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Experimental and Numerical Investigation of Effect of Coal Rank on Burn-off Time in Pulverized Coal Combustion

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Thermogravimetry (TG) for two different coal ranks, Loy Yang coal and Newlands coal, was carried out in an atmospheric air environment. Detailed parameters of the heterogeneous oxidation reaction for each coal rank were estimated by analyzing the TG results. Heat and mass transfer of a single pulverized coal particle that was heated at a constant temperature were numerically simulated. In this calculation, the decrease in the mass ratio caused by the oxidation reaction was considered. The numerically analyzed results were compared and the influence of particle parameters (coal rank, initial particle diameter, oxygen concentration) on burn-off time was examined.

1. Introduction

Recently, because of increasing energy consumption by emerging nations, it has become difficult to maintain the supply of high-rank coals such as bituminous coal. Therefore, the development of technologies to utilize low-rank coal such as brown coal is highly desirable. In addition, the improvement of environmental and operational performance and fuel diversification for pulverized coal-fired generation are required. To achieve high efficiency in pulverized coal combustion furnaces and burners, detailed estimation of burn-off time for pulverized coal particles is important. Many studies on pulverized coal combustion have been previously carried out. The basic experimental approach including the estimation of properties of the combustion reaction rate using thermogravimetry (TG) 1) and drop tube furnace (DTF)2) 3) has been carried out. The numerical approach for pulverized coal combustion was first considered in the 1940's4). This approach has been subsequently developed and extended to include the coupled simulation of pulverized coal char particles and fluid flows in several experimental apparatus5) 6). Furthermore, to discuss the effect of convection of the product due to combustion on the mass transfer rate of the oxidant, heat and mass transfer around a single char particle during combustion has also been studied7).

On the basis of these results, in this study, the parameters of the heterogeneous chemical reaction rate of Char–O_2 for coals of two ranks, i.e., Loy Yang coal and Newlands coal are estimated using TG to investigate the influence of different coal ranks on burn-off time for coal particles. Furthermore, heat and mass transfer around a single pulverized coal particle that is exposed to a simplified heating environment are numerically simulated to investigate the effect of different coal ranks with different reactivities on burn-off time.

2. Experiment

In general, in order to estimate parameters of the chemical reaction rate, TG1) or DTF2)3) is used. In this study, a TG-DTA2000SA (Bruker AXS) thermal analyzer was employed to perform TG analysis on Loy Yang coal and Newlands coal. Note that Loy Yang coal and Newlands coal are classified as low-rank coal and bituminous coal, respectively. Table 1 shows the experimental conditions for TG performed in an atmospheric air environment.

Table 1 Experimental conditions.

Char particle diameter [μm]	125 – 150
Char generation condition [K/min]	100
Sample weight [mg]	0.5
Maximum temperature [K]	1,473
Heating rate [K/min]	100

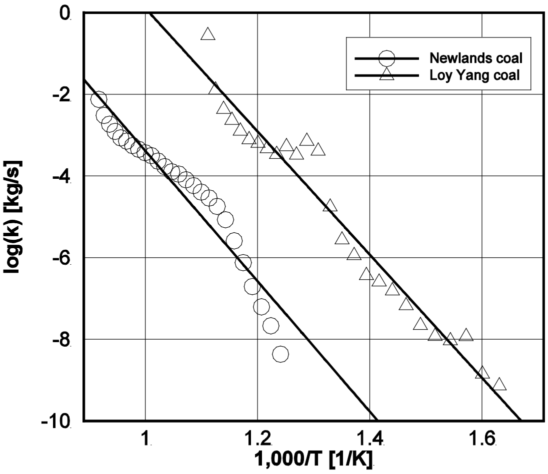


Fig. 1 Arrhenius plots for each coal.

Arrhenius plots for each coal rank obtained by analyzing the TG results are shown in Fig. 1. The detailed estimated parameters of the heterogeneous oxidation reaction are obtained from the laminar approximation of the Arrhenius plots, as shown in Table 2. Note that the chemical reaction is assumed to be a first-order reaction.

Table 2 Estimated reaction parameters.

