INVESTGATING COARSE-GRAINING EFFECTS ON CFD-DEM SIMULATIONS OF FLUIDIZED AND SPOUTED BED REACTORS

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Abstract

Discrete Element Method (DEM) simulation for industrial-scale applications involving particles inflate the computational costs excessively. Coarse grain model can help to reduce the computational demand. On the other hand they introduce a modeling error into the simulation. In this study we are investigating different coarse graining models and quantify the effect on different parameters and their fluctuation like pressure drop and expansion height in a fluidized and spouted bed. Comparison is done against DEM simulation without coarse graining and against experimental data and a reasonable agreement is found.

Keywords

CFD-DEM simulation, coarse graining, fluidized bed, spouted bed.

Introduction

Since its introduction (Cundall and Strack, 1979), the Discrete Element Method (DEM) has proven to be a valuable method for the analyzing and understanding particulate flows. Supported by the continuously increasing computational power, CFD-DEM simulations have found their way into the chemical and process industry for various applications like solid suspension in mixing vessels (Eppinger et al., 2017), fluidized and spouted beds (Baran et al., 2015), granular transport and coating applications in rotary drums.

The major shortcoming of the DEM, however, is its computational cost that increases with the amount of particles involved, their material properties (stiffness) and size. This hinders the application of CFD-DEM simulation to large-scale systems of industrial size. To overcome this shortcoming a coarse grain (CG) model has been described (Sakai et al., 2010). Using straightforward scaling rules, a group of particles gets replaced by a representative coarse parcel. This effectively reduces the number of particles that need to be processed and subsequently shortens the computational time.

The trajectories of the parcel are calculated analogously to the discrete element method (DEM) by solving the Newtonian laws using appropriate contact and fluid interaction models. The particle-particle, particle-wall and particle-fluid interaction forces must be scaled out for reasons of energy conservation or similarity considerations. In the past, a variety of scaling rules have been developed, but a systematic comparison of these has not previously taken place.

In this work two different contact scaling methods are examined for a fluidized and for a spouted bed reactor. The results are compared against experimental results and against a DEM simulation without coarse graining. The

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results are compared with regard to pressure loss as well as frequency, RMS and mean vertical vertical particle position. Furthermore, the influence of the coarse grain parcel to particle diameter ratio is examined.

Methods

In this investigation the software tool Simcenter STAR-CCM+ was used for the coupled CFD-DEM simulation. The built-in DEM solves for each particle Newton's law of motion in each time step. The particle-particle and particle-wall interaction is taken into account based on Hertz-Mindlin model (spouted bed) or the linear-spring-dashpot model (fluidized bed). Momentum exchange between the background gas phase and the DEM particles is calculated based on Gidaspow drag model.

Two include coarse graining (CG), three different approaches were used.

- Particle-based CG with l^3-scaling (CG-L3): Contact forces are calculated based on particle diameter and mass and are scaled with the l^3-approach). DEM time step is based on the particle properties.
- Parcel-based CG with l^3-scaling (PBCG-L3): Contact forces are calculated based on particle diameter and mass and are scaled with the l^3-approach. DEM time step is based on the parcel properties, resulting in significantly larger time steps.
- Parcel-based CG with l^2-scaling (PBCG-L2):Contact forces are calculated based on particle diameter and mass and are scaled with the l^2-approach. DEM time step is based on the parcel properties.

For the fluidized bed a rectangular geometry (150x150x700mm) with 1.1 million particle with a constant diameter of 1.52 mm and two different gas superficial velocities (1.2 and 1.6 m/s) were used.

For the spouted bed a geometry with dimensions and physical settings according to Salikov et al. (2015) were used (235k particles with a diameter of 1.8 mm).

Results and discussion

Figure 1 shows a snapshot of the different CG methods for the fluidized bed compared with a DEM simulation without CG. In general it can be stated that bed expansion and pressure drop are well predicted for all investigated CG methods, but depending on the CG factor the dynamic of the system cannot be captures which can be seen in Figure 2 as deviations in the RMS values for the respective parameter.

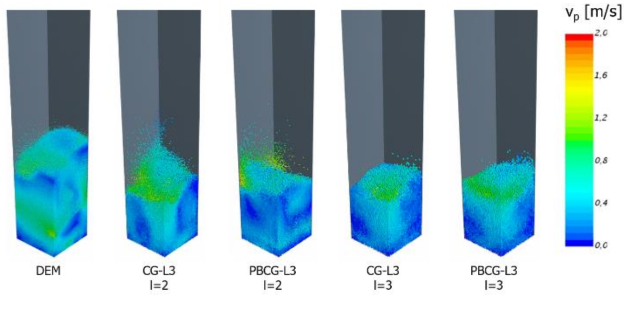

Figure 3 Comparison of the particle dynamics for different CG methods

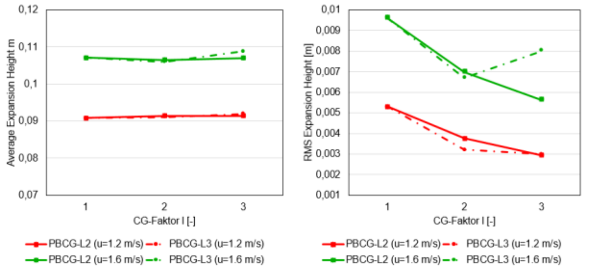

Figure 1: Average and RMS expansion height for different CG methods.

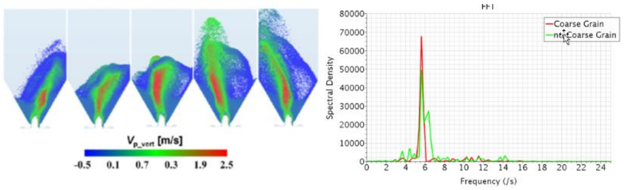

Figure 2: Left: snapshots of the spouted bed for different times. Right: Spectral density of the spouting bed.

Similar results were found for the spouted bed reactor: While the results for pressure drop, expansion height and spouting frequency agree well with the experimental data for all investigated CG factors, the dynamic behavior of the small particles cannot be captured accurately.

Conclusion

Different CG methods were investigated in a fluidized and spouted bed reactor and it can be show that accurate results with a significant reduction in runtime can be achieved at the expensive of accuracy of the dynamics of the fine particles.

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