The Influence of Binary Drag Laws on MP-PIC Simulations of Segregation

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ABSTRACT

Gas-fluidized beds with particles of different sizes and/or densities are common in industry, and known to exhibit segregation under some operating conditions. A key component of both Eulerian and Lagrangian models used to study segregation is the drag force. Monodisperse drag laws have been traditionally employed in polydisperse systems using *ad-hoc* assumptions due to the lack of adequate drag laws for polydisperse systems. van der Hoef *et al.* (2005) developed a drag force correlation for binary mixtures based on Lattice-Boltzmann simulations. This model was used in conjunction with the Gidaspow drag model (1994) in a Multi-Phase Particle-in-Cell (MP-PIC) framework to evaluate the effect the binary drag law has on simulations of binary mixtures. In this effort, a system with two species that differ only by size is considered. For the drag law without the binary correction, the simulation results show total segregation for all gas velocities examined. When using the drag law with the binary correction, however, a relatively homogeneous mixture is obtained for the higher velocities and segregation is observed as the gas velocity is decreased. These trends were confirmed with two-dimensional simulations employing the discrete element method (DEM). Collectively, the simulation results indicate that the form of the drag law plays a crucial role in the qualitative and quantitative nature of segregation predictions.

KEYWORDS: Segregation, MP-PIC, Binary Mixtures, Binary Drag Law

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I. INTRODUCTION

Gas-fluidized beds with particles of different sizes and/or densities are common in industry, and known to exhibit segregation under some operating conditions. Numerous studies have been carried out to investigate the segregation behavior in fluidized beds. The degree of segregation depends on the differences in density and size of the particles, as well as the gas velocity (Chiba *et al*., 1979). For systems composed of equal density particles, small particles tend to concentrate near the surface of the bed while large particles fall to the bottom (Rowe and Nienow, 1976; Wu and Baeyens, 1998; Goldschmidt *et al.*, 2003). Segregation by size increases with increasing bed height, decreasing size of fines, increasing mean size, and as the gas velocity approaches the minimum fluidization velocity of the smaller particle (Geldart *et al.*, 1981). For systems composed of different density particles, denser particles tend to fall to the bottom of the bed. For these systems, a large degree of segregation is present at low gas velocities and this degree of segregation decreases as velocity increases (Rowe and Nienow, 1976). A phenomenon which is not well understood is layer inversion, which refers to systems in which a given species may behave as either flotsam or jetsam, depending on the operating condition (Rasul *et al.*, 1999).

Mathematical models have been used to study segregation in gas-solid fluidized beds. Both Eulerian (van Wachem *et al.*, 2001a; Huilin *et al.*, 2003; Cooper and Coronella, 2005) and Lagrangian (Hoomans *et al.*, 2001; Limtrakul *et al.*, 2003; Feng *et al.*, 2003; Bokkers *et al.*, 2004; Dahl and Hrenya, 2005) models have been able to predict segregation with a certain degree of success and have provided insight on the contributing mechanisms. van Wachem *et al.* (2001a) used binary models for drag and solid phase stress in an Eulerian framework to predict layer inversion. The inversion phenomenon was explained via a change in the dominating mechanisms of the system with gas velocity. Namely, at low gas velocities the segregation is dominated by gravity and drag force and at high velocities by gradients in the granular temperature and granular pressure.

A key component of both Eulerian (continuum) and Lagrangian (discrete) models is the drag force, which couples the fluid and solid phases. In monodisperse systems, previous researchers have found that the use of different drag laws significantly impacts the simulation results, for example by modifying the bed expansion and solid concentration in the bed (van Wachem, *et al.*, 2001b). Numerous experimental studies have been carried out to measure drag force in different monodisperse systems and several correlations have been proposed. These correlations have been developed from packed-bed measurements (Ergun, 1952, Macdonald *et al.*, 1979), settling experiments (Richardson and Zaki, 1954, Syamlal and O'Brien, 1994), fluidized-bed experiments (Wen and Yu, 1966), and Lattice-Boltzmann simulations (Koch and Hill, 2001; Benyahia *et. al.* 2006). Traditionally, the drag force in polydisperse systems has been described by extending the monodisperse drag laws using *ad-hoc* assumptions. Recently, Pirog (1998) developed a drag force correlation for polydisperse systems based on a voidage-velocity correlation obtained from settling and creaming experiments in liquid-solid systems. van der Hoef *et al.* (2005) developed a drag force correlation for binary mixtures based on Lattice-Boltzmann simulations of low gas flow past arrays of random spheres. van Wachem et al. (2001a) and Dahl and Hrenya (2005) used Pirog's (1998) correlation in conjunction with the Ergun (1952) and the Wen and Yu (1966) drag models to describe drag force in binary systems. The focus of the present work is to determine the impact of various drag laws on simulations of fluidized beds composed of binary mixtures, with special emphasis on the prediction of segregation patterns. As described below, the simulations performed as part of this work indicate the critical role of the drag force in predicting segregation.