	Newlands coal	Loy Yang coal
A_{exp} [1/s]	537,132	3,937,277
E [J/mol K]	137,305	125,383

3. Numerical simulation

3.1 Reaction models for char combustion

The following surface reaction of the pulverized coal is considered as the heterogeneous reaction.

$$\mathrm{C} + 0.5\mathrm{O_2} \rightarrow \mathrm{CO} \tag{R1}$$

The overall reaction rate, r, is estimated considering the effect of not only the chemical reaction rate, r_c, but also the mass transfer rate of the oxidant to the surface of the char particle, r_m, as follows:

$$\frac{1}{r} = \frac{1}{r_{\mathrm{c}}} + \frac{1}{r_{\mathrm{m}}} \tag{1}$$

The chemical reaction rate is estimated by:

$$r_{\mathrm{c}} = A \cdot \exp(-E/\mathrm{R}T)\ \cdot P_i \cdot m_{\mathrm{p}} \tag{2}$$

where A, E, R, T, and P_i are pre-exponential factor, activation energy, gas constant, temperature, and partial pressure of the oxidant, O_2. In this study, the aforementioned parameters of the heterogeneous oxidation reaction are used. Because TG is performed in an atmospheric air environment (i.e., $P_{i,\mathrm{exp}} = 0.21$) in order to treat another O_2 partial pressure environment, the pre-exponential factor that is obtained from the experiment is transformed as follows:

$$A = A_{\mathrm{exp}} / P_{i,\mathrm{exp}} \tag{3}$$

The mass transfer rate is estimated from Mulcahy's models[8)] on the basis of some assumptions:

$$\begin{aligned} r_{\mathrm{m}} &= (D_{\mathrm{i},0}/0.5d_{\mathrm{p}})(\rho_0/M)(T/T_0)^{0.75} \\ &\quad \cdot \{-\ln(1-\gamma f_{\mathrm{v,i}})/\gamma\} \cdot M_{\mathrm{c}}/|\nu_{\mathrm{i}}| \cdot S_{\mathrm{p}} \end{aligned} \tag{4}$$

where $D_{\mathrm{i,0}}$, d_{p}, ρ_0, M, $f_{\mathrm{v,i}}$, γ, v_{i}, M_{c} and S_{p} are the diffusion coefficient of the oxidant, O_2, at the standard condition, particle diameter, gas density around the particle, averaged gas molecular weight, mole fraction of the oxidant, O_2, non-dimensional parameter, which is equal to −1 in case of the reaction (R1), stoichiometric coefficient of the oxidant, O_2, molecular weight of char, and surface area of the particle, respectively. The validity of these models has been confirmed by Matsushita *et al.*[7)].

3.2 Government equations

Three heat transfer rate terms to be considered: Q_{conv}, Q_{rad}, Q_{reac}, which are the rates of convective heat transfer, radiation heat transfer, and reaction heat transfer, respectively. Thus, the energy equation of a particle is expressed as follows:

$$m_{\mathrm{p}} C_{\mathrm{p,p}} \frac{\mathrm{d}T_{\mathrm{p}}}{\mathrm{d}t} = Q_{\mathrm{conv}} + Q_{\mathrm{rad}} + Q_{\mathrm{reac}} \tag{5}$$

where $C_{p,p}$ is the specific heat of the particle.

The mass transfer rate to the particle surface due to the reaction is expressed as follows:

$$\frac{\mathrm{d}m_{\mathrm{p}}}{\mathrm{d}t} = -r \tag{6}$$

where γ is overall reaction rate.

Coal char is porous and the mass transfer of a char particle due to the reaction occurs to not only the particle surface but also the pores. However, in this study, to investigate burn-off time and focus on the effect of different coal ranks with different reactivities, a simplified surface reaction model, in which a non-porous spherical particle with no change in its diameter is assumed. This assumption does not affect burn-off time much especially in Loy Yang coal, because the surface reaction is dominant due to reaction field with high temperature.

3.3 Basic assumptions and calculation conditions

To simplify the problem, the following assumptions about the particle have been considered. The particle has no internal temperature distribution and is heated at a constant temperature of an ambient gas and solid wall. The particle does not contain any volatile matter. The contribution percentage of reaction heat generated on the particle surface is set in half and half to the gas phase and the solid phase. The calculation conditions are listed in Table 3. The diameters of the char particles are 10, 15, 100, and 150 μm. The ambient gas temperature and wall temperature are 1,500 and 1,200 K, respectively.

