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## 고온 유동장 내 석탄 단입자 연소과정의 특성화를 위한 수치적 연구

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### A numerical model for combustion process of single coal particle in hot gas

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#### ABSTRACT

With the experiment observation of single particle combustion, this model is built for the numerical analysis of the process. It's about the single coal particle combustion process under different conditions with reasonable assumptions. The model can express the mass, radius, density, temperature changing with different particle sizes, oxygen concentration and gas temperature. It also includes the flame sizes change in different condition and the diffusion of each species. The result shows the characters of the combustion.

**Key Words** : single coal particle combustion, model, flame size, diffusion

To follow the speed of development, no matter for the life style of people or the industrial development, the need of energy becomes larger day by day. In this case, increasing the efficiency of electricity generation becomes an important topic in our life. Though there're lots kinds of new energy catch the sight, coal is still a main source of energy for many countries. To use it efficiently, first of all, we should understand the whole process of coal combustion and the influence of environment to it. By the experimental observation, we can understand the whole process directly with the phenomenon and know the change in different environment by observation. While making a model of it is another way to know the inner principle and a way to understand it mathematically. With this basic understand, we can burn it in a more suitable condition, and know how to adjust the environment with different condition.

In industrial application, the coal is burned in the furnace of a boiler, and instead of the single coal particle, actually it is burned with a pulverized coal. There're a lot of researches about the pulverized coal combustion model while there's no experiment about the single

coal particle, although it can also know the tendency and the influence of different environment, but by observing the single particle combustion, we can see the whole process more clearly and also can find the flame size change during the combustion.

In this study, the model is based on the experiment about single particle enters the hot gas flow done by Hookyung Lee[1] which can be seen as the simulation about the condition coal particle combustion in the furnace. The model can give the information about the temperature and mass changing with time, as well as the inner gradient of it and the density and radius change. It can also show the influence of oxygen concentration, gas temperature and particle size to the combustion and the flame size change with these differences.

The experiment is about injecting a single coal particle at room temperature and to the environment of hot gas composed with propane, air and extra oxygen at 1240K enclosed by walls assumed to be the same temperature as the gas. The single particle combustion process can be divided into four parts, heating up, including the water evaporation, devolatilization, volatile combustion and char combustion. This model is mainly focused on first three parts,

especially the volatile combustion part including the soot combustion. In the model, treat the particles as a symmetric sphere and the temperature is the same at the same radius [2]. Assume no gravity and the particle has zero relative velocity with respect to the gas hence the Nusselt number is 2 [3]. The particle receives heat by convection from the hot gas and radiation from the walls, as well as the homogeneous and heterogeneous chemical reactions happened later. The hot gas temperature is also changed by the influence of particle temperature and volatile combustion. Assume that the heat influences the temperature of the gas around particle till 50 times of particle radius. The heat exchange between hot gas and walls are small enough to ignore compared to that between particle and hot gas [4]. In the model, when the particle temperature reaches 400K, the water evaporation starts and at 600K, the devolatilization starts, and after it reaches 800K, the volatile ignition starts, after all the volatiles separated out, the char combustion starts, but not involved in the current model. And the flame sheet size is decided by the diffusion of gas and soot during this period. Assume all the chemical reactions happened on the surface, and ignore the tar and soot mechanism, assume soot come out with gas in the devolatilization period.

Water evaporation rate is calculated by Eq.(1).

$$\frac{dm_w}{dt} = \dot{W} = k_m \pi d_p^2 \left( \frac{x_{w,0} - x_{w,\infty}}{1 - x_{w,0}} \right) \quad (1)$$

Where  $x$  is the ratio of evaporation partial pressure and total pressure and  $k_m$  is the kinetic parameter of evaporation,  $d_p$  means the diameter of particle.

