Thousand-Fold Speedup of Discrete-Particle-Based Computer-Aided Reactor Design and Scale-up

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ABSTRACT

Multiphase flows are widely encountered in industries like refinery, pharmacy, energy, and turbomachinery. A discrete approach to model the behavior of these flows can accurately predict most observed behaviors, but tracking large numbers of particles makes these simulations too slow to be practical or even useful to industrial engineers. Therefore, we propose an approach to drastically increase the computational speed of these simulations. First, we propose an accurate coarse-grained method to lump many particles into a computational parcel while conserving energy dissipation during collisions. Second, we use a novel hard-sphere approach that can correctly predict packed regions in fluidized beds and others systems. This method is validated by the simulation of a bubbling fluidized bed. Then, it is used to simulate a pilot-scale riser and help the design and scale-up a leaching reactor for extracting rare earth elements from coal-byproducts. This demonstrates the ability of computational fluid dynamics (CFD) to cheaply and accurately design and scale up industrial reactors.

Keywords: computational fluid dynamics (CFD), coarse-grain, time driven hard sphere, scale-up, multi-phase flow

1 INTRODUCTION

Particulate matter is the second-most manipulated material in industry after water and has been observed and studied by scientists and engineers since the earliest of human civilization. In fact, we commonly distinguish between the different phases of early human civilization by referring to granular matter (e.g., Stone Age, Copper Age, and Iron Age). Therefore, there has always been a fascination with the behavior of granular flows that range from solid-like to gas-like depending on the concentration and energy of the system. Industrial systems that handle particulates consist mostly of fluidized beds that are efficient and safe because of high mass/heat transfer mechanisms that lead to uniform characteristics of a product. In fact, fluidized beds are so efficient that Scott Fogler mentioned in an undergraduate chemcial reaction textbook that “the virtues of fluidized-bed reactors drove its competitors from the market.” A discrete approach to model these flows can accurately predict most observed behaviors but suffers mainly from tracking large number of particles that make these simulations too slow to be practical or even useful to industrial engineers. Therefore, we developed an approach to drastically increase the computational speed of these simulations. First, we propose an accurate coarse-grained method to lump several grains into a computational parcel while conserving energy dissipation during collisions. Second, we use a novel hard-sphere approach that can correctly predict packed regions in fluidized beds and others systems. This method is validated by simulating a small bubbling fluidized bed and comparing the results with a much slower but highly accurate discrete particle method based on soft-sphere collision model. For large-scale systems, more particles can be packed into a parcel and the speedup increased to more than a thousand-fold while maintaining a reasonable accuracy. Therefore, this method is then used to simulate a pilot-scale riser section of a circulating fluidized bed as well as the scale-up of a leaching reactor for extracting important rare Earth elements used in many high-technology systems. This work demonstrates the reliability of this technique to speed up computer-aided design and scale-up of multiphase flow reactors.

2 METHOD

The major assumptions of the coarse-grained parcel method (CGPM) are shown in Figure 1, where the reduction of computation cost is obtained by lumping W grains into a parcel [1-3]. Specifically, all particles making a CGP experience the same drag force as they move collectively (Figure 1, b). These particles also have the same reaction rates and temperature, as they share the same fluid species (Figure 1, c). However, the collision must be calculated using the diameter of the CGPs to avoid unphysical overlaps among parcels (Figure 1, d). To further reduce computation cost, the collision process is handled with a more efficient time driven hard-sphere method. The over-packing problem caused by inelastic collapse is solved by adding a correction term after particle collisions. This correction algorithm takes only few iterations and is targeted toward reducing the maximum overlaps between particles in the granular assembly. This algorithm achieves similar void fractions at packing as the more accurate soft-sphere collision approach, but at a very low computation cost. This newly proposed method is hereby called coarse grained hard sphere method (CGHS). The details and validation of this method can be found in a recent publication [4].

