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COMPUTATIONAL MODELLING OF CHAR COMBUSTION BASED ON THE STRUCTURE OF CHAR PARTICLES

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ABSTRACT

The successful design and operation of coal combustion systems depends on the proper application of many facets of fundamental knowledge. This knowledge is conveniently expressed by the governing equations of each particular phenomenon which is relevant to the process. It is the main purpose of the fundamental scientific research in this field to identify the pertinent physics and chemistry of these phenomena and model that by solving appropriate transport equations.

In this paper we will particularly consider aspects of char combustion system modelling which are amenable to treatment by modern computational fluid dynamic codes. Fluent CFD software has been used to model the combustion of char particle. A diffusion limited rate and the intrinsic models are employed to model char combustion. The structure of coal is considered by employing appropriate shape factor. A Lagrangian approach is used to trace the particles. The P-1 radiation model is used for computing the influence of radiation. The char burnout rate computed based on the above models is then validated against the experimental results.

INTRODUCTION

Coal is one of the cheapest fuels and is available in sufficient quantities in Australia. The reserves of higher ranking coals, i.e., anthracite and coking bituminous coals are less as compared to the low ranking bituminous coal and lignite. On the other hand the demand for high ranking coals is more for metallurgical use and for use as fuel in power plants. It is expected that high rank coal will last for about 80 years while the low ranking coal are sufficient for more than 800 years. Because of the cheap price of coal, so far much attention was not paid to improve the efficiency of coal consuming equipment. However, the new restrictions on generating "clean" energy have encouraged the designers on manufacturing more efficient devices. It is estimated that the overall efficiency of coal consuming plants on an average is only about 18%. There is therefore, much scope to improve the efficiency of such equipment. CFD modelling has shown to be an efficient way on modelling pulverised coal combustion systems (Eghlimi and Sahajwalla, 1997).

Coal is not a homogeneous substance. It is characterised by wide variations in its properties and composition including the rank of the coal. CFD modelling of pulverised coal combustion furnaces based on the ultimate and proximate analysis has shown to provide reasonably accurate temperature and species concentration distribution in a number of applications (Sahajwalla, et al, 1997). However, the new challenges in making coal combustion devices to run more efficiently have made combustion modelers to consider other parameters influencing the combustion process.

To characterise coal, different methods have been proposed over time. Hensel (1981) presented the coal data on a moisture and dry ash-free basis. This method had the advantage that the rank of the coal can be determined by this comparative method, which eliminates the requirement that bed moisture be accurately known. With increasing rank, both aromaticity and molecular cluster size increase (Solum et al., 1989) and the vitrinite of coal also increases accordingly. The information of the vitrinite reflectance of coal can specify rank, caloric value, volatile matter content and the gas or oil yield of a coal.

Neavel (1981) classified coal according to its grade. The rank, type or petrographic constitution and inorganic content of coal affect its value. Coal types can be classified into seven groups as the following:

1. Chemical analysis, including proximate and ultimate analysis,
2. Physical properties, including density, porosity and pore structure and surface area,
3. Mechanical properties, namely hardness, elasticity, strength, friability and grindability,
4. Thermal properties including calorific value, heat capacity, free swelling, agglomerating properties, and thermal conductivity,
5. Electrical properties, including resistivity, electrical conductivity,
6. Ash analysis including ash elemental and mineralogical analysis,
7. Petrograph and vitrinite reflectance.

Commercial CFD codes, more or less include some of the above characteristics. The following sections identify the coal properties and discuss the significance of each specification. The models available in Fluent CFD software have been used for this modelling.

PROBLEM DESCRIPTION

The heating and combustion of char particles in a drop tube furnace (DTF) has been numerically studied. The furnace that was used in this investigation was an electrically heated DTF (Figure 1). It consists of coal feeding system, sampling probe, gas distribution system and high temperature furnace. The ultimate analysis of the char studied here is shown in table 1.