II. MODEL DESCRIPTION

To assess the relative merits of the various drag laws, simulations were performed using a novel alternative for modeling fluid-solid systems, namely the Multi-Phase Particle-in-Cell (MP-PIC) method (Andrews and O'Rourke, 1996). This implementation is a combination of the Eulerian and Lagrangian models for the solid phase. In Eulerian models, the solid phase is treated as a continuum via an analogy based on kinetic theory from which good qualitative results have been obtained. The advantage of these models is the minimum computational requirement; the challenge lies in the development of closures, which become more difficult for increasingly complex (e.g., polydisperse) systems. Lagrangian models provide an alternative in which each particle and collision is individually tracked, which has the advantage of making it simple to incorporate particles of different sizes and species. The disadvantage is that even two-dimensional simulations with only thousands of particles require considerable computational effort (Hoomans *et. al.*, 2001), making it computationally prohibitive for three-dimensional systems of industrial sizes. The MP-PIC model possesses advantages of both approaches; particles are grouped in parcels that are individually tracked, but the particle-phase stress is calculated from an Eulerian description, which thereby eliminates the need to resolve individual collisions between particles. Since particles are tracked in groups and individual collisions are not resolved, the modeling of many-particle systems is performed in a more computationally efficient manner than a strict Lagrangian treatment. In this effort, Arena-flow™ is being used as the framework for performing the MP-PIC simulations (Snider, 2001).

The governing equations for the MP-PIC treatment are given below. The equation of continuity for the fluid is:

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon u_f) = 0 \tag{1}$$

where ε is the fluid volume fraction and u_f is the fluid velocity. The fluid momentum balance is:

$$\frac{\partial(\varepsilon u_f)}{\partial t} + \nabla \cdot (\varepsilon u_f) = -\frac{1}{\rho_f}\nabla p - \frac{1}{\rho_f}F + \varepsilon g + \varepsilon \mu_f \nabla^2 u_f \tag{2}$$

where ρ_f is the density of the fluid, p is the fluid pressure, F is the rate of momentum transfer per unit volume between the fluid and particles, g is the gravitational acceleration, and μ_f is the fluid viscosity. The force balance for a cloud of particles is given by:

$$\frac{du_p}{dt} = \beta(u_{f,p} - u_p) - \frac{1}{\rho_p}\nabla p + g - \frac{\nabla \tau_p}{\nu \rho_p} \tag{3}$$

where u_p is the particle velocity, β is the drag force coefficient, $u_{f,p}$ is the fluid velocity at the particle position, ρ_p is the particle density, τ_p is the particle stress, and ν is the solid volume fraction. The interphase momentum transfer is given by:

$$F = \frac{1}{V}\sum_{k=1}^{N}\left[\beta(u_{f,p_k} - u_{p_k}) - \frac{\nabla p_{f,p_k}}{\rho_{p_k}}\right] n_k m_k \tag{4}$$

where V is the volume, N is the number of clouds, $p_{f,pk}$ is the fluid pressure at cloud k position, n_k is the number of particles in cloud k, and m_k is the mass of a particle in cloud k. The solid-phase stress is an extension of the Harris and Crighton (1994) stress and is given by:

$$\tau_p = \frac{P_s \nu^b}{max\left[\nu_{cp} - \nu, \alpha(1-\nu)\right]}\delta \tag{5}$$

where P_s, b, α are constants, ν_{cp} is the solid volume fraction at closest packing, and δ is the Kroneckel delta.

