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Assessing the capability of continuum and discrete particle methods to simulate gas-solids flow using DNS predictions as a benchmark

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ABSTRACT

Gas–solids flow in a three-dimension periodic domain was numerically investigated by direct numerical simulation (DNS), computational fluid dynamic-discrete element method (CFD-DEM) and two-fluid model (TFM). DNS data obtained by finely resolving the flow around every particle are used as a benchmark to assess the validity of coarser DEM and TFM approaches. The CFD-DEM predicts the correct cluster size distribution and under-predicts the macro-scale slip velocity even with a grid size as small as twice the particle diameter. The TFM approach predicts larger cluster size and lower slip velocity with a homogeneous drag correlation. Although the slip velocity can be matched by a simple modification to the drag model, the predicted voidage distribution is still different from DNS: Both CFD-DEM and TFM over-predict the fraction of particles in dense regions and under-predict the fraction of particles in regions of intermediate void fractions. Also, the cluster aspect ratio of DNS is smaller than CFD-DEM and TFM. Since a simple correction to the drag model can predict a correct slip velocity, it is hopeful that drag corrections based on more elaborate theories that consider voidage gradient and particle fluctuations may be able to improve the current predictions of cluster distribution.

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1. Introduction

The multi-scale nature of gas-solids flow is caused by the intra-phase and inter-phase nonlinear interactions. In 1757, Leonhard Euler established a set of partial differential equations to describe the flow of incompressible and frictionless fluids. In 1821, the French engineer Claude-Louis Navier introduced the element of viscosity (friction) for more realistic and vastly more difficult problem of viscous fluids. The Navier-Stokes equations, along with boundary conditions, are still unsolved and were designated a Millennium Problem (https://www.britannica.com/science/Navier-Stokes-equation). Currently, it can only be solved by numerical methods using computation fluid dynamics (CFD) where flow profiles are resolved at the numerical grid scale. Apart from solving Navier-Stokes equations directly, the lattice Boltzmann method (LBM) [1] solves the discretized Boltzmann equation on regular lattices. The incompressible Navier–Stokes equations can be derived from the lattice Boltzmann equation in the limit of small Mach number via Chapman–Enskog procedure.

Physical laws governing the movement of a single particle were established by Newton in 1687 with the publication of "The Mathematical Principles of Natural Philosophy," or the Principia. However, the collective movement of tremendous number of particles under non-equilibrium conditions still lacks a general governing law. Although their movement can be tracked one by one using discrete method, this leads to large computation cost, which becomes too expensive to simulate industrial processes.

Until now, these two problems are still not fully solved. And together they have been listed as one of the 125 big questions in the 125th-anniversary issue of Science [2] asking that "Can we develop a general theory of the dynamics of turbulent flows and the motion of granular materials?". These two problems are inherent to gas-solids flow and raise another question: how to calculate the interaction force between gas and particles?

Currently, only very small scale problems can be accurately solved by direct numerical simulation (DNS) [3,4]. In DNS, the CFD grid and time steps are so small that the local fluctuation of fluid velocities can be captured without any turbulence model. Also, in small scale problems, it is affordable to track the individual movement of a small number of particles. As for the gas-solids interactions, the CFD grids can resolve the shape of each individual particle and no-slip boundary condition applies at the surface of these particles. The drag force acting on particles can be directly calculated at sub-particle scale. In DNS, the gas phase is usually the bottleneck due to large number of grids and small time steps. To solve real world problems, a much larger CFD grid

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and time-step must be used. This method has been reviewed by several researchers [5].

In 1967, Anderson and Jackson [6] developed the first mathematical descriptions of the gas-solids flow using the continuum approach. The volume averaged Navier-Stokes equations were established for both gas and solids phases. Lately, the granular kinetic theory closures [7] were first used by Sinclair and Jackson [8] to predict gas-solids flow in the riser section of a circulating fluidized bed. This two-fluid model (TFM) has been widely used since these groundbreaking works. However, general constitutive relations for granular materials are still literally debatable and the interactions between gas and particles can only be described by drag models derived from experiment [9], DNS [10] or energy minimization multi-scale method [11–15]. This last method was reviewed by several researchers [16,17].

In 1993, Tusji et al. [18] coupled the CFD with discrete element method (DEM). In CFD-DEM [19], the gas phase equations are same as in TFM but the particles are tracked individually by newton's law of motion. This method avoids the complexity of deriving continuum closures for granular flows and can also be accelerated by supercomputers [20–22], hard sphere model [23,24] and coarse grained models [25–28]. But it still depends on closure models for drag force [29]. It has been reviewed by several researchers [30–33].

Typically, the above three different methods are used at different scales, as well as the DNS for small scale, CFD-DEM for lab scale, and TFM for industrial scale reactors. The CFD-DEM and TFM are usually validated through macro-scale properties like pressure drop, solid flux and solid velocities. However, it is difficult to ensure a thorough validation because there are many uncertain parameters [34] in these simulations like spring constant, restitution coefficient, and friction coefficient. Also, not all the effects can be fully considered during the simulation, for example, the effect of cohesion forces [35], particle shapes [36] and particle size distributions [37]. In this research, the exact same gas-solids system is simulated with DNS, CFD-DEM, and TFM. The DNS results are regarded as the most accurate data and used to validate the CFD-DEM and TFM.

