Simulation of Combustion and Alkali Metal Distribution in Zhundong High Alkali Coal Boiler Based on Computer Control System

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Abstract. Restricted by Xinjiang's special geographical location, economic conditions, transportation and other factors, Zhundong coal can't be sent out on a large scale, which seriously hinders the development of Zhundong coal base. Meanwhile, due to the coal-forming history and Xinjiang's special natural geographical environment, the alkali metal content in Zhundong coal is generally over 2%, which is much higher than that of power coal in other parts of China. In this paper, based on computer control system, the combustion and alkali metal distribution in Zhundong high alkali coal boiler are simulated, and the morphological distribution characteristics and migration laws of alkali metals such as Na and K in pulverized coal combustion process of high alkali coal, low alkali coal and their two coal samples are deeply studied. Combustion characteristics and heat flow distribution, the simulation results show that the flue gas temperature at the furnace outlet is 895.07℃, and the flue gas temperature near the wall is low, which is helpful to alleviate the slagging and contamination in the furnace.

Keywords: Computer control, Zhundong high alkali coal, Numerical simulation, Alkali metal

1. Introduction
The coal with alkali metal content greater than 0.5% belongs to high alkali coal, which has certain reserves in China, Australia, the United States, Germany and other places. China also has a significant impact on the world in the consumption revolution of energy from the right side of the country, among which the reduction of coal consumption is the key factor. Problems such as environmental pollution and ecological destruction caused by the development and utilization of energy (especially fossil energy) have become increasingly prominent, and the global climate change caused by energy emissions poses new challenges to human survival and economic development mode [2]. The whole coal field in Zhundong region of Xinjiang covers an area of about 13,000 square kilometers, which is the largest in the world at present. It is predicted that there is a coal reserve of 0.39 trillion tons here, which accounts for 17.8% of the whole Xinjiang region and 7% of the whole country. Li Caiyun et al. [3] summarized the coal quality of Zhundong Coalfield, and thought that Zhundong coal had low ash content, the volatile content in coal was in the middle and high level, and the content of sulfur,
phosphorus and chlorine in coal was low, which was obtained from the perspectives of coal petrology and coal chemistry. Zhang Tian et al. [4] selected a boiler blended with Zhundong coal in Xinjiang, adjusted the operation of the boiler by changing the blending ratio, and concluded that the increase of blending ratio of Zhundong coal would have a bad influence on the operation of the boiler.

Because the content of Na and K in high alkali coal in Zhundong area of Xinjiang is 3–5 times of that of conventional known power coal, the sublimation and condensation of Na and K salts will cause serious contamination and slagging on the water wall and high temperature heating surface of boiler furnace, which will cause great instability. The research is based on computer control system. By dividing different reaction interfaces between pulverized coal combustion process and high-temperature slag, and analyzing the chemical composition and mineral composition of coal ash in each reaction interface, the release and capture characteristics and action mechanism of alkali metals in high-alkali coal under high-temperature slag combustion conditions are studied. The chemical reaction model adopts EDC model, summarizes and simplifies the reaction mechanism in the furnace in this simulation, and obtains the reaction mechanism package used.

2. Numerical Simulation of Combustion Process of a Single Swirl Burner

2.1 Design coal quality
Zhundong coal has the characteristics of high moisture content, low ash content, high volatile matter, medium and high calorific value, low sulfur, low ridge and low chlorine, so Zhundong coal belongs to high quality power coal. While the basic oxides are mainly Fe₂O₃, CaO, MgO, Na₂O and K₂O. The characteristics of acid oxide are: it can increase the melting temperature of ash, and the more it is, the higher the melting temperature will be; on the curve of volume rate change, the inflection point of rate abrupt change appears for the first time. After volatiles are analyzed, they are mixed with the surrounding air, and start to burn at a certain temperature and concentration, and the combustion and precipitation of volatiles are carried out simultaneously. The design coal type is Xinjiang Zhundong high alkali coal, and its coal quality composition and calorific value are shown in Table 1.