Table 3 The calculation conditions.

Char particle diameter [μm]	10, 15, 100, 150
Initial particle temperature [K]	300
Gas temperature [K]	1,500
Wall temperature [K]	1,200
O_2 concentration [%]	5, 10

3.4 Results and discussion

Fig. 2 shows the calculated Arrhenius plots of the char particle having a diameter of 150 μm between 1,000 and 2,000 K. Note that O_2 concentration is set at 5 %. For Newlands coal, transition from chemical to mass transfer control starts at around 1,200 K and completes at around 2,000 K. On the other hand, for Loy Yang coal, the transition starts at 1,000 K and completes at around 1,500 K. This indicates that the transition of the coal having a higher reaction rate begins from a lower temperature region.

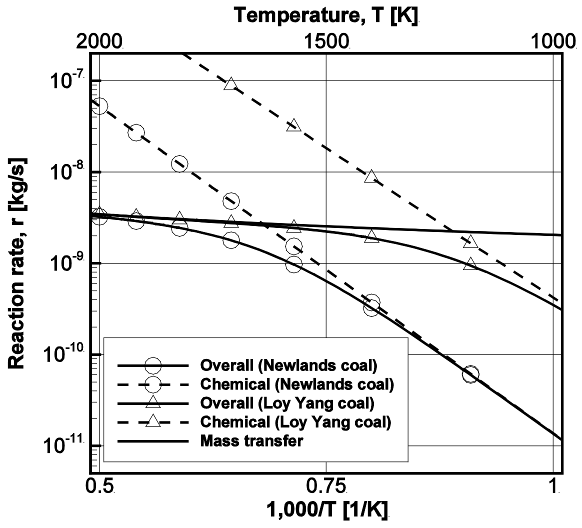


Fig. 2 Effect of coal rank on reaction rate. d_p: 150 µm, O_2: 5 %.

From these facts, use of coal as fuel in the actual pulverized coal furnaces can be influenced by the transition from chemical to mass transfer control in both ranks of coal. In addition, as shown later, the reaction rate effect on the mass transfer of particles starts at around 1,200 K.

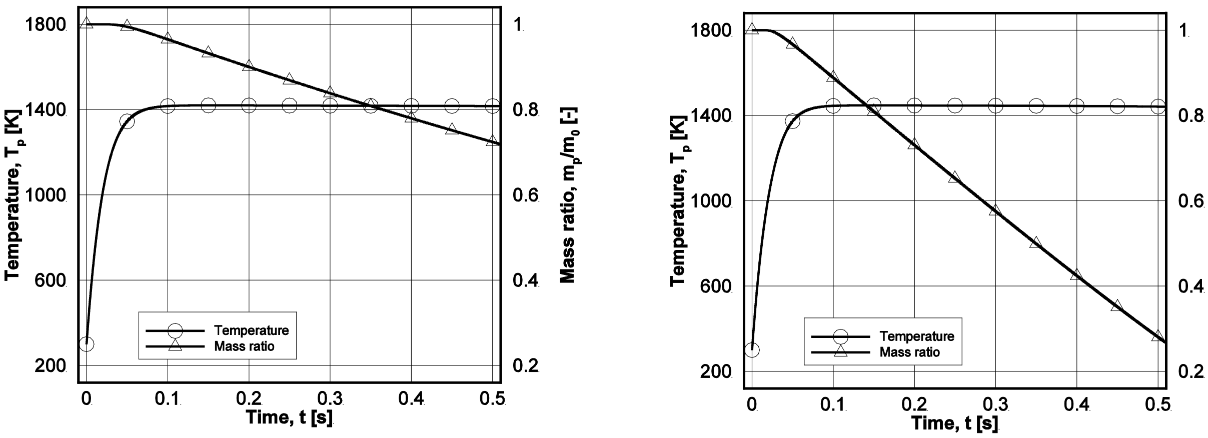
The time histories of the particle temperature and the mass ratio for each coal rank under calculation conditions are shown in Figs. 3 and 4. Fig. 3 shows that, the particle is rapidly heated and temperature increase is completed in about 0.1 s. By comparing Fig. 2 and 3, it is evident that the particle temperature for each coal rank reaches the region where the transition from chemical to mass transfer control starts. However, because the temperature region that the reaction rate of Loy Yang coal is higher, the mass ratio in case (b) decreases more rapidly.