In this work, a new drag force law for binary systems is used, which combines the approach taken by Gidaspow (1994) and the recent work of van der Hoef *et al.* (2005). The former is a "stitching" together of monodisperse drag laws for the packed (Ergun, 1952) and fluidized (Wen and Yu, 1966) regions, whereas the latter provides a correction to monodisperse drag laws for binary systems in order to account for the presence of particles with different diameters. Dahl and Hrenya (2005) modified the Gidaspow (1994) drag law to remove the discontinuity generated when changing between the Ergun (1952) and the Wen and Yu (1966) correlations by doing a linear interpolation over a transition region; in the present work, this same approach is used. The van der Hoef *et. al.* (2005) expression is used to correct the Gidaspow (1994) drag law to account for the presence of different sized particles.

For polydisperse systems, van der Hoef *et al.* (2005) proposed the following expression for the dimensionless drag force:

$$F_i = \left((1-\nu)y_i + \nu y_i^{\,2} + 0.064(1-\nu)y_i^{\,3}\right)F\left(\nu, \langle Re\rangle\right), \quad yi = \frac{di}{\langle d\rangle} \tag{6}$$

where y_i is the diameter ratio between the diameter of species $_i$ diameter and the average diameter , F_i is the non-dimensional drag force of species i, F is the non-dimensional drag force calculated from monodisperse expression at the total solid volume fraction and average Reynolds number of the binary system, which is defined as:

$$\langle Re\rangle = \frac{\rho_g U \langle d\rangle}{\mu} \tag{7}$$

The average diameter is calculated from:

$$\langle d\rangle = \left[\sum_i^s \frac{x_i}{d_i}\right]^{-1}, \quad x_i = \frac{\nu_i}{\nu} \tag{8}$$

where x_i is the ratio between ν_i, the solid volume fraction of species i, and the total solid volume fraction. For a single particle at low Re, the inertial effects are negligible and the drag force takes the Stokes–Einstein form, so it is convenient to define the dimensionless drag force as:

$$F_i = \frac{F_{di}}{3\pi\mu d_i U}, \quad F = \frac{F_d}{3\pi\mu\langle d\rangle U} \tag{9}$$

III. RESULTS AND DISCUSSION

When using a monodisperse drag law in polydisperse systems, several *ad-hoc* modifications are typically made, such as replacing the particle diameter by a species diameter and assuming that the individual species drag force is equal to the drag force of a monodisperse system at the same volume fraction (van der Hoef *et al.*, 2005). These modifications have no physical basis but have been used due to the lack of adequate drag models for polydisperse systems.

The proposed binary drag law, the van der Hoef *et. al.* (2005) binary correction to the Gidaspow (1994) monodisperse drag law, presents a drastically different behavior for polydisperse system than the *ad-hoc* extension of the Gidaspaw (1994) drag law to binary systems. In latter approach, the drag force does not depend on the composition of each species. For example, for a system with a superficial gas velocity of 0.1 m/s and total solid volume fraction of 0.6 composed of 100 and 200 micron particles with density of 2600 kg/m^3; the drag force coefficient of a small particle is 156.9 s^{-1} while for a large one is 39.7 s^{-1} (regardless of the composition of each species in the mixture). The corresponding drag force coefficients using the former approach do depend on the composition. The dependency of both drag laws as a function of the solid volume fraction of the small particles can be seen in Figure 1. The plot shows that for the proposed drag law there is considerable difference in the drag force coefficients of both species as composition changes.