According to the strong slagging and contamination characteristics of Zhundong coal, the relevant key prevention and control technologies are designed. The boiler plays an extremely important role in burning Zhundong coal completely and utilizing Zhundong coal at low cost for a long time. Should be an important factor, the reaction occurs before Na release at low temperature, but the opposite at high temperature, which leads to the difference of Na content in gas phase at different temperatures [5]. Under suitable process conditions, the Na content in Zhundong coal can be reduced to below 2% (calculated by ash), and the removal efficiency is as high as 73.75%. The upgraded coal quality meets the requirements of modern coal-fired boilers [6].

| Table 1 Coal Quality Analysis of Design Coal |
|---------------------------------------------|
| Name     | Unit | Numerical |
| Carbon   | %    | 55.13     |
| Hydrogen | %    | 2.54      |
| Oxygen   | %    | 9.2       |
| Sulfur   | %    | 0.47      |
| Moisture | %    | 0.81      |
| Volatile matter | %    | 30.88    |
| Ash content | %    | 12.45    |
| net calorific power | MJ/kg | 18.83   |

2.2 Calculation area selection and grid division
Because high-alkali coal has serious fouling and slagging characteristics, in order to ensure that the fouling and slagging of blended coal can be controlled, it is necessary to deeply study the migration law of Na and K during the combustion of high-alkali coal, low-alkali coal and their different
proportions of blended coal and their influence on the melting characteristics of coal ash. But the advantage is that the focus of attention is more prominent, and it is convenient to examine the influence of the key parameters of the burner on the combustion process in a core area at its outlet. The combustion characteristic curve of coal pillar has a common characteristic in air atmosphere, that is, at a certain temperature, the internal stress of coal pillar increases, which leads to a slight expansion of the volume. Before that, the volume of coal pillar basically remains unchanged, showing the inflection point of the first rate abrupt change on the volume change rate curve. At the corresponding temperature, it deposits on the wall, and then causes the related slagging and contamination problems. And the corresponding Na content in gas phase decreases. The occurrence forms of Na in bottom slag are almost unchanged, while the proportion of water soluble Na in fly ash increases. The alkali metal content in fuel will change accordingly, and the blended fuel needs to be adjusted accordingly. The geographical location and traffic conditions in Xinjiang greatly limit the stability and economy of blended fuel.

In this paper, a multi-working condition simulation with variable operating parameters is carried out for a single burner, and the boundary conditions are introduced below with the tangential wind speed of 5.5m/s as a typical working condition, as shown in Table 2

| Projects                          | Unit | Numerical |
|----------------------------------|------|-----------|
| Primary wind speed               | m/s  | 17        |
| Primary air temperature          | K    | 349       |
| Inner secondary wind speed       | m/s  | 25        |
| External secondary axial wind speed | m/s  | 27.01     |
| External secondary radial wind speed | m/s  | 6         |
| External secondary rotation speed | m/s  | 4.4       |
| Central wind speed               | m/s  | 7         |
| Secondary air temperature        | K    | 584       |
| Coal feeding amount              | kg/s | 3         |
| Average particle size of pulverized coal | μm  | 80        |
| Wall temperature                 | K    | 800       |

Minerals in coal refer to inorganic non-coal substances and inorganic elements existing in coal organic compounds. A large number of data show that Na content in coal decreases with the increase of mining depth from topsoil, overlying strata of coal seam to coal seam, that is, the composition content of alkali metals in coal in different mining depths in the same mining area is different. In this paper, the separation structure of primary air is retained in the burner structure, and the inlet diversion part of internal and external secondary air is ignored. However, various flares which have a great influence on the combustion process are considered, and encryption treatment is carried out at the inlet of each nozzle. The most important problems to be solved when burning lignite in utility boilers are slagging on the heating surface mainly based on radiation heat transfer and contamination on the heating surface mainly based on convection heat transfer in the furnace. After adding a certain proportion of NaCl to Zhundong coal, the catalytic action of alkali metal Na is obviously enhanced in the middle and late combustion stage, which makes the burnout temperature advance by nearly 200℃, and the burnout obviously advances. In addition, the corresponding temperature decreases obviously when the coke combustion rate is the highest.

3. Prediction of Alkali Metal Conversion and Concentration Distribution in Furnace

3.1 Transformation path of alkali metal in furnace
In the combustion process of Zhundong high alkali coal in the furnace, alkali metal substances are precipitated from pulverized coal after it enters the furnace, and then react in the flue gas. The contents of Na₂SO₄, Na, K and Cl, which are the main substances forming the initial deposit, vary greatly with
different coal types in Zhundong. The influence of ashing temperature on the precipitation of Na and K in coal is related to the occurrence forms of Na and K, which vary with different coal types. According to the chemical reaction mechanism, the volatile gaseous alkali metal can react with silicon-aluminum minerals before and after volatilization to form nonvolatile aluminosilicate, so kaolin, diatomite, active bauxite, oil shale semicoke and coal-fired fly ash rich in silicon-aluminum minerals can be used as additives to alleviate contamination [7]. The formed ash deposits will seriously hinder the convective heat transfer between flue gas and steam, flue gas and air. The formation process of ash deposition is an extremely complicated hydrodynamic process [8]. More importantly, the entrained-flow gasifier can adopt the characteristics of high temperature and high pressure, which determines that it has the greatest potential to improve the production capacity in unit time and unit volume, and represents the mainstream trend of coal gasification technology development [9].

