Numerical simulation of the effect of different NaCl concentration on boiler flame combustion process

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Abstract—Zhundong coal has been widely concerned because of its high alkali metal content, which brings great danger to the combustion of boiler. Therefore, it is extremely necessary to study the laws and characteristics of alkali metal influencing combustion in the burning process of zhundong coal. A gas-solid two-phase flow combustion model of pulverized coal containing NaCl was established by using Fluent software and FactSage software in a hot experimental combustion furnace. The influence of different NaCl content in pulverized coal on pulverized coal combustion process was discussed. The results show that with the increase of NaCl content in pulverized coal from 0 to 1% and 2%, the flame center temperature in the furnace increases about 80°C and 120°C under the same coal content, so it can be concluded that the increase of NaCl content can promote the combustion process of pulverized coal in the furnace. At the same time, it can be calculated that, with the increase of NaCl content, the flame range of the combustion region inside the furnace increases by 1/3. Because NaCl is decomposed by heat during combustion to help combustion, and the radiation heat transfer increases, the flame radiation range inside the furnace will increase.

1. Introduction

As an important pillar of China's national economic development, coal power is still the main power supply in China for a period of time to come. "Zhundong Coal" is currently the largest integrated coal field in China, with an estimated coal reserve of 390 billion tons, which is of great significance to the modern industrialization process of the energy industry. Zhundong coal, however, high volatile coal, the characteristics of high moisture content, high alkali content, Na in zhundong coal and its compound content is higher, zhundong coal ash content usually contains about 5%, the highest can reach 15%, the content of alkali metal (ash) overall 5% or more, some of the alkali metal content as high as 10%\textsuperscript{[1]}. Wei Xiaofang et al.\textsuperscript{[2]} studied Australian high-sodium coal and found that most of the existing forms of sodium in coal are water-soluble NaCl salts. In the study of zhundong coal, Chen Chuan et al.\textsuperscript{[3]} found that sodium in these high-sodium coals is mainly water-soluble sodium, with less organic sodium and insoluble sodium. Song Jinling\textsuperscript{[4]} used mixed coal to control the change of alkali metal content of experimental coals, and found that the coal sample with higher alkali metal content had stronger catalytic effect on pulverized coal combustion, which was faster and more intense, and had stronger reaction ability in the early stage of combustion.

In this paper, by calculating the content of alkali metals in ash after conversion, 1% and 2% NaCl were added to raw coal to simulate different concentrations of alkali metals in pulverized coal\textsuperscript{[5]}. Fluent software is used for numerical simulation of a hot state experimental combustion table to realize numerical simulation calculation of combustion state in the furnace, and obtain the combustion
state, flame distribution and temperature distribution in the furnace. The influence of NaCl on the combustion process in furnace was analyzed by referring to the simulation results.

2. Introduction to experimental combustion furnace

The research object is a hot experimental combustion furnace. The diameter of the combustion furnace shell is 380mm, the external insulation layer is about 120mm, and the height of the furnace is 1200mm. The top area is the burner nozzle, the burner is the center of the primary air, the outer layer is adjacent to the secondary air structure layout, the primary air nozzle diameter is 20mm, the secondary air nozzle diameter is 10mm ring, the secondary air pipe in the insulation layer close to the outer wall of the furnace, depending on the temperature of the furnace heating secondary air temperature. The bottom of the combustion furnace is the outlet of water-cooled flue. Along the inner wall of the furnace, 8 auxiliary heating tubes with length of 800mm and diameter of about 80mm are arranged at equal spacing. Natural gas combustion is used for heating, which is used to adjust the temperature of the inner wall of the furnace and keep the furnace temperature constant.

3. Mathematical model and simulation calculation

3.1 Geometric models and grids

The structure of the test furnace was simplified and the auxiliary heating pipe was ignored. Gambit software was used to build a 1:1 3D geometric model and grid the furnace. In order to make the calculation result more accurate and reliable, the hexahedral structured grid is used to divide the grid, and the grid quality is good and meets the requirements of calculation. The total number of grids is 980,000, and the burner area is the starting point for the calculation of furnace combustion. The flow, heat transfer and other conditions are complicated, which have a great impact on the combustion, temperature field and velocity field in the furnace. Therefore, in order to improve the accuracy of calculation, the encryption method is adopted in the division of the regional network. The grid layout of primary and secondary air nozzles and the overall model is shown in Figure 1.