Element	Wt% (daf)
C	95
H	1.01
O	0.9
N	2.1
S	0.99

Table 1: Ultimate analysis of coal

The density of particles is taken to be 1120 kg/m^3. In the reaction zone (Figure 1) the temperature is fixed to 1373 K. The reaction zone has been modelled with a feeding rate of 1077 ml/min from the sides with 35% O_2 and 65%N_2 and the inlet temperature of 537K. At the centre, the inlet gas is 100% N_2 with the mass flow rate of 145 ml/min and the inlet temperature of 537K. The feed rate of particles from the centre is 4.2E-6 kg/s.

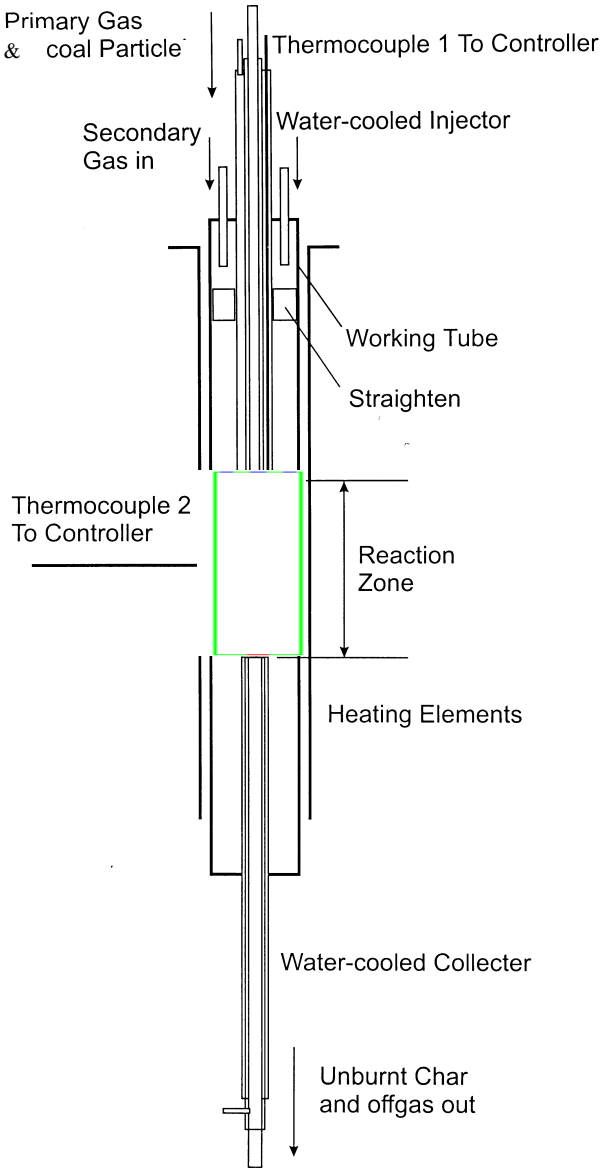

Figure 1: Schematic Diagram of Drop Tube Furnace

Chemical Analysis

In proximate analysis the percentage of fixed carbon, volatile matter, ash and moisture are presented. In ultimate analysis the absolute measurement of the elemental composition of char are shown. It has been shown by a number of investigators including Sahajwalla, et al., 1997, that the proximate and ultimate analysis provide reasonable temperature and species concentration in pulverised coal combustion devices. The chemical analysis information is quite important in any combustion modelling of coal particles.

Physical Properties

The physical properties of particles include true and apparent density that depends on the porosity. Specification of the porosity of chars and nature of pore structure between macro, micro and transitional pores influence the combustion process. The trajectory of particles is predicted by integrating the force balance on the particle in a Lagrangian reference frame. In this balance the drag force is a function of particle diameter and drag coefficient. Morsi and Alexander, 1972, defined this drag force as a function of Reynolds number and a shape factor which is taken from Haider and Levenspiel , 1989. The shape factor, φ , is defined as:

$$\varphi = \frac{s}{S} \tag{1}$$

where, s is the surface area of a sphere having the same volume as the particle, and S is the actual surface area of the particle. When the coal particles go through devolatilisation and heating process their shape changes. The introduction of shape factor would be the beginning of considering the changes of shape and form of coal particles going through devolatilisation or heating processes. More sophisticated models are required to consider these changes. One of them would be having different shape factors in different temperatures.

