, 0.1% O and 0.082% S. Coal elemental analysis is on a dry ash free base. The influence of ash is not considered in the model, therefore, the composition and quantity of ash is not an important factor in this study. Kinetic rate constants for the HVBA (Hobbs *et al.*, 1993) were taken for the oxidation and gasification reactions at the surface of the coal particle. Oxygen mass fraction was set at two levels, 12 and 20%. Gas pressure was fixed in 1 bar and gas temperature varied with the values set at 900, 1100, 1300 and 1500 K. The parametric study started by analyzing the effect of particle size on ignition for different particle sizes. Predictions are shown in Fig. (4).

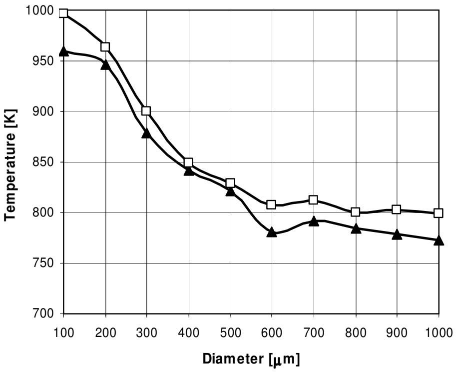

Figure 4: Ignition temperature and type of ignition (□ homogeneous, ▲ heterogeneous) as a function of particle diameter for the bituminous coal.

Gas temperature was set to 1500 K and oxygen mass fraction at 12%. Coal was bituminous. The results show that primary ignition was heterogeneous for all particles sizes, following shortly by gas phase ignition (secondary). In the paper of Du and Annamalai (1994) even particles as small as 20 µm ignited homogeneously for a certain combination of surface and gas phase kinetics. This is not in accordance with the results presented by Howard and Essenhigh (1967) who concluded that particles less than about 65 microns in size experience simultaneously heterogeneous combustion and gas phase reaction. Particle which is less than 15 microns in size appeared to have significant rate of heterogeneous combustion during rapid volatile evolution. In their investigation, particle size ranged from zero to 200 microns. They concluded that ignition was at the particle surface and soon after significant volatile evolution took place. Therefore, the study of the transient ignition process has to take into account the influence of the kinetic parameters for devolatilization, as well as gas phase reactions. Kharbat et al. (1995) studied experimentally the ignition and combustion of isolated coal particles. Thy found that for the temperature range investigated (1027 K, 10% O_2), particle size of 600, 800 and 1000 µm, the ignition of low, medium and high volatiles coals is always heterogeneous. The homogeneous ignition of ejected volatiles occurred only after heterogeneous ignition. The conditions they had in their investigation are, somehow, close to our numerical predictions. Since smaller particles are more prone to ignite primarily at the surface (heterogeneous) we believe the CMVC-CPDNLG model is giving very good results in this kind of investigation. Simplified numerical models, mostly those using two rate equations for the pyrolysis model and isothermal particle as well as constant physical parameters, would give a transition from hetero to homogeneous ignition at about 500 µm (Du and Annamalai, 1994).

For very low heating rates (10 K min^{-1}), particle size ranging from 37 to 4000 µm, the type of ignition for bituminous coal change from hetero-homogeneous to homogeneous combustion. However, they did not mention the particle size for the transition. Our simulations were done up to only 1000 µm. We were concerned with practical coal combustion pulverized systems which operate at much smaller particle sizes, less than 500 µm. As it can be seen, Fig. (4) shows hetero-homogeneous type of ignition, for the diameters investigated. The heating rate, however, is much higher in our predictions, thus favoring slightly heterogeneous ignition.

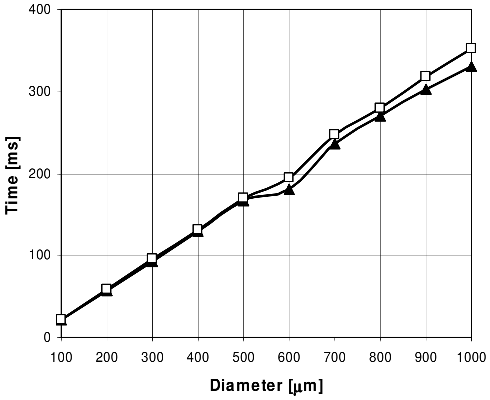

Figure 5: Ignition time and type of ignition (☐ homogeneous, ▲ heterogeneous) as a function of particle diameter for the bituminous coal.

Figure (5) presents the type of ignition and the corresponding time for the bituminous coal at the same condition showed in Fig. (4). As it can be seen, the time for the onset of rapid gas phase reactions (homogeneous ignition) is only a few milliseconds after primary heterogeneous ignition for particles size larger than 500 µm. In the experiments of Kharbat et al. (1995), for particle size of 1000 µm, the calculated time for the heterogeneous ignition was of about 450 ms and the volatile combustion process was apparently completed at 1170 ms. Our predictions, regarding the time for heterogeneous ignition, for the same particle size, but with slightly higher gas temperature and oxygen mass fraction, was at 331 ms. The prediction, thus, are in good agreement to their experimental results.

Figure (6) shows the type of ignition and the corresponding time for the bituminous coal at 1100 K and 12% O_2 (mass fraction). At this lower heating rate we could predict primary homogeneous ignition for particles larger than 500 µm. Smaller the process of ignition is of the type hetero-homogenous, as Fig (6) shows. Rigorously, based on the almost insignificant difference in time between the primary homogeneous and secondary heterogeneous ignition, we would say that ignition was hetero-homogeneous for all particle sizes studied.

