Numerical Assessment on Blended Pulverized Coal Combustion by Large Eddy Simulation
Seongyool Ahn†, Hiroaki Watanabe, Toshiaki Kitagawa

Pulverized coal is one of major energy resources for last centuries, and the range of coal quality is getting wide which involves higher volatile matter and humidity, and lower fixed carbon. These differences have potential possibility giving a damage on a furnace. So, it is crucial to understand the effect of fuel composition on combustion characteristics to prevent physical damages and improve combustion efficiency.

Many researches have been performed to improve understanding of the effect of fuel composition on pulverized coal combustion. Lisandy et al. [1] investigated unburned carbon and NO formation characteristics from low-rank coal combustion in a drop-tube furnace experimentally and numerically. They revealed that higher thermal NO is formed at peak temperature whereas NO formation is suppressed during low-stoichiometric-combustion. Mätzing et al. [2] modeled grate combustion of biomass and low rank fuels with numerical approach. The new model captured key quantities such as ignition delay time, ignition rate, reaction front velocity and mass conversion rate properly comparing to experiment. Although many researches have been performed and are performing, much of it is still disclosed.

The purpose of this study is, therefore, to investigate the effect of fuel composition on combustion characteristics of different rank of coals by numerical analysis. Two coals were employed for this study which have different fuel ratios as 1 and 2. Simulations were carried out for a pilot-scale turbulent pulverized coal combustion furnace, and validated by comparison with experiment. The combustion characteristics of each coal are discussed based on simulation results in terms of gaseous temperature, velocity and composition.

To solve the LES equations, the FFR-Comb. package is employed which is extended by NuFD, Central Research Institute of Electric Power Industry, Kyoto University and Kyushu University [3]. The governing equations for gaseous phase are given by

\[
\frac{\partial \rho_i \hat{u}_i}{\partial t} + \frac{\partial \rho_i \hat{u}_i \hat{u}_j}{\partial x_j} = \frac{\partial \hat{p}}{\partial x_i} + \frac{\partial \tilde{\sigma}_{ij}}{\partial x_j} + S_{\text{mom},i} + \tau_d \frac{\partial T}{\partial x_i}.
\]

where \(\rho_i\) is density, \(\hat{u}_i\) is velocity, and \(\sigma_{ij}\) is viscous stress tensor of the gas phase, respectively while \(\tau_d\) denotes the SGS effect. \(T\) represents the thermal diffusivity. \(Y_k\) is the kth species and \(D_k\) is the diffusivity. \(\hat{\rho}_i\) denote the spatial averaging and Favre-filtering, respectively. \(S_{\text{int}}, S_{\text{mom}}\) and \(S_h\) are source terms attributable to interactions between gaseous phase and particles.

The governing equations for particles are written as below in the order of position, velocity, and temperature.

\[
\frac{d x_{i,p}}{d t} = u_{i,p},
\]

\[
\frac{u_{i,p}}{d t} = f_d (\hat{u}_i - u_{i,p}),
\]

\[
\frac{d T_p}{d t} = \frac{Q_p + (d m_p/dt)/L_v}{m_p C_v},
\]

where \(x_{i,p}\) and \(u_{i,p}\) denote the location and the velocity of the particle, respectively, \(f_d\) is the drag force term, and \(\tau_p\) is the response time of the particle. \(T_p\) and \(C_v\) are the particle temperature and the specific heat of the particle, respectively. \(L_v\) is the latent heat of vaporization at \(T_p\). Interactions between the
two phases are solved by the Particle-Source-In Cell (PSI-CELL) model [4,5].

A single postulated species, CaHbOc, is introduced to explain released gases during devolatilization process.

\[
dV/dt = K_v (V^* - V), \quad (8)
\]

\[
K_v = A_v \exp(E_v/(RT_p)), \quad (9)
\]

where \( V^* \) and \( V \) are the volatile matter content of the proximate analysis and total amount of released volatile gases from a particle respectively. \( R \) is the universal gas constant and \( A_v \) and \( E_v \) indicate pre-exponential factor and activation energy, respectively. The values of \( A_v \) and \( E_v \) are determined by the FLASHCHAIN software [6] and set to 2021 s\(^{-1}\) and 31.1 kJ/mole, respectively, in this study.

Combustion of gaseous phase is explained by a simple global kinetic mechanism consists of three steps, as below:

\[
\text{CaHbOc} + d \text{O}_2 \rightarrow x \text{CO} + y/2 \text{H}_2\text{O}, \quad (10)
\]

\[
\text{CH}_4 + 3/2 \text{O}_2 \rightarrow \text{CO} + 2 \text{H}_2\text{O}, \quad (11)
\]

\[
2 \text{CO} + \text{O}_2 \rightarrow 2 \text{CO}_2, \quad (12)
\]

where \( d, x \) and \( y \) are determined by the species conservation of the oxygen component. Particle combustion is calculated by a single step reaction, as presented in the following equation.

\[
2C(s) + O_2 \rightarrow 2\text{CO}, \quad (13)
\]

where \( C(s) \) denotes the carbon component in the char. The combustion rate of (13) is determined by Field’s model [7]. The reaction rate of the kinetics is built by the scale similarity filtered reaction rate model (SSFRRM) for turbulent flow field [8].

