Powder Technology 256 (2014) 39–51

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

A new blended acceleration model for the particle contact forces induced by an interstitial fluid in dense particle/fluid flows

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ARTICLE INFO

Article history:
Received 17 October 2013
Received in revised form 5 January 2014
Accepted 31 January 2014
Available online 7 February 2014

Keywords:
Mathematical modeling
Multiphase flow
Particulate processes
Computation
Complex fluids
MP-PIC

ABSTRACT

We use the Multi-Phase Particle-in-Cell (MP-PIC) numerical method to simulate binary fluidized beds and find that experimentally measured separation of the two particle types in such beds can be explained by including a new contact force model in MP-PIC that accounts for the inhibition of relative motion between particles of differing sizes or densities. Without the new contact force model, we find that there is poor agreement between experimentally measured and MP-PIC calculated particle separation. In the new contact force model, individual particle accelerations are a blend between the particle acceleration of the original MP-PIC method, appropriate for rapid granular flows, and an average particle acceleration that applies to closely packed granular flows, and we call the new model the "blended acceleration" model. In this paper, we develop the equations of the blended acceleration model, detail its numerical implementation, verify correct implementation by comparing with an analytic solution for one-dimensional binary beds, and compare MP-PIC calculation results with three sets of measurements of particle separation in binary beds.

1. Introduction

This work grew out of the desire to explain experimental measurements of steady particle separation in binary fluidized beds, where under some flow conditions the two particle types separate and under others very little separation occurs [3,6,8]. The accurate prediction of the separation of differing particle types in fluidized beds is very important for the prediction of fluidized bed performance. Binary fluidized beds have been extensively studied experimentally because phenomena that occur in poly-disperse beds can be more easily measured in the simpler situation of a bed with two types of particles. Yet, even in binary beds a rich variety of phenomena can occur [8]. In contrast to mono-disperse beds, in binary beds fluidization occurs over a range of gas velocities. Particles that tend to rise to the tops of such beds are sometimes called flotsam, and those that tend to sink are called jetsam. Typically, as the fluidizing velocity is increased, a state of maximum separation of flotsam and jetsam materials is reached. Further increases in the fluidizing velocity, result in re-mixing of flotsam and jetsam materials and, in some cases, even in a nearly uniformly mixed bed. This re-mixing is invariably accompanied by bubbling in the bed, and, evidently, bubbling is a necessary part of the re-mixing process. Subsequent reductions in the fluidizing velocity result in the bed materials separating again.

To simulate binary beds numerically and help explain the observed particle separation phenomena, we use the Multi-Phase Particle-in-Cell (MP-PIC) method [1,13]. MP-PIC is a particle/fluid numerical method that is widely used for the numerical calculation of three-dimensional, two-phase flows in which the particle phase may occupy a significant volume fraction of the two-phase mixture, up to a closely packed state in which particles are in sustained contact with each other. To calculate the particle phase, MP-PIC solves a transport equation for a particle distribution function (PDF), which is similar to the Boltzmann equation of gas dynamics [16]. In particle/fluid flows, however, in addition to having a distribution of spatial positions and velocities like the molecules of the Boltzmann equation, particles may have a distribution of sizes (diameters) and other attributes, such as density or temperature, and MP-PIC accounts for distributions of these additional particle attributes by including them as independent variables of the PDF. It is this capability to account for size- and density-distribution effects that makes MP-PIC well suited for the current study and, more generally, for the simulation of practical fluidized beds. Solution of the PDF equation in MP-PIC is coupled to solution of Navier–Stokes equations for the fluid phase by volume displacement terms, as well as aerodynamic drag and other fluid–particle interaction terms.

A recent development of the MP-PIC method is the inclusion of a Bhatnagar–Gross–Krook (BGK) collision model [9,10,11]. This collision model predicts local damping of relative particle motions and the relaxation of particle velocity distributions to isotropic, Gaussian

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http://dx.doi.org/10.1016/j.powtec.2014.01.084
0032-5910/

distributions. Coefficients in the relaxation times associated with the new collision terms have been chosen to replicate expressions for the particle-phase shear viscosity and the collision decay rate of granular temperature that are commonly used in particle continuum-fluid models for particle/fluid flows [4,5].

At the beginning of this work, we postulated that including the effects of particle collisions in MP-PIC calculations could help explain the experimental results in binary beds. When not using our recently developed BGK particle collision model, MP-PIC calculations reproduce the bed bubbling observed in experiments, but, in contrast to experiments, always give complete particle separation. We reasoned that since particle collisions damp relative motion between particles, including the effects of collisions in MP-PIC calculations should slow particle separation in bubbles and could result in the re-mixing observed in binary beds.

Based on similar reasoning, others have studied the effects of particle collisions on separation in binary beds, but have had limited success in comparing with experiments. In particle-continuum-fluid models for the particle phase, separate phase equations can be solved for each particle type, and collisions between different particle types are accounted for through so-called "particle–particle drag" terms. Syamlal [14] studied the effects on particle separation of using alternative forms of the radial distribution function, which enters into formulas for particle collision frequencies. He found that, for some forms of the radial distribution function, initial particle separation rates were predicted fairly accurately, but that equilibrium separation concentrations were not well predicted.