The parametric investigation also studied the influence of oxygen mass fraction on ignition. Our predictions show that increasing O2 mass fraction from 12 to 20% did not change the type of ignition. For smaller particles we observed hetero-homogeneous ignition and, for larger particles, a slight tendency to primary heterogeneous type of ignition. As before, the time between the events are very short and we would say that the ignition phenomenon is better characterize, for the particle size range investigated, as hetero-homogeneous.

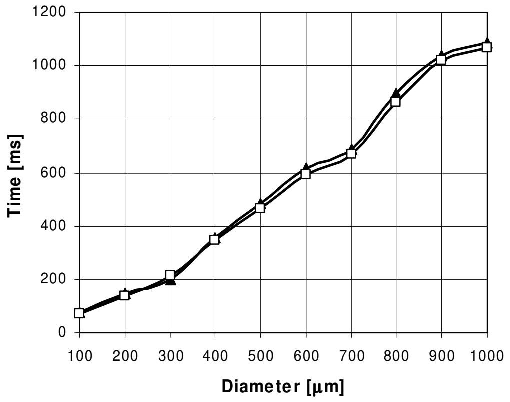

Figure 6: Ignition time and type of ignition (□ homogeneous, ▲ heterogeneous) as a function of particle diameter for the bituminous coal.

Ignition of anthracite coal was also investigated. For 1300 K, 14% O_2 mass fraction, for different particles sizes (100 to 1000 µm) the type of primary ignition was also hetero-homogeneous.

As regarded to the transition of ignition phase, our results are neither in accordance with the predictions of the continuous model of Du and Annamalai (1994) nor to that of the flame sheet model of Annamalai and Durbetaki (1977). For bituminous coal, the former found TIP size to be about 500 µm and the latter, 105 µm. However, both models assumed isothermal particles and the global rate expression for volatiles (CH_4) oxidation was based on one step conversion.

Du and Annamalai (1994) investigated the effect of kinetic parameters on the transient ignition mode. Primary homogeneous ignition was predicted even for small particles when combining fast combustion kinetics for gas with slow surface reactions. On the other hand, ignition was always heterogeneous when using slow volatiles kinetics combined with fast surface reactions. This suggests a strong influence of the kinetic parameters chosen, as well as some of their model assumptions. The CMVC-CPDNLG model, however, calculates the temperature distribution inside the particle and, at lower heating rates, the phenomenological pyrolysis model gives more realistic predictions for volatiles evolution as well as species distribution. In the CMVC model, the local rate of production of volatiles is a function of the temperature history of that control volume. Therefore, the volumetric rate of volatile evolution from our predictions is much less that where it is assumed uniform coal particle temperature. In addition to this, coal heat capacity is not constant but increases as the local temperature increases, thus retarding the heating of the interior of the particle. It is expected, then, lower production of volatiles in the CMVC-CPDNLG model which, thus, favored heterogeneous ignition.

The global mechanisms for volatile combustion in the CMVC model differ from that employed by Du and Annamalai (1994). The two-step mechanism used here is more realistic for gas phase ignition than one-step models as pointed by Sloane and Ronney (1992). They criticized the use of one-step model for hydrocarbon oxidation in predicting minimum ignition energy. The reason is, predominantly, due to the fact that one-step models were tailored to reproduce the integrated heat release in the flame front, as to enable the model to reproduce burning velocity. The conclusions were supported by calculations, which showed that the homogeneous induction times for one-step model and detailed chemical models are drastically different, although all the models reproduce well steady planar burning velocity. The kinetic constants of the two-step model, used here, were fitted as to give better agreement with detailed mechanism in a broad range of equivalence ratios (Westbrook and Dryer, 1981). Therefore, we may expect that ambient factors for gas phase ignition, as predicted from our model, are different compared to those from the continuous model presented by Du and Annamalai (1994). Neglecting all of these observations greatly favors homogeneous ignition for larger particles.

In the review of Essenhigh *et al.* (1989), particles smaller than 650 µm are reported to have no volatiles flame but instead ignition was observed to take place only at the surface of the particle. They also mentioned that the ignition was of the char, not of the whole coal. Ignition occurred only after a clear pyrolysis pulse had been released. This experimental observation is very difficult to simulate in the model. The surface reactivity we are employing is for the char derived from the specific coal. Therefore, it is indirectly assumed by the model that the outer surface has released all the volatiles although it might not be the case. However, the small amount of volatiles released before heterogeneous ignition greatly contributes for the surface ignition since the heat released in the gas phase increases the gas temperature near the particle. Our results agree with the observations discussed in the review of Essenhigh *et al.* (1989) that, at high temperature, the heterogeneous ignition may take place simultaneously with pyrolysis.

Although the mixture around the particle would favor gas phase ignition, the surface of the particle acts as a cold wall, thus retarding homogeneous ignition. As soon as the surface ignites, the heat produced by the combustion of the mixture, around the particle, is transferred at lower rates to the particle, thus, increasing the local temperature to the gas phase ignition temperature.

This parametric study will continue as to investigate lignite coal and biomass transient ignition as well as different rate equations for char oxidation, pyrolysis heat of reaction and others. The results will be published in the near future.

5. CONCLUSIONS

The CMVC-CPDNLG model showed results that are not in full agreement with previously published models. Pyrolysis model (more phenomenological) and the temperature distribution inside the particle were the main reason for the discrepancies. In addition, the usage of a two step global mechanisms for volatiles oxidation and a correction for the heat value of such devolatilization products are deemed more appropriate for this analysis. Most of the predictions indicated that the primary ignition mode was hetero-homogenous. Only at low heating rates and oxygen mass fraction, gas phase ignition was observed to take place firstly.

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