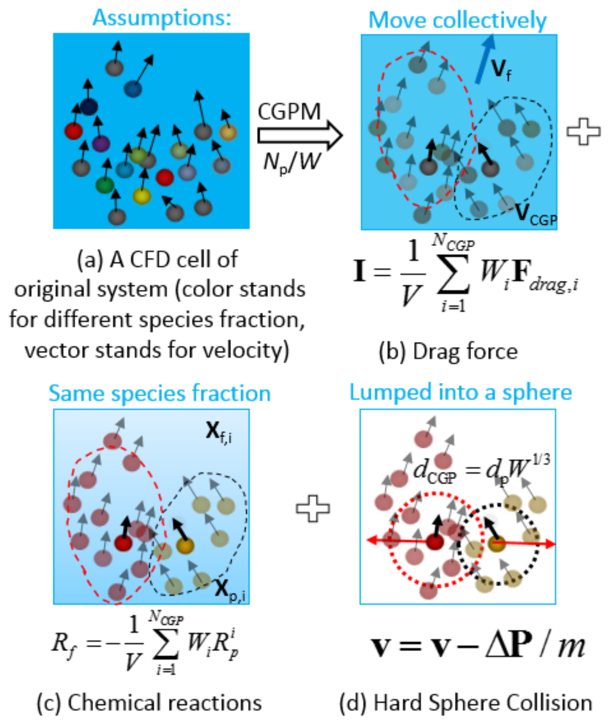


Figure 1: CGHS model description

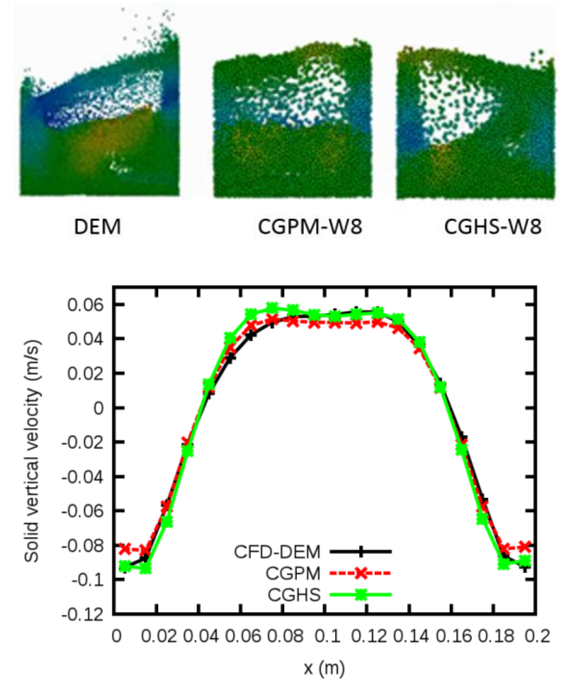


Figure 2: Comparison of results obtained with coarse CGPM and CGHS methods

3 RESULTS

As shown in Figure 2, the proposed method is verified by simulating a small bubbling fluidized bed. The results of CGPM and CGHS compare well with the most accurate particle tracking using soft-sphere collision method (CFD-DEM) with a speedup of 30 and 125 times, respectively. The speedup of CGPM is mainly due to the reduced number of tracked particles (8 times) while the CGHS gains further acceleration by using larger particle tracking time steps.

For large-scale systems, W can be increased to hundreds and even thousands with a reasonable accuracy [5]. Thus, this method can be used to simulate pilot and industrial-scale fluidized beds. As shown in Figure 3-4, a pilot-scale cold-flow riser is simulated with CGHS. Qualitatively, the particles distribution across the riser width shows the well-known core-annular flow regime where particles tend to concentrate preferably at the wall region [6]. Quantitatively, computed time-averaged radial profile of particles vertical velocity compares well with experiment data obtained with fiber optic probe (FO) and high speed PIV (HSPIV). The detailed experiment setup can be found at https://mfix.netl.doe.gov/challenge-problem-iii-2010/.

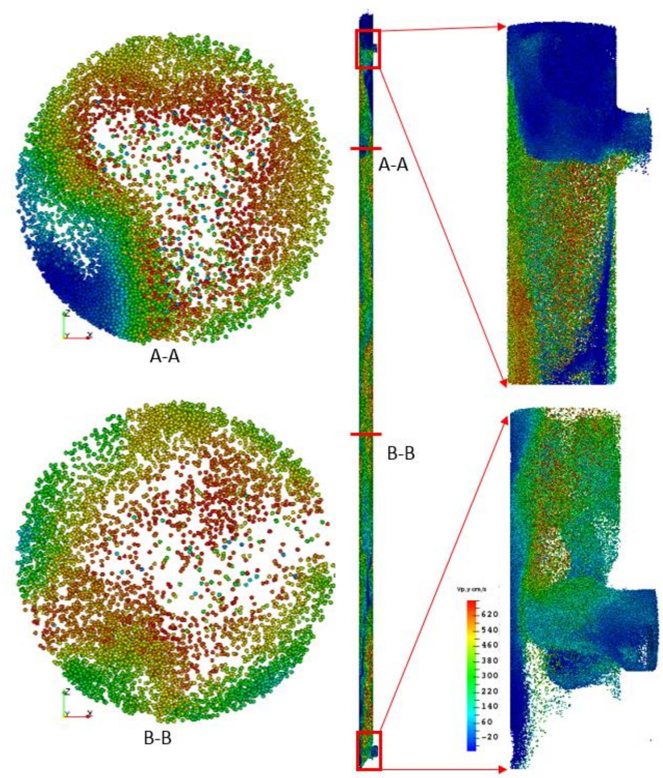


Figure 3: Particle distribution of a pilot scale riser (H = 16 m, D = 0.3 m) simulated with CGHS

