

## Prediction of flow behavior of micro-particles in risers in the presence of van der Waals forces

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### Abstract

Flow behavior of gas and micro-particles in riser is predicted within the framework of the classical Euler–Lagrange approach. The Newtonian equation of motion considering the effect of van der Waals forces is solved for each simulated particle in the system. Particle collisional dynamics is modeled by means of the direct simulation Monte Carlo (DSMC) method. The influence of van der Waals forces on the particle collisions is investigated. The effect of interparticle collisions on the particle concentration and velocity distributions is presented. These numerical results allow one to understand the effect of the considered parameters on the flow behavior of micro-particles agglomerations.

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### 1. Introduction

Micro-particles in which surface forces play an important role in the mechanical behavior of particles are classified to the Geldart group C [1]. Strong cohesive forces between micro-particles promote the fluidization of aggregates of primary particles [2]. Properties of the fluidized aggregates, rather than those of primary particles, determine the hydrodynamic behavior of risers. Experiments indicated that the elutriation rate of group C particles decreased with the increase of the particle mean diameter under the condition of a given superficial gas velocity in the fluidized bed [3]. Sound waves, mechanical vibration, gas pulsation, and magnetic and centrifugal fields have been applied to provide external forces to improve the fluidization of fine particles [4–7]. Experimental results indicated that with assistance of external forces the bed of agglomerates can be readily fluidized, and the flow structures of channeling or slugging disappeared and the bed expanded uniformly.

On the other hand, Mikami et al. [8] simulated the fluidized behavior of cohesive particles using a discrete numerical simulation model considering the effect of liquid bridge force and particle–particle interaction force in a two-dimensional bubbling fluidized bed. Helland et al. [9] simulated the flow structure of

cohesive particles in a two-dimensional riser by a hard-sphere discrete particle model. Rhodes et al. [10] analyzed the influence of the magnitude of the cohesive force of particles on fluidization characteristics in terms of the change in the ratio of the minimum bubbling to minimum fluidization velocities by a discrete element method. Kuwagi and Horio [11] investigated the mechanism of agglomeration in a bubbling fluidized bed of cohesive fine particles by a two-dimensional discrete element method. Ye et al. [12] studied the fluidization behavior of Geldart A particles by use of a soft-sphere discrete particle model considering the interparticle van der Waals forces. The particle circulation and bubble flow were predicted in the bubbling fluidized bed.

Turbulent particle agglomeration is an important mechanism especially for micro-particles flow [13]. For such small particles, Brownian motion and gravitational settling generally are negligible compared to turbulence-induced motion. Moreover, van der Waals interaction dominates in fluidized transport system of micro-particles, so that they tend to stick together to form particle aggregates when they collide with each other. The lack of detailed information in the open literature concerning the motion of micro-particles has hindered further investigation of flow behavior of micro-particles in the riser. A better understanding of the flow behavior of micro-particles is therefore of great importance in applications involving mixing and transporting of micro-particles. The purpose of this study is to investigate the effect of van der Waals forces on the flow

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## Nomenclature

$a_i$	local area of a particle $i$ ( $\text{m}^2$ )
$A$	Hamaker constant (J)
$B$	Boltzman's constant (J/K)
$c_{\text{do}}$	drag coefficient
$d$	particle diameter (m)
$D$	diameter of riser (m)
$e$	coefficient of restitution of particles
$e_w$	coefficient of restitution between particle and wall
$f_c$	collision frequency of particles ( $\text{s}^{-1}$ )
$f_d$	drag force (Pa)
$F$	time fraction (s)
$g$	gravity ( $\text{m s}^{-2}$ )
$G_s$	solid mass flux ( $\text{kg m}^{-2} \text{s}^{-1}$ )
$h$	height of riser (m)
$\hbar$	Planck's constant (J s)
<b>I</b>	unit vector
$m$	particle mass (kg)
$n$	particle number density
ns	number of real particle/simulated particle
$N$	refractive index
$p$	fluid pressure (Pa)
$p_{ij}$	collisional probability
$P_p$	material limiting contact pressure (Pa)
$r$	position, distance from center (m)
$R$	random number, radii of particle and riser
$s$	local area of a particle ( $\text{m}^2$ )
$t$	time (s)
$T$	absolute temperature (K)
$u_g$	gas velocity, superficial gas velocity ( $\text{m s}^{-1}$ )
$v$	particle velocity ( $\text{m s}^{-1}$ )
$x$	location along lateral direction (m)
$y$	location along vertical direction (m)
$z_0$	contact distance (m)