At the initial stage of combustion, the volume of Zhundong coal has obviously expanded. When the temperature rises to 895.07℃, the combustion volume of coal pillar has expanded to twice the original volume. By comparing the distribution of intermediate products of the two ways, the proportion of the two ways in NaCl sulfation was analyzed. Therefore, it is necessary to consider two aspects: total sodium of coal entering the furnace and pollution intensity trend of coal ash. Theoretically, burning Xinjiang Zhundong high alkali coal is easy to catch fire, but it is easy to be seriously polluted, so the outlet flame of its burner should be more similar to direct current, not too diffuse, and the phenomenon of "flash" caused by too diffuse flame should be avoided. NaCl showed catalytic action at the initial stage of combustion, especially in the middle and late stage of combustion, and it was proportional to the increase of NaCl. The subsequent intermediate products are generated by the highest concentration at the outlet of the burner and then decreased with the rising temperature of the flue gas, and gradually decrease; The content of Na in ash and bottom slag is quite different. Higher combustion temperature will also lead to an increase in NOx production, which is not conducive to pollutant emission control. There are still some problems such as iron precipitation and high temperature corrosion in cyclone combustion of liquid slag discharge.

3.2 Influence of load change on alkali metal
The combination of water-soluble alkali/alkaline earth metals in solids with solid matrix is weak and has strong solubility, so most of water-soluble alkali/alkaline earth metals can be easily removed by water washing. This combustion mode retains the advantages of pulverized coal combustion mode, overcomes the disadvantage of high ash content in pulverized coal combustion flame, and can effectively control the amount of fly ash in flue gas. Therefore, in the traditional process, most of the pollution sources come from the organic matter which is not completely decomposed in coal. Although the decrease of flue gas temperature can reduce the specific heat capacity of flue gas, it is still necessary to modify the cross-sectional area of flue gas in a corresponding proportion Water washing can effectively remove Na from Zhundong coal. Increasing water washing temperature and prolonging water washing time can improve the removal rate of Na, but the combustion characteristics of Zhundong coal after water washing become worse. At present, it is considered that the reason is that after the furnace load is higher than 80%, the load ratio of furnace outlet smoke temperature is at a higher level, so the influence of temperature on its reaction generation has been lower than the sensitivity at lower load, which is increased due to other factors.

In the practical application of Zhundong Coal, the contamination phenomenon of Zhundong Coal will be reduced under low load. In this section, the concentration of Na2SO4 at furnace outlet under different loads is compared. Average concentration of Na2SO4 at furnace outlet under different loads is shown in Figure 1.
Under low load, the change of load is sensitive to the change of flue gas temperature at the furnace outlet. In the process of sulfation in high temperature zone, the average concentration of Na$_2$SO$_4$ at the outlet is increased due to low temperature and high sulfation degree of NaCl. However, due to the decrease of load, the total amount of flue gas in the furnace decreases, and the total amount of Na$_2$SO$_4$ near the furnace outlet decreases with the decrease of load.

After adding a certain proportion of NaCl, Zhundong coal shows the phenomenon of intensified combustion, and this phenomenon of promoting combustion reaction is more obvious in the middle and late combustion period. When coal ash is in plastic fluid, it has strong contamination characteristics; It also affects the opposite water wall, or overlaps with the high temperature zone of the opposite burner outlet flame, resulting in too high temperature level and a large amount of nitrogen oxides. When burning in oxygen atmosphere, the oxygen flow rate is 500ml/min. With the increase of temperature, pulverized coal goes through the stages of moisture removal, volatile matter precipitation and coke combustion. The CO$_2$-H$_2$O pretreatment technology at normal temperature and pressure can remove 88% of Na in high alkali Zhundong coal, including all water soluble Na and most organic Na. The decrease of smoke temperature reduces the heat transfer temperature difference of heating surface, so it is necessary to increase the area of heating surface at the tail; The decrease of flue gas temperature will reduce the grade of flue gas, which will also lead to the decrease of efficiency.