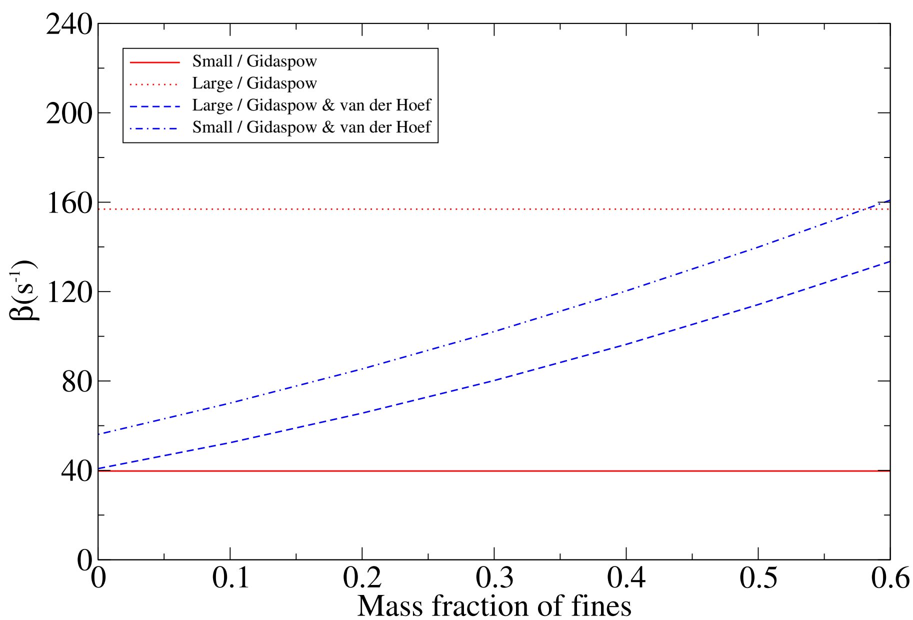

Figure 1. Drag force coefficients for a binary mixture of 100 and 200 micron particles, both with a density of 2600 kg/m^3. The total solid volume fraction is 0.6 and the superficial gas velocity is 0.1 m/s. The coefficients are shown as a function of the solid volume fraction of the small particles using both the *ad-hoc* extension of the Gidaspow (1994) drag law to binary systems and the van der Hoef *et. al.* correction (2005) to Gidaspow (1994).

To assess the impact of both drag laws on the segregation behavior of a system with only a size difference (both particle have the same material density), simulations were performed for defluidizing beds, the model parameters are given in Table 1. The initial condition was a uniformly mixed bed 40 cm with both species at a solid volume fraction of 0.15. The initial gas velocity was set to 0.15 m/s, and was decreased in steps of 0.025 m/s in periods of 0.2 s. The gas velocity was then kept constant for 2 s, and time-averaged properties were calculated over the second half of this period. In an attempt to isolate the effect of the drag force, the simulation study was performed at low velocities, in which the drag force is a dominating force for segregation (van Wachem et al., 2001a).

Variable	Value
Column diameter	10 cm
Cell dimensions	1 cm x 1 cm x 1 cm
d_s	100 μm
d_l	200 μm
ρ_s	2600 kg/m^3
ρ_l	2600 kg/m^3
n_s	28,986 particles/cloud
n_l	3,623 particles/cloud
N_s	30,720 clouds
N_l	30,720 clouds
μ_f	1.789e-5 kg/m/s
ρ_f	1.225 kg/m^3
P_s	10 Pa
b	3
α	1e-8
v_{cp}	0.6

Table 1. Simulation parameters.

As depicted in Figure 2, both drag laws predicted the minimum fluidization velocity to be between 0.03 and 0.05 m/s. Both drag laws also predict a pressure drop equal to the total weight of the bed divided by its area for gas velocities above 0.05 m/s (i.e., in the fully fluidized region). As the gas velocity decreases, a defluidized layer of coarse particles forms in the bottom of the bed. For a gas velocity of 0.025 m/s, a slightly smaller pressure drop was calculated by the drag law with the binary correction. More particles are in the defluidized layer in the simulation without the binary correction, resulting in the lower pressure drop. In terms of bed expansion, both models present similar bed heights for all gas velocities.