3.2 Mathematical model

3.2.1 Realizable K-\( \varepsilon \) model

The K-\( \varepsilon \) two-way equation model\(^7\) is selected to simulate the gas-solid two-phase flow of pulverized coal in the furnace. For the three-dimensional steady convection and diffusion problem, the governing equation is as follows:

\[
\frac{\partial}{\partial x} (U\phi) + \frac{\partial}{\partial y} (\rho V\phi) + \frac{\partial}{\partial z} (\rho W\phi) = \frac{\partial}{\partial x} \left( \Gamma_\phi \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma_\phi \frac{\partial \phi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \Gamma_\phi \frac{\partial \phi}{\partial z} \right) + S_\phi \tag{1}
\]

Where: \( \phi \) is the general dependent variable; \( \Gamma_\phi \) is the transport coefficient; \( S_\phi \) is the source term of general dependent variable; \( \rho \) is the gas phase density.
Equation (1) gives the transport equations of continuity and momentum and energy and turbulent kinetic energy and turbulent dissipation rate. The transport equation of turbulent kinetic energy $K$ and turbulent kinetic energy dissipation rate $\varepsilon$ for k-ε model can be written as follows:

$k$ equation:
\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_m + S_k
\]  

(2)

$\varepsilon$ equation:
\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho C_1 \varepsilon - \rho C_2 \frac{\varepsilon^2}{k+\nu\varepsilon} + C_{1\varepsilon} \frac{\varepsilon}{k} - \varepsilon G_b + S_\varepsilon
\]  

(3)

Where: $\mu_t$ is turbulence viscosity coefficient; $\mu$ is the laminar viscosity number; $G_b$ is turbulent kinetic energy due to buoyancy; $Y_m$ is turbulence dissipation caused by pulsating expansion of compressible fluid; $Y_m = 2 \rho \varepsilon \frac{k}{\alpha T a}$ is sound velocity; $S_k$ is the source term; $C_1 = \max \left[ 0.43, \frac{\eta}{\eta + 5} \right]$; $\eta = \frac{Sk}{\varepsilon}$; $C_{1\varepsilon}$, $C_2$ are constants; $\sigma_k$, $\sigma_\varepsilon$ are the turbulent Prandtl numbers of turbulent kinetic energy and its dissipation rate respectively. In Fluent, as the default constant value, $C_{1\varepsilon} = 1.44$, $C_2 = 1.9$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.2$.

### 3.2.2 Component transport and chemical reaction models

Component transport and chemical reaction were used to simulate the combustion process of pulverized coal with different concentrations of NaCl. The component transport model was selected as the finite rate/vortex dissipation model [6], indicating that chemical reaction was of finite reaction rate, and the reaction rate was controlled by both chemical reaction itself and turbulent mixing.

The reaction equation of pulverized coal combustion is calculated based on the coal quality characteristics used in the simulation in Fluent software, as shown in Formula (4) and Table 1.

\[
C_{1.53}H_{1.69}O_{0.56}N_{0.0275}S_{0.0137} + 1.68O_2 \rightarrow 1.53CO_2 + 0.84H_2O + 0.013N_2 + 0.012SO_2
\]  

(4)

Combined with the pure matter thermodynamics database in FactSage software, the thermal physical property parameters of eight optimized compounds containing Na were queried, as shown in Table 2. The 7-step elemental reactions of NaCl combustion reaction process were established, as shown in Table 3. The elemental reaction rate depends on Arrhenius’ law [7]:

\[
k = A \cdot T^\beta \exp[-E/(RT)]
\]  

(5)

Where: $k$ is the rate constant; $A$ is the pre-exponential factor; $T$ is temperature; $\beta$ is the index; $E$ is the activation energy, J/mol; $R$ is the gas constant, taking 8.314J/(mol·K).

### Table 1 Industrial analysis and elemental analysis of coal used in simulation

| Industrial analysis/% | Elemental analysis/% | Heat value (MJ·kg⁻¹) |
|-----------------------|----------------------|----------------------|
| FC, ar | V, ar | A, ar | M, ar | C, ar | H, ar | O, ar | N, ar | S, ar | | |
| 31.2 | 39.6 | 5.2 | 24.0 | 52.51 | 2.13 | 11.36 | 0.48 | 0.52 | 18.57 |

### Table 2 Reaction mechanism of optimized sodium-containing substances

| No. | elemental reaction | A | n | E/R |
|-----|-------------------|---|---|-----|
| 1   | NaCl+H₂O=NaOH+HCl [8] | 1.7E14 | 0 | 0 |
| 2   | NaCl+NaCl=(NaCl)₂ [8] | 8.0E13 | 0 | 0 |
| 3   | NaO₂+HCl=NaCl+HO₂ [8] | 1.4E14 | 0 | 0 |
| 4   | Na+HCl=NaCl+H [8] | 1.3E15 | -1 | 5030 |
| 5   | Na+Cl=M+NaCl+M [8] | 1.1E20 | -1 | 0 |
| 6   | NaCl+SO₃(+)M=Na₂SO₄(+)M [8] | 1.0E14 | 0 | 0 |
| 7   | NaHSO₄+NaCl=Na₂SO₄+HCl [8] | 1.0E14 | 0 | 0 |
4. Simulation results

