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Assessment of CFD-DEM solution error against computational cell size for flows through a fixed-bed of binary-sized particles

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ABSTRACT

Computational cell size is a crucial factor for accuracy in Computational Fluid Dynamics (CFD) - Discrete Element Method (DEM) simulations of particle-fluid interactions. In the present study, we investigate how simulation results change with computational cell size and mixture composition, for calculation of drag force over a fixed bed containing a binary-sized particle mixture. To investigate the complex solution convergence behavior, the simulation results are examined for several definitions of dimensionless computational cell size. Several regimes of consistent behavior, across three investigated mixtures, are identified and a consistently optimal cell size range is identified. We find that both the difference between simulated solution results and published experimental results, and the standard deviation of the void fraction profile, show consistent trends when plotted against the dimensionless computational cell size based on the Sauter-mean particle diameter. Grid-refinement studies are performed across all grid solutions, and the Grid Convergence Index (GCI) is analyzed as a predictor for the grid solution error. Correlations between simulation error and GCI are not strong, likely because of incongruence of the solution trends with typical asymptotic convergence. Alternatively, a correlation between change in solution value on successively refined grids and finer-grid solution error is shown to be adequate for the current results.

1. Introduction

Particle processing operations are prevalent in industries such as food processing, coal processing, plastics manufacturing, mineral processing and pharmaceuticals. Many varieties of equipment, including fixed-beds, hoppers, conveyors, fluidized beds, and spouted beds, are used to move and process particles into their final desired form. Each step of the process has to be well understood in order to most efficiently produce a consistent, high-quality product.

Experimental investigation of particle processing operations are often hampered by the complicated, multi-scale phenomena present in granular flows [1,2], and the opaque nature of granular mixtures [3]. Methods of non-invasive measurement of the flows are currently in limited use [2–4], and require much development and validation before they can be prevalently used.

Computational simulation of granular flows has shown great success, with many different approaches continuing to be developed [5]. One of the most common approaches is the coupled Computational Fluid Dynamics (CFD) - Discrete Element Method (DEM). The CFD-DEM procedure calculates particle trajectories individually, while the fluid properties are computed on a standard CFD computational grid. The coupling involves calculation of the mass displacement and momentum transfer between phases, and is computed on the same computational grid as the CFD calculation [6].

There are many published studies investigating the cause of differences between CFD-DEM results and experimental data [7,8]. The modeling choices investigated as possible causes of this difference include drag law [9–12], boundary conditions [13], 2D modeling of 3D systems [14,15], particle properties [9,10,16-19], porosity calculation method [20,21], and coupling model [14,22]. However, all of these studies have either ignored the effect of the computational cell size in their grid, or only compared solutions using several dissimilar computational cell sizes. In 2007, Beetstra et al. [13] reported that computational cell size had a larger impact on their results than the choice of drag law, indicating that the effect of computational cell size cannot be neglected.

An important complication exists in computational cell size choices for CFD-DEM simulations. While pure CFD studies can simply choose a cell size that is sufficiently small, cell size choice for CFD-DEM simulations is bounded by two critical cell sizes [23]. The simulation solution diverges from the exact solution of mathematical model when the cell size is larger than an upper-critical cell size,

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and this solution-divergence behavior is also present when the cell size is smaller than a lower-critical cell size. If the chosen computational cell size is outside of the area bounded by the two critical cell sizes, the solution is likely to have a large error.

The present study is part of our continuing work to determine the optimal cell size for CFD-DEM models. Ultimately, we want to know if the average cell size can be non-dimensionalized by a reference particle diameter such that the optimal dimensionless cell size remains constant. Knowledge of such a constant optimal dimensionless cell size would save substantial time and computational resources that are currently required to determine the model-specific optimal cell size. An optimal dimensionless cell size could also be used to analyze published CFD-DEM studies for discrepancies caused by use of non-optimal cell sizes.

In the present study, we examine the simulation results for fluid flows through fixed-beds of three different particle mixtures. We model the experimental setup of Formisani et al. [24] for flow through a fixed-bed containing different weight fractions of fine particles. The empirical expressions we have for drag laws compare well with the experimental data, ensuring small mathematical errors originating from the drag law. The experimental description provided by Formisani et al. [24] includes well defined flow conditions, boundaries, and particle mixture properties. Simulation results for this setup are calculated on computational grids of varying average cell size. The total drag force, calculated from the solution on each grid, is compared to the experimental data to determine the error. This error is plotted against the different definitions of dimensionless computational cell size, to investigate the possible presence of a consistently optimal dimensionless cell size, or cell size range. Finally, we analyze simulated trends of void fraction with dimensionless cell size, to explain divergence of the simulation results from the experimental values.

