

# Numerical modeling of flow and reaction characteristic in chemical looping combustion system

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## Abstract

CO<sub>2</sub> is the primary greenhouse gas causing global warming which has aroused increasing alarm all over the world. Fossil fuels used for power generation account for a large amount of anthropogenic CO<sub>2</sub> emission which may greatly affect the global climate. According to IPCC 2013 report, carbon dioxide concentrations primarily from fossil fuel emissions have increased by nearly 40% since pre-industrial times, and it is likely to be responsible for the average increase in the global temperature observed during the past 150 years. It is a great challenge to capture CO<sub>2</sub> from power plant. Interest has arisen in capturing and sequestering CO<sub>2</sub> generated in fossil fuel combustion.

Chemical looping combustion, introduced in 1983, is a promising technology to capture CO<sub>2</sub> release into the atmosphere at a low cost. It provides an inherent feature of isolating CO<sub>2</sub> in the flue gas, which avoids the CO<sub>2</sub> diluted by nitrogen. This is accomplished by using two reactors, where subsequent oxidation and reduction reactions take place respectively. The direct contact between air and fuel is circumvented, thus, the flue gas leaving the fuel reactor only includes CO<sub>2</sub> and H<sub>2</sub>O. After the condensation of H<sub>2</sub>O, almost pure CO<sub>2</sub> is obtained with a small energy loss.

Numbers of CFD studies, which offer the capacity of studying a system under conditions over its limits, were carried out on chemical looping combustion. It can be applied to various systems to obtain a beforehand idea of the process design, development and scale-up. The reaction of coal in CLC is complex and can be divided into pyrolysis, gasification and combustion et al. Until now, most studies focus on the fuel reactor or air reactor, individually. We can find few papers present the simulation of the full loop structure with reaction for chemical looping system and the integrated effect on complete process is missing.

Thus, the purpose of this work attempts to fill the gap by developing a computational model for coal-fired chemical looping combustion system with full loop structure. The heterogeneous and homogeneous reactions are coupled with the multiphase computational fluid dynamics model. For the fuel reactor, the two-equation model and shrinking-core model are adopted for the coal pyrolysis and char gasification, respectively. The circulating behavior of oxygen carrier is first investigated under different operating conditions. The products from fuel reactor are analyzed and compared with experimental data to validate the accuracy of model. Conversion efficiency of fuel, carbon capture efficiency and oxide oxygen fraction are studied to evaluate the system. Then heat and mass transfer characteristic, gas-solid flow patterns, specie distributions and other important parameters are investigated for better understanding the operation of CLC system.

**Keywords:** numerical model; chemical looping combustion; gasification; simulation