The Brownian and Saffman's lift force due to the size of the coal particles are negligible and not included in the present study.

Mechanical Properties

Most of the mechanical properties of char particles, referenced in literature, such as friability, grindability and dustiness are process related not combustion related. The elasticity of coal particles in an Eulerian approach for dense concentration might play an important role depending on the geometry. In the present study the particle-particle interactions are not considered. In terms of boundary condition an elastic collision has been applied for wall boundaries.

Thermal Properties

The heating value of char is taken to be 32.9 MJ/kg. Due to a low value of volatile the swelling of char, which is an indication of plastic and caking properties, is taken to be negligible.

Electrical Properties

Electrical resistivity, treating char as a semiconductor, is not included in this study. Also the electrostatic polarisability and magnetic susceptibility of char particles are not included in this modelling.

Ash Properties

The ash percentage is 18.9 based on proximate analysis that contributes in inert heating calculations. Major elements found in char ash such as SiO_2, Al_2O_3, and Fe_2O_3 are not included in the calculation. The ash fusibility and mineralogical analysis of char are not considered here.

Petrographic and Sample Properties

The influence of maceral composition, sample history, sample location and seam information are not included in this study.

CHAR COMBUSTION MODELLING

The volatile component of the char is very low. Therefore, more attention is given to char combustion modelling. After and during the evolution of remaining volatile, the surface reaction of chars occurs. Two different heterogeneous surface reaction rate models of combusting chars are investigated.

The first model is a diffusion limited surface reaction model based on the work done by Baum and Street, 1971. In this model it is assumed that the surface reaction proceed at a rate determined by the diffusion of the gaseous oxidant to the surface particle:

$$\frac{dm_p}{dt} = -4\Pi D_p D_{i',m} \frac{m_O T_p \rho_g}{S_b (T_p + T_\infty)} \qquad (2)$$

$D_{i',m}$ = Diffusion coefficient for oxidant in the bulk (m^2/s)

m_0 = Local mass fraction of oxidant in the gas

ρ_g = Gas density

S_b = Stoichiometry coefficient

D_p = Current particle diameter

T_p = Char temperature

The diffusion limited rate model assumes that the diameter of the particles does not change and the kinetic contribution to the surface reaction rate ignored.

The second model assumes the order of reaction is equal to unity. This model is known as intrinsic model and is based on the work done by Smith, 1982. It includes the effects of both diffusion and chemical reaction. The diffusion rate R_1 is computed via:

$$R_1 = C_1 \frac{[(T_p + T_\infty)/2]^{0.75}}{D_p} \qquad (3)$$

where C_1 is a constant. The chemical rate R_2 is explicitly expressed in terms of the intrinsic chemical and pore diffusion rates:

$$R_2 = \eta \frac{D_p}{6} \rho_p A_g k_i \qquad (4)$$

A_g is the specific internal surface area of the char particle, which is assumed to remain constant during char combustion. η is the effectiveness factor which is the ration of the actual combustion rate to the rate attainable if no pore diffusion resistance existed (Laurendeau, 1978):

$$\eta = \frac{3}{\Phi^2}(\Phi \coth \Phi - 1) \qquad (5)$$

where Φ is the Thiele modulus:

$$\Phi = \frac{D_p}{2}\left[\frac{S_b \rho_p A_g k_i P_O}{D_e C_O}\right]^{0.5} \qquad (6)$$

C_O is the concentration of oxidant in the bulk gas and D_e is the effective diffusion coefficient in the particle pores. Neglecting the pore size distribution, D_e is defined as:

$$D_e = \frac{\theta}{\tau^2}\left[\frac{1}{D_{kn}} + \frac{1}{D_O}\right]^{-1} \qquad (7)$$

