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Research on the Effect of Coal Ash Slag Structure Evolution on Its Flow Behavior During Co-gasification of Coal and Indirect Coal Liquefaction Residue

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Abstract : Entrained-flow gasification technology is considered the most promising gasification technology because of its clean and efficient utilization characteristics. The stable fluidity of slag at high temperatures is the key to affecting the long-period operation of the gasifier. The diversity and differences of coal ash-slag systems make it difficult to meet the requirements for stable slagging in entrained-flow gasifiers. Therefore, coal blending or adding fluxes has been used in industry for a long time to improve the flow behavior of coal ash. As a by-product of the indirect coal liquefaction process, indirect coal liquefaction residue (ICLR) is a kind of industrial solid waste that is usually disposed of by stacking or landfilling. However, this disposal method will not only occupy land resources but also cause serious pollution to soil and water bodies by leachate containing toxic and harmful metals. As a carbon-containing matrix, ICLR is not only a kind of waste but also a kind of energy substance. Utilizing existing industrial gasifiers to blend combustion ICLR can not only transform industrial solid waste into fuel but also save coal resources. Moreover, the ICLR usually contains a unique ash chemical composition different from coal, which will affect the slagging performance of the gasifier. Therefore, exploring the effect of the ash addition in ICLR on the coal ash flow behavior can not only improve the slagging performance and gasification efficiency of entrained-flow gasifier by using the unique ash chemical composition of ICLR but also provide some theoretical support for the large-scale consumption of industrial solid waste. Combining molecular dynamics simulation with Raman spectroscopy experiment, the effect of ICLR addition on slag structure and fluidity was explained, and the relationship between the evolution law of slag short/medium range microstructure and macroscopic flow behavior was discussed. The research found that the high silicon and aluminum content in coal ash led to the formation of complex $[SiO_4]^{4-}$ tetrahedron and $[AlO_4]^{5-}$ tetrahedron structures at high temperature, and the $[SiO_4]^{4-}$ tetrahedron and $[AlO_4]^{5-}$ tetrahedron were connected by oxygen atoms to form a multi-membered ring structure with high polymerization degree. Due to the action of the multi-membered ring structure, the internal friction in the slag increased, and the viscosity value was higher on the macro-level. As a network-modified ion, Fe2+ could replace Si4+ and Al3+ in the multi-membered ring structure and combine with O2-, which will destroy the bridge oxygen (BO) structure and transform more complex tri cluster oxygen (TO) and bridge oxygen (BO) into simple non-bridge oxygen (NBO) structure. As a result, a large number of multi-membered rings with high polymerization degrees were depolymerized into low-membered rings with low polymerization degrees. The evolution of oxygen types and ring structures in slag reduced the structure complexity and polymerization degree of coal ash slag, resulting in a decrease in the viscosity of coal ash slag.

Keywords : ash slag, coal gasification, fluidity, industrial solid waste, slag structure
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