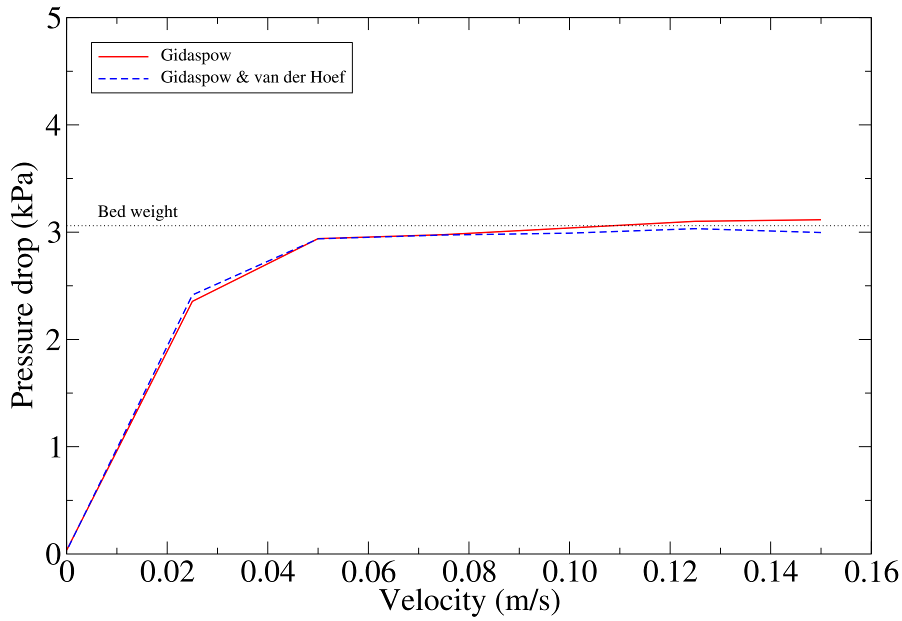

Figure 2. Fluidization curves for MP-PIC simulations of a binary mixture of 100 and 200 micron particles both with density of 2600 kg/m^3 using both the Gidaspow (1994) and the van der Hoef *et al.* (2005) correction to Gidaspow (1994) drag laws.

The axial segregation profiles at several velocities are presented in Figure 3. For the drag law without the binary correction, the simulation results show total segregation (i.e., complete separation of species) for all gas velocities examined. Specifically, the small particles segregate on top of the big particles at the initial velocity and remained unmixed as the velocity is decreased. When using the drag law with the binary correction, however, a relatively homogeneous mixture is obtained for the higher velocities and segregation is observed as the gas velocity is decreased below 0.1 m/s. At a velocity of 0.075 m/s the binary drag law presents partial mixing; *i. e.*, a layer of small particles is present at the top of the bed, a layer of large particles is present at the bottom, and the middle portion of the bed has both components present. At the final state a total segregation is present.

To verify that the results obtained with the MP-PIC approach were not influenced by the semi-empirical, solid-phase stress model (Snider, 2001) used in Arena-flow^{TM}, two-dimensional, discrete-particle simulations of a bidisperse fluidized bed were carried out following the development by Dahl and Hrenya (2005). In this treatment, individual particle collisions are resolved and hence no solid-phase stress model is required (unlike the MP-PIC approach). The Lagrangian simulations were done for a binary mixture of 1000 and 2000 micron particles, having the same diameter ratio as the MP-PIC simulations, both with density of 2600 kg/m^3 and with a superficial gas velocity of 1.5 m/s. The particles were considered inelastic and frictionless. For this strictly Lagrangian formulation, a higher degree of segregation was observed when using the model without the binary correction as seen in Figure 4; this behavior qualitatively mimics that obtained in the MP-PIC simulations.

