Meso-scale Investigation of the Effect of Van der Waals Interaction on Fluidization of Fine Solids

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Abstract

Interparticle forces can influence the overall performance of a gas-solid fluidized bed. The Van der Waals interparticle force contributes to the pressure drop overshoot observed for fine particles during the transition from fixed to fluidized bed state. Experiments show a hysteretic behavior between the increasing and decreasing velocity path pressure-drop curves. In this work, we propose an approach to investigate at the meso-scale the effect of Van der Waals force on fluidization of fine solids and its contribution to the pressure overshoot phenomenon. The proposed methodology aims at building a CFD-DEM database to guide developing a solid stress closure for a two-fluid model, which allows the macro-scale model to account for the effect of Van der Waals adhesive force on the hydrodynamics of fluidization and to predict the hysteresis in the bed pressure drop.

An Approach for Predicting the Pressure Drop Hysteresis

Gas-solid fluidized beds are broadly employed in industrial chemical and petrochemical processes. Van der Waals adhesive force is the dominant interaction force between fine particles in fluidized beds operating at dry ambient conditions. The influence of this interparticle force on the fluidized bed hydrodynamics is still far from being thoroughly understood. Thus, the main goal of this study is to provide mesoscopic numerical data that extends our knowledge about the effect of Van der Waals force on the fluidization hydrodynamics and its contribution to the experimentally observed pressure drop hysteresis.

In our previous work (Badran et al. 2021), we accounted for the Van der Waals force through a gradient of adhesive particle pressure in the solid phase momentum equation under the Eulerian-Eulerian framework. We proposed two adhesive pressure models and checked their ability to produce an overshoot in the bed pressure drop of fine particles. The first adhesive pressure model derived in the framework of the kinetic theory of rapid granular flows failed to produce the overshoot due to the dominant effect of multiple and long duration contacts in the fixed-bed flow. Another closure based on the coordination number was then proposed, which gave an adhesive contribution much larger than the one of the kinetic theory model and was able to create the pressure drop overshoot. This adhesive pressure model did not predict a hysteretic behavior between the fluidization and defluidization cycle curves because it does not account for the history effect. In order to get the hysteresis, the contact network destruction and formation should be considered (the coordination number evolution).

The structural changes of the contact network during the fluidization and defluidization cycles can be captured by a fabric tensor, R_{ij}, defined as (Zhang et al. 2010):

$$R_{ij} = \frac{1}{N_p} \sum_{k=1}^{N_p} \sum_{c=1}^{c_k} n_{k,i}^{c} \, n_{k,j}^{c} \tag{1}$$

where N_p is the number of particles in the bed, c_k is the number of contacts on particle k, and $n_{k,l}^{c}$ is the lth component of the unit branch vector pointing from the center of particle k to a contact point c. The trace of the fabric tensor, R_{ij}, is the mean number of contacts per particle. CFD-DEM

simulations can be performed using the code YALES2 (Dufresne et al. 2020) to determine the evolution of the fabric tensor during fluidization and defluidization cycles.

The Van der Waals force can be taken into account in the CFD-DEM model by adding an adhesive force term, $\boldsymbol{F}_{q\to p}^{ad}$, to the particle equation of motion. The adhesive force exerted by particle q with center at $\boldsymbol{x}_q$ on particle p with center at $\boldsymbol{x}_p$ can be written as (Elimelech et al. 1998):

$$\boldsymbol{F}_{q\to p}^{ad} = \frac{A}{6d_p}\frac{1}{(2\xi+\xi^2)^2}\frac{1}{(1+\xi)^3}\boldsymbol{n}_{pq} \tag{2}$$

where A is the Hamaker constant, $\xi = \|\boldsymbol{x}_q - \boldsymbol{x}_p\|/d_p - 1$ is the dimensionless distance between the two particle surfaces, and $\boldsymbol{n}_{pq}$ is a normal unit vector along the line of centers of two interacting particles. For distance between the surfaces of two particles smaller than a typical interatomic distance S_0, Eq. (2) is no longer valid and the Van der Waals force is set to a constant and maximal value in order to represent the physical repulsive nature and avoid the singular attractive force when the surface separation distance is equal to zero. When the spheres are nearly touching, the force in Eq. (2) can be simplified to:

$$\boldsymbol{F}_{q\to p}^{ad} = \frac{A}{6d_p}\frac{1}{(2\xi_0+\xi_0^2)^2}\frac{1}{(1+\xi_0)^3}\boldsymbol{n}_{pq} \approx \frac{A}{6d_p}\frac{1}{4\xi_0^2}\boldsymbol{n}_{pq} \tag{3}$$

with $\xi_0 = S_0/d_p$ is a minimum dimensionless separation distance between two particle surfaces.

In addition to the fabric tensor, R_{ij}, the structural evolution of the system can be explored by means of collisional stress tensor, σ_{ij}. In an averaging volume V, the macroscopic stress may be computed as (Zhang et al. 2010):

$$\sigma_{ij} = \frac{1}{V}\sum_{k=1}^{N_s}\sum_{c=1}^{c_k} r_{k,i}^c f_{k,j}^c \tag{4}$$

where N_s is the number of particles whose centers lie within the averaging volume V, c_k is the number of contacts on particle k, $\boldsymbol{r}_k^c$ is the branch vector from the center of particle k to a contact point c, and $\boldsymbol{f}_k^c$ is the contact force acting on particle k. The solid stress distribution and evolution in the presence of adhesion can be determined from CFD-DEM simulations using Eq. (4).

Data provided by meso-scale simulations through the fabric and collisional stress tensors may guide postulating a continuum evolution equation for the coordination number or developing a particle stress closure in order to predict the hysteresis in the bed pressure drop at the macro-scale.

Conclusion

This work presents an approach to extract from meso-scale simulations information about structural and stress changes during fluidization and defluidization of adhesive particles. These data can be employed to model the Van der Waals force at the macroscopic scale, which provides additional insights into its effect on the hydrodynamics of gas-solid fluidized beds.

References

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