4.1 Effect of NaCl concentration on flame temperature
It can be seen from observation that with the increase of NaCl content in coal, the temperature of the flame center, zone and zone in the furnace also rises. When NaCl content increases from 0 to 1%, the flame center temperature rises by about 80°C; when NaCl content increases from 0 to 2%, the flame center temperature rises by about 120°C. When NaCl content increases from 0 to 1% and 2%, the overall furnace temperature increases by about 50°C. The temperature distribution of furnace flame is shown in Figure 2. Researchers think that electron transfer theory is the main reason why alkali metal acts on carbon atoms in pulverized coal and promotes the catalytic combustion of pulverized coal. Electron transfer refers to the heating of alkali metal thermal decomposition and activated enough, leave the electrons in the metal ions, metal a cationic hole, cause the change of the carbon surface electronic structure, so the metal ions change is incentive structure, coal molecular changes structure is the result, so that volatile release intensifies, and accelerate damage the structure of the carbon, accelerates a pulverized coal combustion. At the same time, in the flame burnout region, the flame temperature also increased with the increase of NaCl content, but the increase was less, because most of NaCl had already reacted and only a few remained.

![Fig.2 Flame combustion temperature at different NaCl content](image_url)

4.2 Effect of NaCl concentration on flame combustion range
Through calculation, it can be found that with the increase of NaCl content in coal, the combustion range of the flame in the furnace also expands. When NaCl content increases from 0 to 1% and 2%, the combustion radius of furnace flame increases from 4.5cm to 6.8cm, and it can be calculated that the flame combustion range on the cross section is about S=81.6cm². The combustion length of the furnace flame increases from 26cm to 38cm, and the combustion range of the flame can be simplified into a cylinder with the same radius in terms of the combustion length. The radius is obtained by measuring respectively, and it can be known that the overall combustion range is expanded by about V=897.6cm³. The flame temperature distribution in the cross-section of the furnace is shown in Figure 3. It can be seen from Figure 4 that NaCl enters the furnace mainly at the position 0-35cm at the nozzle of the burner, where the coal powder carrying NaCl decomposes into Na⁺ ions and Cl⁻ ions at high temperature and releases a large number of free electrons to promote combustion.
5. Conclusion
Based on the results and discussions presented above, the conclusions are obtained as below:

(1) As the content of NaCl added to pulverized coal increases from 0% to 1% and 2%, the flame center temperature in the furnace also increases to about 80℃ and 120℃, so it can be concluded that NaCl content can promote the combustion process of pulverized coal in the furnace. The increase of NaCl on the temperature of the furnace is mainly reflected in the main combustion region, because in the burnout zone, most NaCl has been completely decomposed, and there is less decomposition through the burnout zone, so the increase of the ambient temperature in the furnace is small.

(2) With the increase of NaCl content in pulverized coal from 0% to 1% and 2%, the overall combustion range of the flame in the furnace is about 897.6cm³, and the flame combustion range on the cross section is about 81.6cm².

(3) Through the research of this paper, we can more deeply understand and explore the combustion characteristics and promoting combustion mechanism of alkali metals in the combustion process of zhundong coal, which can provide experimental and theoretical basis for the large-scale development and utilization of zhundong coal in the next step.

References
[1] Chen Xinwei, Zhuang Xinguo, Zhou Jibin, et al. Coal quality characteristics and distribution law of Zhundong Coalfield[J]. XINJIANG DIZHI, 2013, 31(01): 89-93.
[2] Wei Xiaofang, Liu Tiefeng, Huang Jiejie, et al. Changes in the form of sodium in high salt Australian coal during pyrolysis[J]. Journal of Fuel Chemistry and Technology, 2010, 38(02): 144-148.
[3] Chen Chuan, Zhang Shouyu, Liu Dahai, et al. The form of sodium in high sodium coal in Xinjiang and its influence on combustion process[J]. Journal of Fuel Chemistry and Technology, 2013, 41(07): 832-838.

[4] Song Jinling. Experimental study on the effect of alkali metals in high alkali coal on coal combustion characteristics[D]. Shanghai Jiao Tong University, 2015.

[5] Ling Zhongqian, Zeng Xianyang, Hu Shantao, et al. Numerical simulation of optimization of SCR flue gas denitration system for power plant boiler. Journal of Chinese Society of Power Engineering, 2014(1): 50-55.

[6] Zhizhong Kang, Xian Ding. Numerical analysis on combustion process and sodium transformation behavior in a 660 MW supercritical face-fired boiler purely burning high sodium content Zhundong coal[J]. Journal of the Energy Institute, 2020, 93(2).

[7] Ji Jie Qiang, Cheng Leming, Liu Yanquan, et al. Chemical kinetic simulation of high temperature form of sodium in zhundong coal[J]. Journal of Chinese Society of Power Engineering, 2017, 37(10): 780-787.

[8] Peter Glarborg, Paul Marshall. Mechanism and modeling of the formation of gaseous alkali sulfates[J]. Combustion and Flame, 2004, 141(1).

[9] Lusi Hindiyarti, Flemming Frandsen, Peter Glarborg, Paul Marshall. An exploratory study of alkali sulfate aerosol formation during biomass combustion[J]. Fuel, 2007, 87(8).