## Greek symbols

$\alpha$	dielectric constant
$\varepsilon_g$	porosity
$\varepsilon_s$	solid concentration
$\theta$	granular temperature ( $\text{m}^2 \text{s}^{-2}$ )
$\mu_{\text{lam,g}}$	laminar viscosity of gas phase (Pa s)
$\mu_t$	turbulent viscosity of gas (Pa s)
$\nu_e$	absorption frequency ( $\text{s}^{-1}$ )
$\rho_g$	gas density ( $\text{kg m}^{-3}$ )
$\rho_s$	particle density ( $\text{kg m}^{-3}$ )
$\sigma$	standard deviation
$\tau_g$	gas stress tensor (Pa)

## Subscripts

g	gas phase
$i$	index of particle
n	normal direction
s	particles

behavior of micro-particles in a riser through DSMC simulation. The distributions of velocity and concentration of particles in the riser are analyzed. It is expected that the results of this study would stimulate further discussion and development of the micro-particle interaction models in risers. This would eventually enable new insights into the mechanism of agglomerate micro-particles in risers to be revealed.

## 2. Eulerian–Lagrangian gas–solid flow model

### 2.1. Continuity and momentum equations for gas phase

The Euler–Lagrangian method computes the Navier–Stokes equation for the gas phase and the motion of individual particles by the Newtonian equations of motion. For the gas phase, we write the equations of conservation of mass and momentum [14,15]:

$$\frac{\partial}{\partial t}(\rho_g \varepsilon_g) + \nabla \cdot (\rho_g \varepsilon_g u_g) = 0 \quad (1)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon_g \rho_g u_g) + \nabla \cdot (\varepsilon_g \rho_g u_g u_g) \\ = -\varepsilon_g \nabla P - S_{p-g} - (\varepsilon_g \nabla \cdot \tau_g) + \varepsilon_g \rho_g g \end{aligned} \quad (2)$$

where  $u_g$  and  $\rho_g$  are gas velocity and density, respectively.  $\varepsilon_g$  is porosity, and  $S_{p-g}$  the interaction drag force acting on a particle. The interaction force between the two phases should be equal and has reverse direction. The value can be determined by

$$S_{p-g} = \frac{\sum_{i=1}^N a_i f_{d,i}}{\sum_{i=1}^N a_i} \quad (3)$$

where  $a_i$  is the area of particle  $i$  in the cell. The drag force,  $f_{d,i}$ , is calculated by Eq. (7). The stress tensor of gas phase can be represented as

$$\tau_g = \mu_g [\nabla u_g + (\nabla u_g)^T] - \frac{2}{3} \mu_g (\nabla \cdot u_g) \mathbf{I} \quad (4)$$

The gas turbulence is modeled using a simple subgrid scale (SGS) model. The model was first used and proposed by Deardorff [16] for channel turbulence flow. The SGS model simulates the local Reynolds stresses arising from the averaging process over the finite-difference grid by about the crudest of methods, that involve an eddy coefficient with magnitude limited in some way by the size of the averaging domain. This domain is considered to be the grid volume in a detailed numerical integration. Then the eddy coefficient becomes a “subgrid scale” coefficient:

$$\mu_g = \mu_{\text{lam,g}} + \rho_g (C_t \Delta)^2 \sqrt{S_g : S_g} \quad (5)$$

where  $\Delta = (\Delta x \Delta y)^{1/2}$  and  $S_g = (1/2)[\nabla \cdot u_g + \nabla \cdot u_g^T]$ . Deardorff suggested  $C_t$  be in the range of 0.1–0.2 [16]. In this study  $C_t = 0.1$  was used in the simulations.

### 2.2. Particle motion equations

The particle motion is subject to Newton's equation of motion. Basset, Magnus and Saffman forces should not be included in the Newtonian equations of motion anyway since

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