D_O is the bulk molecular diffusion coefficient and θ is the porosity of the char particle defined as:

$$\theta = 1 - \frac{\rho_p}{\rho_t} \qquad (8)$$

ρ_p and ρ_t are the apparent and true densities of the pyrolysis char respectively. τ is the tortuosity of the pores and is taken to be $\sqrt{2}$ (Laurendeau, 1978). k_i is the intrinsic reactivity, which is of Arrhenius form. D_{kn} is the Knudsen diffusion coefficient:

$$D_{kn} = 97\overline{r_p}\left(\frac{T_p}{M_O}\right)^{0.5} \qquad (9)$$

where T_p is the particle temperature and $\overline{r_p}$ is the mean pore radius of the char particle which is taken to be 150A°. A_g is the specific internal surface area of the char particle. During the combustion process of char, the surface reaction consumes oxygen. This supplies a negative source term during the computation of the transport equation for the species. The effect of radiation heat transfer to the particles is included by using the P-1 model (Cheng, 1964). The emissivity and scattering of coal particles are included in the calculation.

RESULTS AND DISCUSSION

The physical grid used in this study is shown in Figure 2. The grid is dense close to the inlets and outlet. It is shown by Lu, et al. 1999, that char particles going through the

heating process deform. Figure 3 illustrates the heterogeneous form of the particles. As the temperature increases the particles become more porous. This changes the drag force which varies the velocity. Changing the value of shape factor (Equation 1) would somewhat consider this particle deformation.

Figure 2: Physical grid of the drop tube furnace

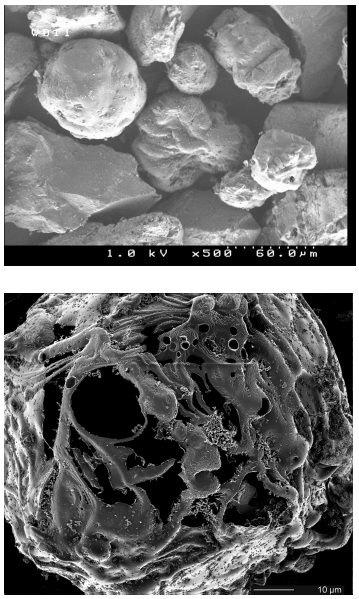

Figure 3: Particle deformation during combustion process

In Figure 4, the experimental data of burn off rate of char particles travelling in the DTF passing the heated zone are compared with the diffusion limited rate and intrinsic model. As shown in Figure 3 and investigated by Lu et al., 1999, the char particles deform completely during the combustion process. This changes in porosity and form would influence the surface reaction rate. As discussed earlier the diffusion limited rate model provides a simple kinetic calculation. On the other, the intrinsic model includes the particles porosity and surface reaction rate in a more sophisticated approach. This corresponds to the result shown in Figure 4.

CONCLUSION

The pulverised coal combustion in a drop tube furnace has been modelled based on two char combustion models. The intrinsic model, that takes account of the apparent and true densities of char during heating process and includes both diffusion and chemical reaction rates, has shown to provide a closer burn off rate to the experimental investigation.

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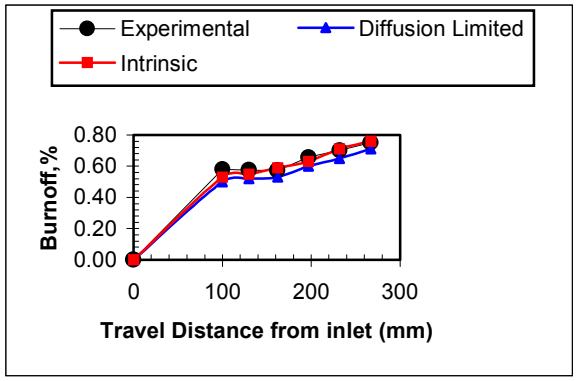

Figure 4: The burn off rate based on different char combustion models

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