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Dynamics of Reactive Particles in Supercritical Water Turbulence

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Extended Abstract

Coal consumption yields over 15 billion tons of CO_2 annually, which is the largest source of CO_2 emissions in the world. Supercritical water gasification (SCWG) is a promising technology to convert coal into hydrogen cleanly, and it could capture the pure CO_2 as well as the inorganic salts synchronously. The large-scale industrial application of SCWG urgently needs to improve the reaction rate of hydrogen production in the reactor, in which the time and space scales of multiphase flow, heat transfer, and chemical reaction are multiple and extremely mismatched. However, the theoretical guidance and basic models are lacking.

In the present research, we established a multi-scale kinetic theory to explain the physiochemical processes in the reactor of hydrogen production, including the heterogeneous and homogeneous reactions inside the micro-scale particles, the interaction between reactive particles, as well as the macro-scale fluidization in the multiphase multicomponent supercritical fluid. The main conclusions are as follows.

1) For the reaction of individual particles, we experimentally found that the reaction mainly occurs in the pores of particles in SCWG[4], which has been unable to be explained by previous researches which ignore the homogeneous reaction and the multi-species diffusion inside the reactive particles. A three-dimensional model coupling reaction and diffusion is thereby proposed to describe the multiple physical processes and chemical fields inside the non-spherical porous particles. We observe that the intrapore reaction inhibits the gasification of reactive particles by slowing down the fluid diffusion and retarding the fixed-carbon steam reforming heterogeneous reaction. Increasing gasification temperature enhances the inhibition by particle intrapore reaction while increasing the mole fraction of H2O weakens the inhibition.

2) For the motion of reactive particles, we found that the aggregation of coal particles significantly reduces the contact area between particles and supercritical water, which is the other key factor to impede the reaction. We proposed a four-way coupled model to analyze the interaction between particles, as well as between particles and supercritical fluids[1]. We found that the flocculation of particles proceeds most rapidly when the fluid and particle time scales are balanced[2]. The Kolmogorov scale of turbulence effectively inhibits the growth of floc. Adjusting the Kolmogorov scale to be close to the particle size can greatly limit the flocculation of coals and improve the reaction rate[3].

3) For the macro-scale fluidization, an optimal slurry feed rate and a temperature control strategy are proposed to achieve the highest reaction rate by balancing the transport rate of fluid species and the aggregation rate of reactive particles. The research found the role of natural convective vortices in the reactor in promoting the fluid-solid reaction. It is clarified that the hydrogen production rate at the reactor outlet increased with the increase of the supercritical water flow rate, and the optimal interval of the ratio of the supercritical water flow rate to the coal slurry feed flow rate was given.

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