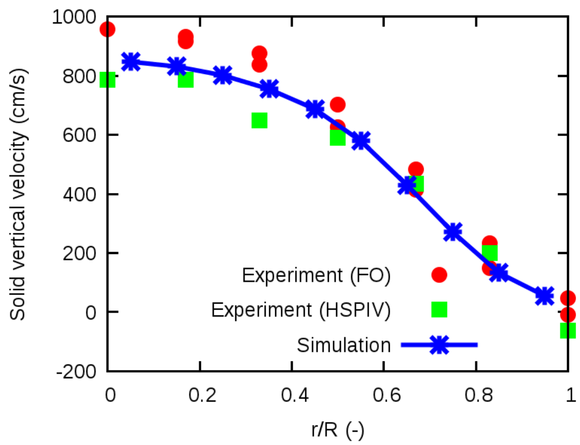


Figure 4: Radial profile of particle vertical velocity

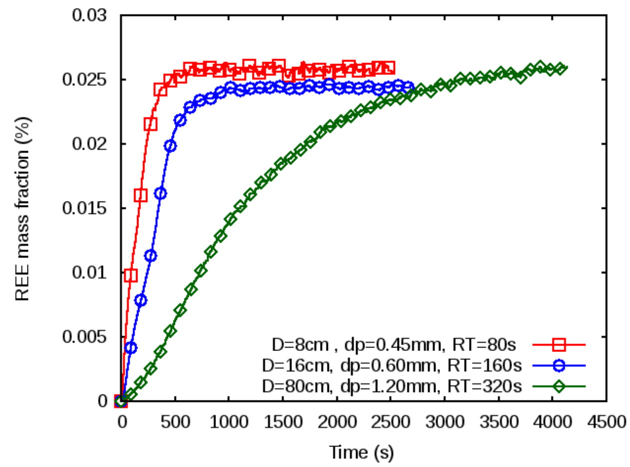
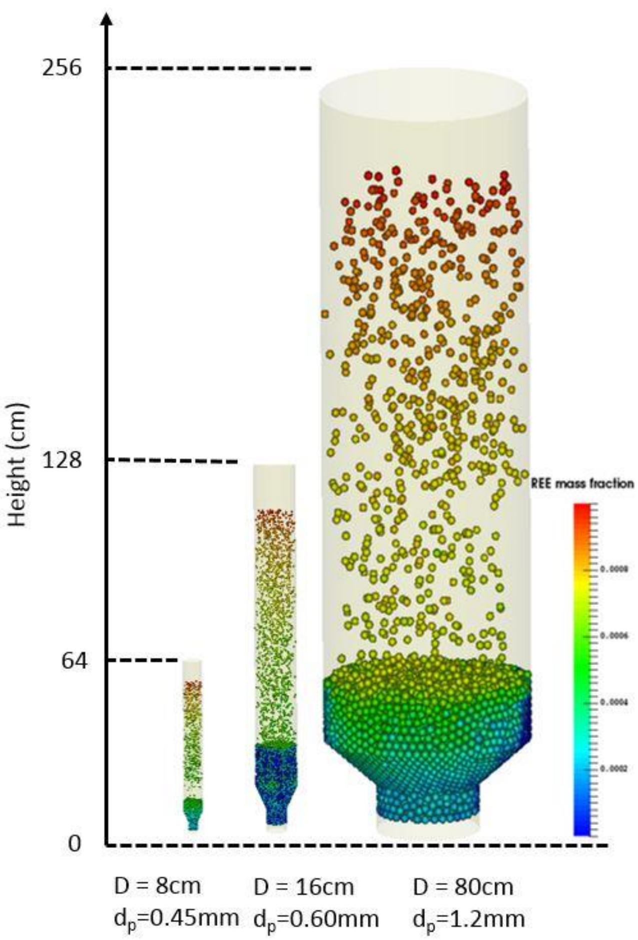


Figure 5: Computer-aided scale-up of REE leaching reactors



The CGHS method is also used to help design a leaching reactor for extracting valuable rare earth elements (REE) from coal-byproducts. This is a continuous counter-current reactor where solid particles made of clay (a byproduct of coal excavation) are fed from near the top of the reactor and flow downward due to gravity, while an aqueous solution containing magnesium sulfate is fed from near the bottom of the reactor. A counter-current ion exchange reaction occurs and valuable REE ions are leached from the clay particles following a shrinking-core model that is limited by inner-diffusion. As shown in Figure 5, the reactor is virtually scaled-up by 2 and 4 times in axial direction and 2 and 10 times in radial direction. The amount of calculated leached REE ions from small to medium to large reactors are: 0.36, 1.45, 36.2 kg/day, respectively based on a targeted 80% extraction efficiency. We were able to conduct many CFD simulations to study the effects of particle size, reactor height, and residence time of particles because of the increased computational speed of this newly developed method to track particles and their collisions. The results of these simulations indicate that larger particles can be used for larger reactors. This is highly desired because using larger particles is cheaper due to the energy savings realized by minimizing grinding of solid material. It was also interesting to notice that our computational results (not shown) could distinguish between different fluidization regimes near the bottom of the reactor that are influenced by the size of the particles.

4 CONCLUSIONS

A newly developed numerical method that tracks the trajectory and collisions of particles in a fluidized bed system was validated and shown to increase significantly the speed of the simulation while maintaining reasonable accuracy for the predictions. Thus it is our hope that this computer-aided reactor design and scale-up tool will help engineers in industry as well as in research laboratorys conduct simulations of complex particle-fluid flows cheaply and accurately. It will reduce the lab-to-industrial development time and help us meet the 21st century challenges in providing cheap and clean energy.

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