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3D/2D CFD particle-resolved and porous media modeling of the heterogeneous combustion of carbon char in a fixed-bed reactor

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Hybrid porous media reactors have been studied for hydrogen production under gasification regimes [1, 2]. From a numerical perspective, heterogeneous combustion processes are complex due to the multiphase phenomena involved in the thermal decomposition of carbon [3]. This work numerically investigates a 3D/2D chemically reacting fixed-bed (CRFB) for non-porous char [4], and a single carbon char particle using both particle/macro-pore-resolved and porous media model (PMM) approaches [5]. The effects of Reynolds number (Re_{in}), inflow gas temperature (T_{in}), and oxidative atmosphere ($Y_{O2,in}$) are evaluated, along with the feasibility of a 2D axisymmetric PMM to represent a 3D particle-resolved approach of carbon char gasification. Additionally, a macro-pore-resolved approach is compared against a PMM using a single carbon char particle to assess the effect of intrinsic chemical reactions. Simulations were performed using the commercial software Ansys Fluent, implementing a six semi-global kinetic scheme, consisting of carbon monoxide combustion, forward and backward water-gas-shift reaction, Boudouard reaction, and two other heterogeneous reactions. The fixed-bed was composed of 85 spherical particles with a 5.6 mm diameter, located in the bed zone and subsequently placed in a stationary position. Results from the CRFB simulations showed a significant role of the inflow gas temperature in the gasification process, particularly for T_{in} = 1300 K. Minimal deviations in the mass fractions of all species were observed for $Y_{O2,in}$ = 0.05, being 3.6% for CO, 5.5% for CO_2 and 0.76% for temperature within the porous zone. At a particle scale, results showed good agreement specially for T_{in} = 2000 K, where the maximum deviation in CO_2 was 1.54%. The effect of variable porosity, tortuosity, effective diffusivity, dispersion, and thermal conductivity is further discussed. Tailoring a PMM approach, making results close to those obtained using a PRS model, opens new possibilities for the accurate and efficient modeling of CRFBs aimed at renewable hydrogen generation [6].

Keywords: Heterogeneous combustion, Fixed-bed reactor, Chemical kinetics, Porous media, Particle-resolved simulation.

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