MOMENTUM, ENERGY AND SCALAR TRNSPORT IN GAS-SOLID FLOWS USING PARTICLE-RESOLVED DIRECT NUMERICAL SIMULATION

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Research Program: Complex Fluid Systems

Introduction

Generation of clean energy from fossil or bio-based fuels is one of the principal challenges of this century. Emerging technologies such as CO_2 capture and chemical looping combustion (CLC) offer the promise of reduced emission of greenhouse gases [2,4]. Gas-solid flows form an integral component of the industrial devices that are used to implement these technologies. For instance both the CO_2 capture and CLC are implemented using fluidized beds, where the solid particles are made to behave like a fluid by the use of high pressurized fluid. Understanding the complex gas-solid flow in these industrial devices is crucial for their successful operation.

The scale-up of the process equipment from laboratory scale to the industrial scale is very difficult. Numerical simulations are being extensively used to aid in the design process of these devices since experiments are often costly and time consuming. The simplest numerical models are the so called zero-dimensional models, where the gas-solid flow device is represented as a single block in the entire process. Global balance equations for momentum, energy and heat transfer are solved and the effect of the gas-solid device on the process as a whole is studied. This method does not provide any details about the gas-solid flow inside the device. Gas-solid computational fluid dynamics (CFD) is the approach that is employed to study the details of the flow in the device. CFD simulations of gas-solid flow devices are usually based on the Eulerian-Eulerian two-fluid approach in which averaged equations for conservation of mass, momentum and energy are written for both the solid and the gas-phase [1]. These equations contain unclosed terms representing the interactions between both phases that need to be modeled. The predictive capability of the zero-

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dimensional models and gas-solid CFD simulations depends on accuracy of the models used for the unclosed terms. Such accurate models for gas-solid flow can be developed using Particle-resolved direct numerical simulation (PR-DNS). The interrelation between these simulation approaches is depicted in Figure 1.



Figure 1. Computational approaches used in gas-solid flow. The level of accuracy and details that can be obtained from the simulation increases from left to right.

Particle-resolved direct numerical simulation

PR-DNS is a first-principles physics-based numerical approach in which the Navier-Stokes equations are solved in the fluid-phase by imposing exact boundary conditions on each particle surface. The most popular PR-DNS approaches employ fixed, uniform Cartesian grids. The specific implementation of PR-DNS used in this work is the Particle-resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (PUReIBM). The has been validated in a PUReIBM approach comprehensive suite of test cases and has been shown to

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be accurate and numerically convergent [3]. In this work we employ PUReIBM to solve for flow past arbitrary arrangements of spherical solid particles in order to develop models for gas-solid momentum, energy and heat transfer.

Gas-solid momentum transfer

The average gas-solid force appears as an unclosed term in the momentum equation for both the fluid and solid phases that is solved in gas-solid CFD simulations. The closure model for the average gas-solid force is popularly known as the "drag law". We study the flow past fixed random assemblies of monodisperse spheres using PUReIBM. The normalized average drag force F is obtained from PR-DNS and a new correlation is proposed in terms of the solid volume fraction ϕ and the Reynolds number based on the mean slip velocity Re_m (see Figure 2) [3].



Figure 2. Drag law for monodisperse gas-solid flow generated from PUReIBM PR-DNS.

Gas-phase kinetic energy

Similar to single-phase turbulence, the gas-phase Reynolds stress appears as an unclosed term in the momentum equation of the gas-phase in gas-solid CFD. This is usually modeled using an eddy viscosity model, for which the kinetic energy in the gas-phase k_f and the dissipation rate \mathcal{E}_f need to be quantified. Such quantification from PR-DNS has not been performed previously. Data from PR-DNS is used to propose an eddy viscosity model for gas-solid flow (see Figure 3).



Figure 3. Eddy viscosity for gas-solid flow.

Gas-solid heat transfer

Accurate prediction of the average gas-phase temperature is crucial for applications such as CLC. The average gassolid heat flux is an unclosed term in the temperature equation of both phases, which is modeled in terms of an average gas-solid Nusselt number. In this work, a novel PR-DNS methodology is developed that is used to obtain a correlation for the average gas-solid Nusselt number in terms of the solid volume fraction ϕ , mean slip Reynolds number Re_m and the Prandtl number Pr.

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