4. Simulation Result Analysis

According to the different composition of coal ash, the viscosity-temperature characteristics of coal ash show different characteristic curves during the heating/cooling process, which can be divided into glass slag, crystal slag, near-glass slag and plastic slag according to the shape of viscosity-temperature characteristic curves. Pulverized coal is carried by primary air and ejected from the nozzle of swirl opposed burner. Most pulverized coal particles are concentrated in the main combustion zone, releasing heat intensively, forming a main combustion zone with higher temperature level, and forming an obvious high-temperature concentrated area at the lower part of OFA nozzle section. In the hearth, when pulverized coal burns, alkali metals such as Na and K sublimated by air flow still stay in the hearth. Under appropriate conditions, complex physics will occur between alkali metals such as Na and K and solid surfaces such as coal ash and heating surface. When the primary wind speed is reduced to 10m/s, the rigidity of the primary wind becomes weaker, which makes it easier to be driven by the external secondary wind, resulting in a large radial diffusion, and the torch shows an open air flow. When the primary wind speed increases to 17 m/s, the forward impact force increases and the airflow shape becomes narrower and narrower; In addition, the content of C1 in Zhundong high alkali coal and its gasification fly ash is as high as 1.24% and 8.04% respectively, which belongs to high chlorine fuel, and will bring serious contamination and corrosion during gasification and combustion.

It is found that when the alkali metal content in lignite ash exceeds 3%, it is necessary to test its fouling and slagging performance, and it is considered that when the $f$ index exceeds 3 ~ 6%, problems will easily occur in boiler operation. The formula for calculating $f$ index is as follows:
In the formula, \( B / A \) is the ratio of alkali to acid, and \( Na_2O \) and \( K_2O \) are the mass fractions of \( Na_2O \) and \( K_2O \) in ash.

As shown in fig. 2. The \( f \) value of contamination index indicates the contamination degree of mixed coal ash with different blending ratio of high alkali coal, and the greater the \( f \) value, the greater the contamination degree; And comprehensively characterize that contamination degree and the contamination/slagging amount of the char coal. Therefore, comprehensive evaluation of high alkali coal-low alkali coal blending ratio the blending ratio of high alkali coal should not be higher than 50%.

According to the advantages of the circulating fluidized bed boiler in resisting contamination and the temperature sensitive characteristics of contamination, the high-temperature flue gas entering the tail flue of the circulating fluidized bed boiler can be cooled below the contamination sensitive temperature range of the coal burned, thus reducing the contamination tendency and realizing the long-term stable operation of the boiler. Taking the outer wall of superheater tube as an example, when flue gas and its fly ash particles flow through the outer wall of superheater tube, the larger particles will not move along the streamline direction of flue gas because of their large inertia, but will directly impact the outer wall surface of superheater tube through the streamline. However, because the reaction process between coal and gasification agent is extremely complex, there are many influencing factors, including metamorphic degree, lithofacies composition, mineral content, surface chemistry, temperature, pressure, heating rate and so on. When the primary wind speed decreases, the duration of burnout process changes obviously. When the primary wind speed is 10 m/s, it is beneficial to coke combustion and can burn out quickly in a short area. At this time, the ash clings to the surface of heating surface can be easily removed (such as soot blower, increasing flue gas flow rate, etc.); However, the injection of a large amount of low-temperature air causes the overall temperature level to decrease, which decreases with the continuous absorption of heat by the flue gas flow wall.

5. Conclusion
In this paper, based on computer control system, high-temperature slag is poured into the surface of high-alkali coal powder to simulate the combustion and alkali metal distribution in Zhundong high-alkali coal boiler. By dividing the different reaction interfaces between pulverized coal combustion process and high-temperature slag, the characteristics and mechanism of alkali metal release, migration and capture of high-alkali coal under high-temperature slag combustion are studied. In the simulation of variable structure, it is not necessary to redraw the grid, but directly adjust these defined structural parameters; The effects of different burn-out height, burn-out air nozzle position and burn-out air rate on the combustion process and pollutant generation in the furnace were simulated.
Especially in the middle and late stages of combustion, it shows a strong catalytic effect. The burnout characteristics show that the average volume change rate increases, the burnout temperature decreases by about 50 ~ 200℃, and the burnout is obviously advanced. More Na₂SO₄ is deposited in advance in the furnace and discharged from the furnace bottom, which is beneficial to reduce the contamination of convection heating surface and realize long-term continuous operation; To provide the necessary theoretical basis and pilot test data for selecting appropriate mixing ratio and guiding boiler design/operation.

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