The devolatilization process is calculated by species ( $\text{CH}_4, \text{CO}, \text{C}_2\text{H}_6, \text{CO}_2, \text{H}_2\text{O}$ ), and the liquid hydrocarbon is represented by  $\text{C}_6\text{H}_6$  [5] with one step mechanism by Arrhenius equations as shown in Eq. (2). The parameter  $k$  and  $E$  is corrected by comprising to the real experiment situation [1] based on previous research [6].

$$\frac{dm_i}{dt} = -k_i \exp\left(-\frac{E}{RT}\right) (m_{ij}^0 - m_{ij}) \quad (2)$$

After reach the assumed ignition temperature, the volatile combustion starts. In this part, the reaction rate is calculated by Eq.(3), and the heat is calculated by the combustion reaction heat.

$$\dot{r}_i = -A_i \exp\left(-\frac{E_i}{RT_g}\right) C_x^a C_y^b \quad (3)$$

While the heat from the gas by convection and from the wall by radiation is expressed

by

$$m_p c_p \frac{dT_p}{dt} = \theta h A_p (T_p - T_g) - \sigma \varepsilon_p A_p (T_p^4 - T_w^4) + \sum_i \dot{r}_i \Delta H_i \quad (4)$$

Where,  $\theta$  is the correction parameter of heat transfer coefficient  $h$ ,  $r$  and  $H$  for chemical reaction.

$$B = \frac{c_{pg}}{2 \pi d_p k_g} \left( \frac{dm_p}{dt} \right) \quad (5)$$

$$\theta = B / (e^B - 1) \quad (6)$$

$$m_g c_g \frac{dT_g}{dt} = h A (T_p - T_g) + N_c \sigma \varepsilon A_{soot} (T_p^4 - T_g^4) + q_{soot} + \sum_i \dot{r}_i \Delta H_i \quad (7)$$

For the gas temperature it is decided by Where,  $N$  is the soot number,  $A$  is the soot particle size which is assumed to be 0.01 of the coal particle size,  $q$  is the soot combustion heat.

$$A_{soot} = (6^{2/3} \pi^{1/3} (\rho_g N)^{1/3} Y_c^{2/3} \rho_g^{2/3}) / \rho_c^{2/3} \quad (8)$$

$$Y_c = C_1 C_2 M_c \beta_c \quad (9)$$

Where,  $C_1=0.35, C_2=1$  is the local molar density

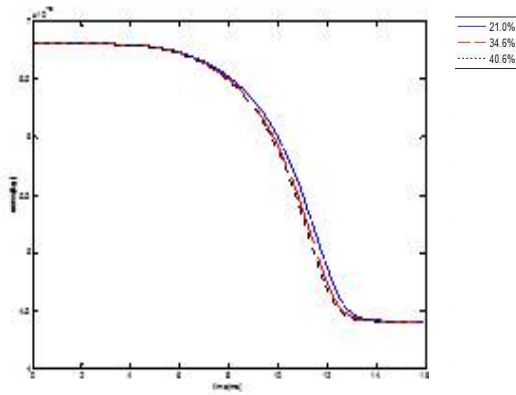
$$\rho_g N = 10^{16}$$

**Table 1** Solid fuel properties.

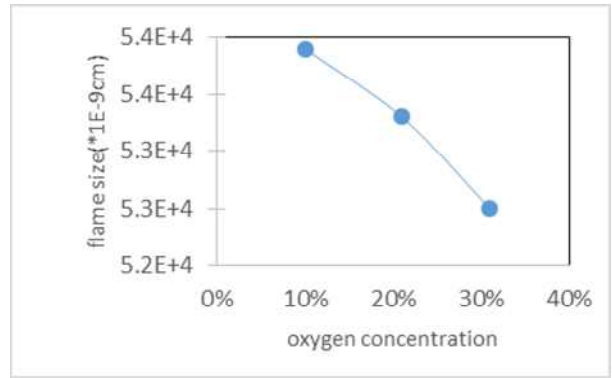
Solid fuel	Proximate analysis [wt.%]		Ultimate analysis [wt.%]	
	W	2.38	C	70.38
Bituminous coal (air-dried)	VM	35.32	H	4.65
	FC	49.62	O	7.91
	Ash	12.68	N	1.48
			S	0.52