As shown in Fig. 4, in the case of the small particle, a similar rapid temperature increase is observed. Due to relatively lower heat capacity, the rate at which temperature increase is achieved is extremely high and temperature increase is completed in about 0.002 s from the start. The maximum temperature of Loy Yang coal is slightly higher for both particle diameters. For this reason, the influence of the higher reaction heat transfer rate because of the rapid progress of the reaction is considered.

The energy balance histories of the particles under the same conditions as those used in Fig. 3 are shown in Fig. 5. For both coal ranks, for the region in which temperature increase is achieved, as shown in Fig. 3, the total energy term is balanced in about 0.1 s. Initially, radiation heat transfer serves as the heating source; however, with temperature increase, it gradually transits to a cooling source. Finally, radiation heat transfer becomes the only cooling source because the ambient gas temperature and wall temperature are set at 1,500 and 1,200 K, respectively. The difference in the other heat transfer terms for each coal rank can be described as follows. For Newlands coal, convective heat transfer is consistently predominant as compared to reaction heat transfer. On the other hand, for Loy Yang coal, due to the influence of its higher reaction rate, reaction heat transfer becomes predominant as temperature increase is achieved. Finally, reaction heat transfer rate decrease slightly because of the decrease in the reaction rate owing to the decrease in the particle mass.

Table 4 summarizes burn-off time considering various particle parameters. In all conditions, it is evident that burn-off time for Loy Yang coal is drastically shorter than that for Newlands coal.

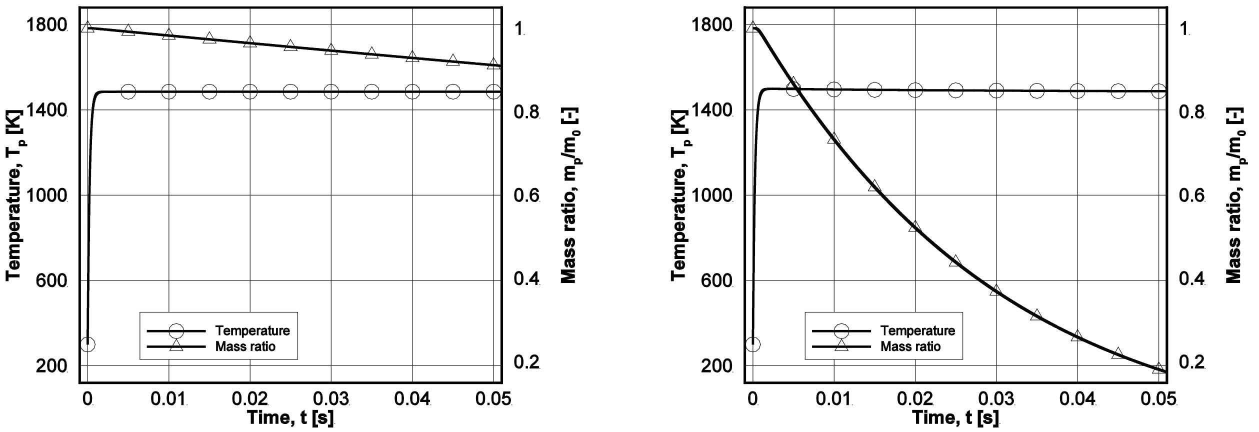
This tendency is more pronounced particularly in the case of small particles, i.e., burn-off time for the 150-µm-diameter particle of Newlands coal is several times



(a) Newlands coal.

(b) Loy Yang coal.