Fig. 1 indicates the numerical domain which is unstructured, and has 8 m length. Fig. 1 (b) shows the burner and inlets consists of 1st inflow, 2nd inflow and 3rd inflow. There is one more inlet at middle of the reactor named OFA. Pulverized coal particles are issued through 1st inflow with carrier gas of air, while additional air is provided by 2nd and 3rd inflows to generate turbulent flow. Staging air is issued at middle of the furnace, which is corresponding to over-fire-air (OFA).

<table>
<thead>
<tr>
<th>Table 1 Fuel property</th>
<th>Newlands coal</th>
<th>Tanitohalum coal</th>
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</thead>
<tbody>
<tr>
<td>Proximate analysis [wt%]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Moisture</td>
<td>2.6</td>
<td>10.9</td>
</tr>
<tr>
<td>Volatile matter</td>
<td>28.5</td>
<td>45.6</td>
</tr>
<tr>
<td>Fixed carbon</td>
<td>57.2</td>
<td>45.7</td>
</tr>
<tr>
<td>Ash</td>
<td>14.3</td>
<td>8.7</td>
</tr>
<tr>
<td>Ultimate analysis [wt %]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbon</td>
<td>73.3</td>
<td>68.7</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.4</td>
<td>4.78</td>
</tr>
<tr>
<td>Oxygen</td>
<td>6.2</td>
<td>15.4</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>1.51</td>
<td>1.53</td>
</tr>
<tr>
<td>Sulfur</td>
<td>0.29</td>
<td>0.74</td>
</tr>
</tbody>
</table>

![Fig. 1](image_url) (a) Whole numerical domain and (b) enlarged image of burner inlets
Two coals are employed in this study to make comparison, and the examined fuel property is presented in Table 1. As shown in the table, the fuel rations of New lands (NL) coal and Tanitoalum (TH) coal are different as 2 and 1, respectively. The size of particles is assumed as 45 µm of diameter. The inlet conditions of the simulations are corresponding to experiments for each case, and the values are summarized in Table 2.

The maximum Courant number is below unity during calculation with time difference of 5 µs. A case consumes approximately 166 h of wall-time with 576 cores in the supercomputing facilities at Research Institute for Information Technology, Kyushu University. The calculation is performed for 300 thousand steps, and time-averaged values are estimated for last 50 thousand steps.

<table>
<thead>
<tr>
<th>Table 2 Inlet conditions</th>
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<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>T [K]</td>
</tr>
<tr>
<td>NL [m/s]</td>
</tr>
<tr>
<td>TH [m/s]</td>
</tr>
</tbody>
</table>

Fig. 2 exhibits gaseous temperature distribution of two coals. As presented in the figure, distributions of the gaseous temperature seem similar over the region. The high temperature gas becomes lower when the OFA is injected in the both cases.

For more detail comparison, time-averaged gaseous temperature is plotted according to central position of the furnace as well as comparison with experiment of NL coal in Fig. 3. The peak gaseous temperature is higher than that of experiment for the both cases, but it becomes similar after the OFA is injected. The both cases have similar temperature distribution, as presented in the plot.

Fig. 4 presents contoured distributions of time-averaged axial velocity for the both simulations. As presented, there are two large recirculating flows at upstream in inside and outside of the flame. There is one more recirculated flow at middle and downstream after OFA injection. The recirculating flow is faster in the case of NL coal at the inside of flame and middle stream than that of TH coal, even though general distribution characteristic is similar in the both cases.

Fig. 5 shows contoured images of mole fraction distributions for oxygen, volatile matters and CO₂ of the cases of NL and TH coals. As expected, more oxygen has been consumed in the case of TH coal due to the lower fuel ratio. Moreover, devolatilized gas and CO₂ are higher in the case of TH coal than that of NL coal. All oxygen remains at upstream is completely consumed when OFA is injected in the case of TH coal.

![Gaseous temperature](image1)

*(a) NL coal and (b) TH coal*

![Gas temperature](image2)

*(Gas temperature of single cases along central position of the furnace)*
Acknowledgements

This study is supported by MEXT (Ministry of Education, Culture, Sports, Science and Technology Japan) as "Priority issue on Post-K computer" (Accelerated Development of Innovative Clean Energy Systems), Project ID: hp160220, hp170273 and hp180203.

References