We found that including the BGK collision model in binary bed calculations resulted in suppressed bed bubbling, and the particle types still separated. As in the experiments, in our calculations it was necessary to have bed bubbling in order to have particle types re-mix. In order to restore the correct bubbling behavior in our bed calculations by varying the coefficients in the collision model, it was necessary to effectively "turn off" the BGK collision model. The reason that the collision model suppressed bed bubbling is that particle collision scattering resulted in large increases in the effective particle-phase viscosity [11]. Our speculation is that the granular temperature is being over-predicted by the current collision model, and this leads to over-predictions of the collision frequency and, hence, of the particle-phase viscosity. Over-prediction of the granular temperature also causes increased damping of relative particle motion, but particle types still separate, albeit at slower rates. We believe that it is incorrect to compute the granular temperature on the grid as is done with the current collision model, because the grid-scale particle velocity fluctuation intensity will also include turbulent particle motions and will over-estimate the granular temperature. These speculations will be the subjects of a future study.

So, we looked for another physical effect that could explain the experimentally observed particle separation phenomena in binary beds, and this led us to consider the role of particle contact forces in suppressing relative particle motion. Regions of closely packed particles occur often in fluidized beds. Some fluidized beds are largely composed of regions of closely packed particles interspersed with bubbles of fluid. It also happens that close packing is brought about in regions of moderate particle loading, by differential accelerations of particles with different sizes or densities causing the particles to clump together. Once brought together in direct contact, the particles have their relative motion inhibited by contact forces.

Until this study, the acceleration equation used by MP-PIC has suffered the deficiency that it allows interpenetrating particle motion in closely packed polydisperse beds, even though such motion is suppressed because of the sustained particle contacts in such beds. By "interpenetrating" particle motion, we mean that the particle phase itself acts as if it were a multi-phase fluid, with a separate phase velocity at each spatial location for each particle size or density. In closely packed beds, in contrast, the particle phase acts as a single phase with a single velocity at each spatial location because interpenetration is precluded by particle contact forces. (In closely packed beds with two widely different particle sizes, smaller particles can move through the interstitial openings between large particles, but we ignore this possibility in this work.)

In this paper we propose a modification of the contact stress term in the MP-PIC particle acceleration equation that gives uniform particle accelerations in closely packed beds. The old contact stress term, currently used in MP-PIC, is proportional to the gradient of a particle contact pressure and is independent of particle size or density. Thus, the old contact stress term does not cancel the different accelerations induced by drag and buoyant accelerations in closely packed beds. The new contact stress term we propose results in a total acceleration that is a blend of the old MP-PIC model acceleration and an expression for the uniform acceleration that particles experience in closely packed beds, and we call the new model the "blended acceleration" model. The blending function, which determines the fraction of each acceleration to use, is a function of particle volume fraction alone and effectively determines the transition between a particle phase that acts as a multi-phase fluid and one that acts as a single-phase fluid. The damping of relative particle motion in the blended acceleration model is not accompanied by any increased particle-phase viscosity or diffusion.

Some authors have attempted to explain the behavior of binary beds by using more complex forms of the particle drag model [7]. The calculations of this paper mostly use the Wen–Yu drag model [17] for monodisperse particle mixtures, but we also use a combined Wen–Yu and Ergun [2] drag model. It was found that, although changing the drag model can make some quantitative differences in separation behavior, especially in beds near minimum fluidization, these differences are small in comparison with the large qualitative differences between calculations using traditional unblended acceleration models for particle acceleration, and using the blended acceleration model of this paper.

This work has the important implication that numerical models of fluidized beds must include the effects of the contact force variations that accompany differential drag and buoyancy accelerations of particles with different sizes and densities. Many current fluidized bed models are based on the so-called kinetic theory of granular flow in which particle–particle interactions are only due to binary collisions and particle contact forces are ignored. Our work implies that in many practical fluidized beds, where there are regions of closely packed particles, contact forces contribute significantly to separation and mixing of particles of different sizes or densities. For example, in commercial processes such as in gasifiers that contain wood-chips and sand, or in TiO_2 production in which beds contain ore and coke, there are large differences in particle sizes and densities, and use of the blended acceleration model is expected to improve the accuracy of numerical simulations of these beds.

The next section of this paper gives the equations of the blended acceleration model. After a brief review of the old MP-PIC acceleration model, we derive the equation for the uniform acceleration at close pack and postulate a particle acceleration equation based on a blending of the old MP-PIC model and the uniform acceleration at close pack.

We next describe the numerical implementation of the blended acceleration model. This implementation is an extension of the original implementation of the MP-PIC method. We retain the important feature of the MP-PIC method that, in the particle acceleration equation, terms are differenced implicitly that are associated with aerodynamic forces, fluid pressure gradient forces, and contact stress gradient forces.

We have implemented the blended acceleration model in the Barracuda© computer code, and we next compare Barracuda results using the blended acceleration model with an analytic solution given in Appendix A and with experiments of binary fluidized beds. The calculations with the blended acceleration model give good agreement with experimental measurements of steady particle separation in binary beds.