Proceedings of the 10th World Congress on Momentum, Heat and Mass Transfer (MHMT 2025)
Barcelona, Spain - April 10 - 12, 2025
DOI: 10.11159/icmfht25.002

Multiphase Reaction Flow and Heat Transfer Of Coal Gasification in Supercritical Water for Hydrogen Production: From Pore to Agglomeration Perspective

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Abstract

Hydrogen production through supercritical water gasification (SCWG) is a promising technology for the low-carbon and efficient utilization of coal. The large-scale industrial SCWG of coal urgently needs to enhance the reaction rate of hydrogen production. The key factor is the heat and mass transfer between supercritical multi-species fluids and porous coal particles, involving fluid-solid heterogeneous reactions, fluid-fluid homogeneous reactions, irregular-shaped particle morphology evolution, and interparticle interactions. In this work, we introduce the experimental technology of particle morphology evolution in the SCWG and the numerical method of multiphase reaction flow. The reaction characteristics of coal particles in supercritical multi-species fluids and the quantitative correlations of the SCWG of coal particles are obtained. This work provides theoretical support for enhancing the reaction rate of coal particles in the SCWG. The main conclusions are as follows:

(1) For the effect of intrapore species concentration in supercritical fluids on the coal particle gasification, we experimentally found that the water-gas shift reaction inhibited the SCWG of coal particles. The intrapore water-gas shift reaction impeded the steam reforming reaction of coal and the non-equimolar multi-species diffusion within the pores of particles. It was clarified that enhancing the transport of reaction products at the solid interface is the key to promoting the reaction rate of coal.

(2) For the evolution characteristics of coal particle morphology in the SCWG, we experimentally found that the particle structural sharpness significantly promoted the reaction rate and numerically reproduced the evolution of irregular-shaped reaction fronts inside the particles. Furthermore, we have obtained the quantitative correlations between particle morphology and reaction rate, thereby providing a theoretical foundation for optimizing the preparation of coal particles in order to enhance the reaction rate.

(3) For the interactions of coal particles in the SCWG, we observed serious agglomeration of coal particles in the hydrogen production. The influence of particle size, temperature, and coal particle concentration on agglomeration was experimentally investigated. The agglomeration, deformation and breakage of coal particles in the SCWG was numerically simulated. We found that the intermediate shear rate of fluid produced maximum aggregate size, and the intermediate temperature of supercritical water enhanced the dispersion of particles. The quantitative correlations between the structure of aggregates and the reaction rate were proposed, providing theoretical support for improving the reaction rate by inhibiting the particle agglomeration.