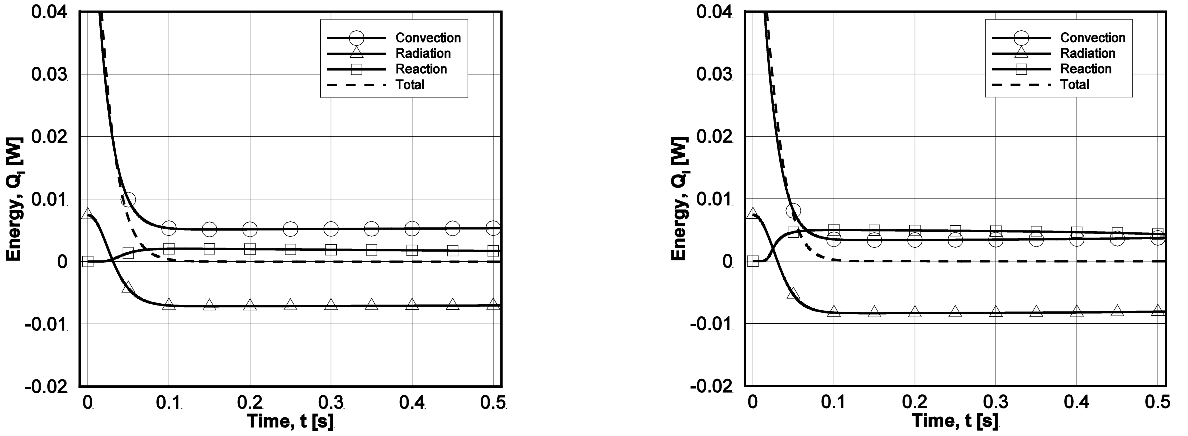
Fig. 3 Time histories of temperature and mass ratio. d_p: 150 µm, O_2: 5 %.



(a) Newlands coal.

(b) Loy Yang coal.

Fig. 4 Time histories of temperature and mass ratio.
d_p: 15 μm, O_2: 5 %.



(a) Newlands coal.

(b) Loy Yang coal.

Fig. 5 Time histories of energy balance.
d_p: 150 μm, O_2: 5 %.

Table 4 Burn-off time for various particle parameters.

Char particle diameter [μm]	O_2 concentration [%]	Burn-off time [s]	
		Newlands coal	Loy Yang coal
10	5	2.358	0.1242
	10	1.178	0.0616
15	5	2.449	0.1305
	10	1.223	0.0642
100	5	4.113	0.4358
	10	2.016	0.2121
150	5	5.218	0.8041
	10	2.536	0.3995

longer than that for Loy Yang coal having the same particle diameter. However, burn-off time for a 15-μm-diameter particle of Newlands coal is approximately 20 times that of Loy Yang coal. From these results, it is evident that the detailed estimation of burn-off time for coals of different ranks is important to achieve not only high efficiency in pulverized coal combustion furnaces and burners, but also fuel diversification for pulverized coal-fired generation.

In addition, it is evident that the influence of different concentrations of oxygen is a simple proportional relationship for all conditions.

4. Conclusions

In order to investigate the influence of different coal ranks on burn-off time, the parameters for the heterogeneous chemical reaction rate of Char–O_2 for Loy Yang coal and Newlands coal were estimated using TG. By analyzing the TG results, detailed parameters about heterogeneous oxidation reaction were estimated.

Furthermore, in order to investigate the phenomena of the char particle in detail, heat and mass transfer around a single pulverized coal particle that is exposed to a simplified heating environment were calculated. By comparing these numerically analyzed results for various particle parameters (e.g., rank of coal, initial particle diameters, oxygen concentration), the qualitative tendency that burn-off time for Loy Yang coal is drastically shorter than that of Newlands coal is found.

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Nomenclature

A	pre-exponential factor	[1/ s]
Cp	specific heat	[J/(kg K)]
D	diffusion coefficient	[m^2/s]
E	activation energy	J/mol K
f	fraction	[-]
k	rate coefficient	[kg/(m^2·s)]
M	molecular weight	[kg/kmol]
m	mass	[kg]
P	partial pressure	[atm]
R	universal gas constant	[J/mol K]
r	reaction rate	[kg/s]
S	surface area	[m^2]
T	temperature	[K]
	Greek symbols	
ν	stoichiometric coefficient	[-]
ρ	gas density	[kg/m^3]
	Subscripts	
exp	expriment	
m	mass	
p	particle	
v	mole	
0	standard condition	

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