**Table 2** volatile species and fraction assumption.

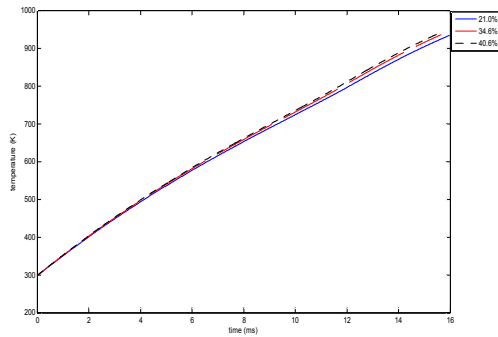
Species	Mass fraction
CH <sub>4</sub>	3.31%
C <sub>2</sub> H <sub>6</sub>	1.82%
CO	9.35%
CO <sub>2</sub>	8.00%
H <sub>2</sub> O	6.92%
SOOT	5.92%



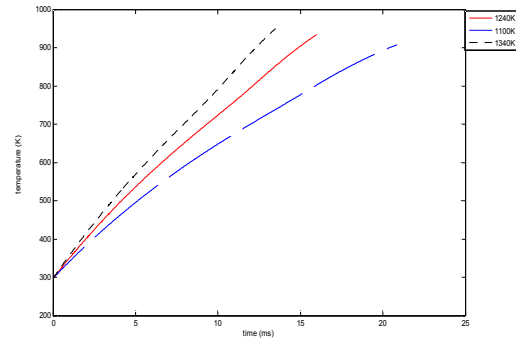
**Fig.1** Mass change of 100um coal particle during heat-up and devolatilization process at different O<sub>2</sub> concentration(21,34.6,40.2%).



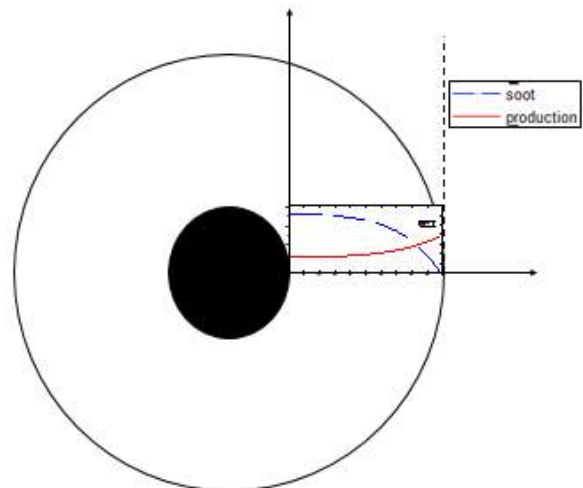
**Fig.3** Temperature change of coal particle at different gas temperature (1100K, 1240K, 1340K) during heat-up and devolatilization process at O<sub>2</sub> concentration of 21%, 100um particle.



**Fig.2** Temperature change of 100um coal particle during heat-up and devolatilization process at different O<sub>2</sub> concentration(21,34.6,40.2%).



**Fig.4** Flame size at different oxygen concentration of 10%, 21%, 30.6%, while particle size 100um.



**Fig.5** Diffusion in flame of soot and production of oxygen concentration at 21%, gas temperature of 1240K, 50um coal particle

From Figs. 1 and 2, we can see that, the devolatilization ended faster and with higher temperature as the oxygen concentration becomes higher, but the time is around 15ms. Fig. 3 shows the temperature change of different gas temperature at oxygen concentration of 21%. We can see that as the gas temperature becomes higher, the combustion process finished faster, and the difference is somehow larger. The final temperature is also different and becomes higher as the gas temperature goes up. Fig. 4 shows flame sizes change with the oxygen concentration while particle size is 100um and the gas temperature is 1240K. We can see that as the oxygen concentration becomes higher, the flame size is smaller. Cause the combustion process finished faster as the oxygen concentration becomes higher, in this way, the temperature goes up quickly so the diffusion rate becomes higher, the volatile reaches the oxygen faster also the ignition temperature will be lower in real situation, so the flame size is smaller. These results are the same as the experiment result which show the character of coal particle combustion process.

This is the basic model of the coal combustion, further work will be concentrated on influence of soot to the whole process.

#### 후 기

본 연구는 KAIST BK21 Plus 사업의 지원으로 수행되었습니다.

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