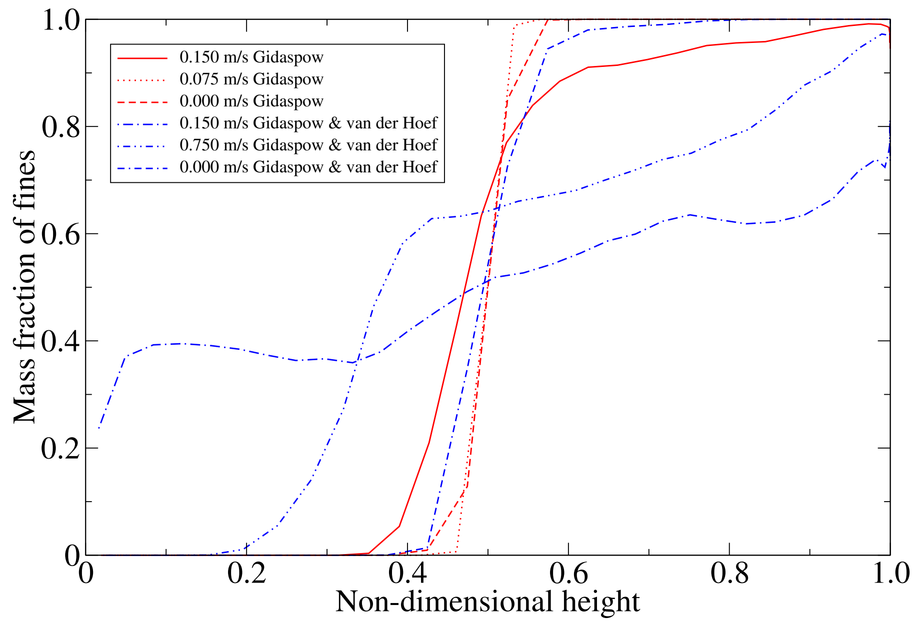

Figure 3. Segregation profiles for MP-PIC simulations of a binary mixture of 100 and 200 micron particles both with density of 2600 kg/m^3 superficial gas velocities of 0.15, 0.075, and 0 m/s for both the Gidaspow (1994) and the van der Hoef *et. al.* (2005) correction to the Gidaspow (1994) drag laws.

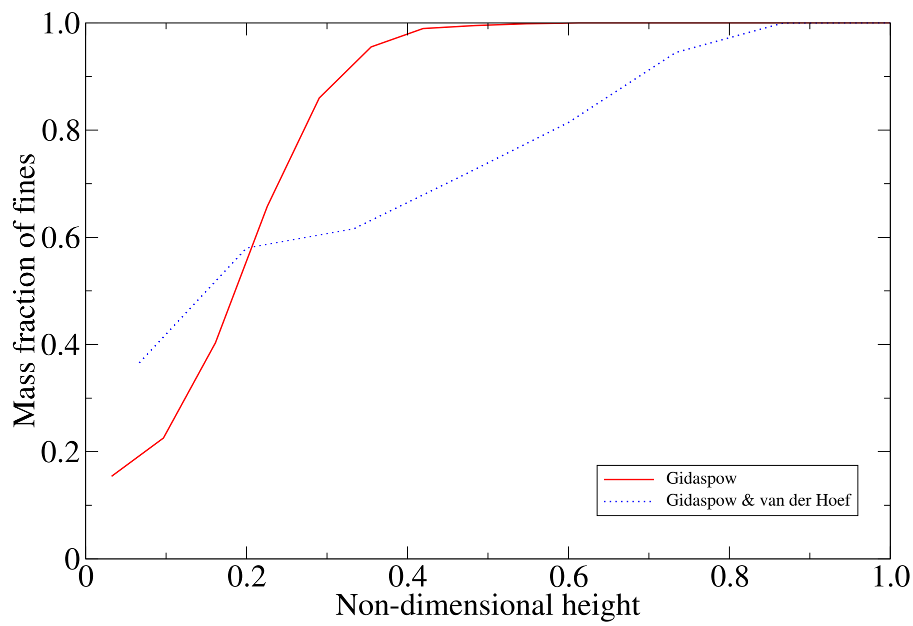

Figure 4. Segregation profile for the Lagrangian simulation following the development by Dahl and Hrenya (2005) for a binary mixture of 1000 and 2000 micron particles both with density of 2600 kg/m^3 and a superficial gas velocity of 1.5 m/s for both the Gidaspow (1994) and the van der Hoef *et. al.* correction (2005) to the Gidaspow (1994) drag laws.

A set of MP-PIC simulations for the system described in Table 1 using the Hill-Koch-Lad drag model presented by Benyahia *et. al.* (2006). Both the *ad-hoc* Hill-Koch-Lad (Benyahia *et. al.*, 2006) and the van der Hoef *et. al.* correction (2005) to the Hill-Koch-Lad (Benyahia *et. al.*, 2006) present the same qualitative results obtained on the first set of simulations. When using the van der Hoef *et. al.* correction (2005) the simulation presents a homogenous mixture at high gas velocities and segregation increases as the gas velocity decreases, the *ad-hoc* model presents total segregation for all the gas velocities examined.

IV. CONCLUSIONS

In summary, both MP-PIC and discrete-particle simulation results indicate that the form of the drag law plays a crucial role in the qualitative and quantitative nature of segregation in binary mixtures. By incorporating the van der Hoef *et. al.* correction (2005) to account for the presence of different size particles into the drag law a more homogenous mixture is present at high gas velocities where the *ad-hoc* monodisperse drag models adapted for polydisperse system predict a higher degree of segregation. This behavior was also found to be true for systems with both size and density differences; a direct comparison between simulations and experiments for a range of parameter sets is detailed in the companion contribution by Joseph *et al*. (2006).

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