We perform grid-refinement studies for the results from simulations across the range of computational cell size. Grid-refinement studies have been consistently used for CFD simulations to calculate numerical error due to finite cell size. We previously applied grid-refinement studies to simulations of flow through a mono-sized, fixed-particle bed with moderate success [23], and are interested in how this process will extend to simulations of flow through binary-sized fixed-particle beds.

2. Mathematical model

The CFD-DEM mathematical model consists of the fluid flow conservation equations, the discrete-particle equations of motion, and coupling expressions to describe how the two phases interact. Here we give a brief overview, as a detailed description has been included in the paper by Volk et al. [23].

The conservation of mass and momentum equations of incompressible flows are modified, to account for the solids fraction in each computational cell and the fluid-solid interacting force [15], as

$$\frac{\partial \varepsilon}{\partial t} + \nabla\cdot(\varepsilon \mathbf{u}_f) = 0, \tag{1}$$

and

$$\frac{\partial(\varepsilon \mathbf{u}_f)}{\partial t} + \nabla\cdot(\varepsilon \mathbf{u}_f \mathbf{u}_f) = -\varepsilon \nabla \frac{p}{\rho_f} - \mathbf{R}_{pf} + \nabla\cdot\tau. \tag{2}$$

The void fraction, ε, and solids interaction term, $\mathbf{R}_{pf}$, are calculated by a coupling routine (to be detailed later) and communicated to OpenFOAM, the CFD solver, at each calculation step [6].

The particle equations of motion, calculated using the DEM solver LIGGGHTS, consist of summing all forces acting on each individual particle, in the form of linear and angular momentum equations, written for particle i as:

$$m_i \frac{dv_i}{dt} = \sum_{j \in S_i^p} F_{ij}^c + f_{grav,i} + f_{g,i}, \tag{3}$$

and

$$I_i \frac{dw_i}{dt} = \sum_{j \in S_i^p} (R_i \times F_{t,ij}), \tag{4}$$

where S_i^p stands for the local set of particles interacting with particle i.

For this application, the fluid-solid interaction term ($f_{g,i}$) is calculated by a coupling routine (see below), gravity ($f_{grav,i}$) is standard and constant, and the particle-particle interactions $\left(F_{ij}^c, F_{t,ij}\right)$ are described by the Hertz contact model [25].

The CFDEM coupling software is used as the coupling routine. The void fraction is first calculated by the divided void fraction method, in which a large number of marker points are evenly distributed on each particle. The computational cell corresponding spatially to each marker point is determined, and each cell is assigned the appropriate fraction of solids volume, based on the marker points it contains [26]. Average particle velocities in each computational cell are gathered from the DEM solver, along with the fluid velocity from the CFD solver. The resultant quantities are used to calculate the fluid-particle interaction force using the Gidaspow drag law. The Gidaspow drag law [27] is a combination of the Ergun Equation [28] when void fraction in the computational cell, ε, is less than 0.8, and the Wen & Yu Equation [29] for larger void fraction values:

$$f_{g,i} = \frac{V_i \beta}{(1-\varepsilon)}[\mathbf{u}_f - \mathbf{v}_i], \text{ where} \tag{5}$$

$$\beta = \begin{cases} \frac{150(1-\varepsilon)^2 \mu_f}{d_p^2} + \frac{1.75(1-\varepsilon)\rho_f}{\varepsilon d_p} \mid \mathbf{u}_f - \mathbf{v}_i \mid & \text{for}(\varepsilon < 0.8) \\ \frac{3}{4} C_d \frac{(1-\varepsilon)\rho_f}{d_p} \mid \mathbf{u}_f - \mathbf{v}_i \mid \varepsilon^{-2.65} & \text{for}(\varepsilon \geq 0.8) \end{cases}. \tag{6}$$

The Gidaspow Drag Law is appropriate to describe fluid-particle interactions in the fluid flow through fixed-particle beds. We find that the calculated values of Gidaspow drag are very close to the experimental data of Formisani et al. [24], with an average 2% difference, and maximum 7% difference. We establish a threshold error for our simulation results based on this known difference between the mathematical model and experimental data. Simulation results with less than 5% error from the experimental data are deemed acceptable, because of the unavoidable errors due to the use of drag law equations. Our goal is now to find an optimal cell size to minimize any additional error caused by cell size.

2.1. Grid-refinement study

The solution value trends with cell size are analyzed using the standard grid-refinement study procedure. The total drag force on the particle bed, at each velocity value of interest, is used as the representative solution value, because the drag force controls system behavior. The rate of solution-convergence and the predicted numerical error in the solution on the finest-grid, known as the Grid Convergence Index (GCI), are calculated based on the relationship between changes in the grid-refinement level and the representative solution value. All possible combinations of grid-refinement levels that feature similar changes in refinement, as well as similar changes in representative solution value, are considered. The full grid-refinement study procedure is described in Celik et al. [30], and