2. Method

Fig. 1 explains the simplifications from DNS to CFD-DEM and TFM. Generally, DNS solves NS equation with no-slip boundary conditions, CFD-DEM solves averaged NS equation for gas phase, and TFM solves averaged NS equation for both phases. In DNS, the gas phase is resolved with CFD grids about 20 times smaller than the diameter of particle. The voidage of each cell is precisely calculated according to the position of particles and can be ranged from 0 (fully occupied by particle) to 1 (not occupied by particle). And the inter-phase interactions can be calculated by immersed boundary method (IBM). All the particles are tracked individually with DEM. For CFD-DEM simulation, the simplifications mainly reside in gas phase and inter-phase interactions. For gas phase, the grid size ranges from several particles to hundreds of particles. Thus, small structures of the flow field can't be captured. The use of coarse grid also changes the methods to calculate voidage. Since the grid size is larger than particle size, the voidage depends on grid size and interpolation methods. The typical value is in the range of about 0.4 (fully packed) to 1.0 (no particle) which is quite different from voidage in DNS which can be as small as 0. For inter-phase interactions, a drag model should be used. However, due to the complex and nonliner behavior of particles, we are still lacking a general and accurate drag model. Although some sub-grid drag models are being developed, the Wen-Yu drag model derived empirically from experiments is still widely used. For TFM simulation, and in addition to the simplifications discussed in CFD-DEM, it also further averages the system in a solids phase and inter-phase. In TFM, the solids phase is assumed to be continuum and solved using Euler method. Also, the particle-particle interactions are modeled by stress closure derived from kinetic theory of granular flow. For this method, it is difficult to precisely account

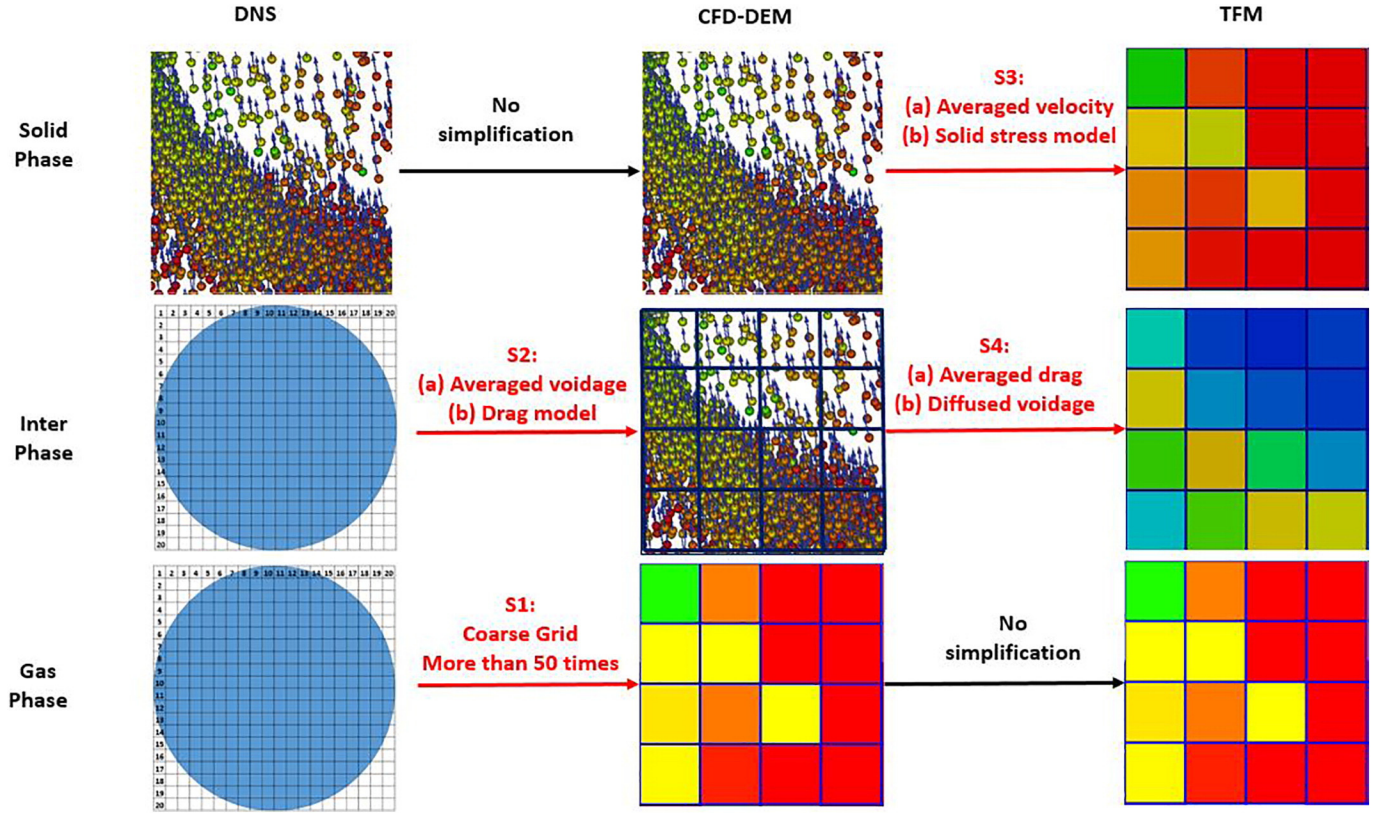

Fig. 1. Simplifications from DNS to CFD-DEM and TFM.