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Computational Simulation of the Influence of Moving Solid Particles on Species Diffusion and Chemical Reactions

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It is well known that the gas-solid system plays a significant role in many industrial processes. It is a complex physical and chemical process, which generally consists of heat transfer, mass transfer, species diffusion and chemical reactions. In this paper, the reaction of methane with air, and the gas flow in a vertical cylinder reactor filled with 0.1 mm alumina particles are computational simulated to study the effect of the inert solid particles on the species diffusion and the chemical reactions. The reaction of methane and air is modelled by a two-step reaction mechanism. There are a continuous fluid phase, being composed of six gases (CH_4, CO, O_2, CO_2, H_2O and N_2), and discrete solid particles in the reactor.

A standard $k-\epsilon$ turbulent model is used for the continuous gas phase. The standard momentum, energy and species diffusion equations are modified by considering the interaction of the solid particles and the continuous gas phase. The mass, momentum, energy, and species conservations of a continuous fluid phase are described by the following generalized equation:

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial(\rho v_x\phi)}{\partial x}+\frac{1}{r}\frac{\partial(r\rho v_r\phi)}{\partial r}=\frac{\partial}{\partial x}\left(\Gamma_\phi\frac{\partial\phi}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\Gamma_\phi\frac{\partial\phi}{\partial r}\right)+S_\phi+S_{p,\phi} \quad (199.1)$$

where the general variable ϕ represents one of the dependent variables as follows: gas velocity components (v_x in x-direction and v_r in r-direction), turbulent kinetic energy (k), eddy dissipation rate (ϵ), enthalpy (h), and mass fraction of chemical species Y_j (j=CH_4, O_2, CO, H_2O and CO_2), and $\phi=1$ for the continuity equation.

Both the finite rate model (FRM) and the eddy dissipation model (EDM) are employed in the present work to calculate the overall chemical reaction rate. The EDM describes the effect of turbulence on the reaction rate. The eddy dissipation reaction rates are calculated based on the work of Magnussen and Hjertager [1]. The FRM describes the effect of temperature and concentration of the species on the reaction rate. The rate of reaction for any reactant is assumed to be given by the Arrhenius expression. The lower rate, out of the eddy dissipation rates and the chemical kinetics rate, is the limiting rate of reaction and is used for the calculations.

The particle phase is simulated by the discrete element method (DEM) [2, 3]. The motion of every individual particle in the system is described by the Newtonian equation of motion, equation (199.2). The left term in equation (199.2) is the change of particle momentum and the right terms are the forces acting on the particle. They are the drag force (term 1), the force (term 2) due to the pressure gradient in the gas, the buoyancy (term 3), and the normal and the tangential particle-particle contact interaction forces (F_n and F_t), respectively.

$$m_p \frac{dv_p}{dt} = 3 \frac{\pi \mu d_p}{\varepsilon_f^2} \frac{C_D \, \mathrm{Re}_p}{24} (v_f - v_p) - V_p \nabla p_f + V_P(\rho_P - \rho_f) g + F_n + F_t \qquad (199.2)$$

In the simulation, the governing equations are solved sequentially. Because the equations are non-linear and coupled, several iterations of the solution loop were performed before a convergence is achieved. The simulation results show that the inert particles change the pattern of gas flow and cause the gas circumfluence in the reaction zone. This enhances the diffusion of the reactants and products and increases the chemical reaction rates. As heat carriers, the hot particles heated in the high temperature region move to the reactor bottom and transfer their heat to the cold methane and air. As the results, the propagation of the reactions starting from the reactor wall is accelerated and, or the reactants are heated to the activation temperature and then the reactions are ignited. The charge of solid particles in a reactor also makes the reactants and products distribute uniformly in the reactor.

References

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