International Journal of Multiphase Flow 73 (2015) 171–206

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

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

Modeling and simulation of particle agglomeration in turbulent flows using a hard-sphere model with deterministic collision detection and enhanced structure models

M. Breuer *, N. Almohammed

Professur für Strömungsmechanik, Helmut-Schmidt-Universität Hamburg, D-22043 Hamburg, Germany

ARTICLE INFO

Article history:
Received 10 October 2014
Received in revised form 10 February 2015
Accepted 20 March 2015
Available online 28 March 2015

Keywords:
Agglomeration
Cohesive force
Van-der-Waals force
Collision time
Hard-sphere model
Deterministic collision model
Particle-laden turbulent flow
Large-eddy simulation

ABSTRACT

The present paper is concerned with the modeling and simulation of particle agglomeration of rigid, dry and electrostatically neutral particles in turbulent gas flows. Based on a deterministic collision model in the framework of an Euler–Lagrange approach for the description of disperse particle-laden flows, the original agglomeration model of Kosinski and Hoffmann (2010) is improved regarding the determination of the collision time. The application area of the agglomeration model is extended towards fully three-dimensional turbulent flows simulated by the large-eddy simulation technique. Additionally, the model is enhanced by introducing three different concepts to model the structure of the arising agglomerate, namely the volume-equivalent sphere model, the inertia-equivalent sphere model and the closely-packed sphere model. Furthermore, the resulting simulation strategy for turbulent particle-laden shear flows is first analyzed and evaluated concerning the three structure models. Then, the performance of the extended agglomeration model is tested by investigating the influence of various simulation parameters such as the restitution and friction coefficients of the particles, the inclusion of the two-way coupling, the subgrid-scale model for the particles, the lift forces, the wall roughness and the particle mass loading on the agglomeration process in a turbulent particle-laden vertical channel flow. In the parameter study solely the closely-packed sphere model is adopted, since it takes the interstitial space between the agglomerated particles into account and additionally satisfies the conservation of mass and angular momentum. Based on the results, it can be concluded that the enhanced agglomeration model using the closely-packed sphere model for the arising agglomerate realistically predicts the physical behavior of the agglomeration process within particle-laden flows.

Introduction

Disperse particle-laden flows play an important role in numerous industrial processes and occur in various natural phenomena. Classical examples are the dispersion of atmospheric pollutants, pneumatic conveying systems of granular flows, gas cyclone separators and pulverized coal firing systems. As the mass loading of the disperse phase increases, there is a certain limit at which the effect of the solid phase on the gas flow becomes important. Here, the interaction between the particulate and the continuous phase has to be taken into account by the so-called two-way coupling. In this regime, it is commonly accepted that the particle–particle interactions still do not play a dominant role. For a higher mass loading, however, the particle–particle interactions can no longer be neglected within a simulation environment leading to the necessity of four-way coupling.

The collision between particles is the first prerequisite for the agglomeration of particles. Note that the particle–wall interaction follows similar rules as the inter-particle interaction, but is excluded in this study. Owing to the variety of relevant physical phenomena, the following considerations are furthermore restricted to dry, electrostatically neutral particles in a gas flow. In this case, the second prerequisite for agglomeration is an attractive force between the particles known as the molecular van-der-Waals force. That is especially important for microscopic particles with diameters in the range of 1–20 μm. Thus, if a collision between particles occurs (first prerequisite fulfilled), it has to be proved whether the cohesive force between the particles (second prerequisite) is strong enough for their agglomeration. This can be achieved either by energy or momentum (impulse) based models and on different levels of complexity allowing strongly simplified considerations or physically more detailed models.

* Corresponding author.
E-mail address: breuer@hsu-hh.de (M. Breuer).

http://dx.doi.org/10.1016/j.ijmultiphaseflow.2015.03.018
0301-9322/

To evaluate the situation after a collision on the energy basis, first ideas were suggested by Löffler and Muhr (1972) and Hiller (1981) in the context of particle deposition in fiber filters. However, their considerations were restricted to a frictionless head-on collision, where the velocity vectors of the approaching particles are collinear. Based on an energy balance of the kinetic energy of the particles before and after the impact, the dissipated energy due to irreversible deformations and the van-der-Waals energy (London, 1937; Hamaker, 1937), a critical relative velocity between the approaching particles is determined. If the actual relative velocity between a collision pair is smaller than this critical value, it is assumed that the colliding particles agglomerate. In the framework of Euler–Lagrange simulations based on RANS and a stochastic collision detection model (Sommerfeld, 2001), this agglomeration model was extensively applied by Sommerfeld and co-workers (Ho and Sommerfeld, 2002; Ho, 2004; Sommerfeld, 2010; Stübing and Sommerfeld, 2010). The assumption of frictionless head-on collisions and the disregard of particle rotation are rather crude constrictions not justified by real conditions. Therefore, Jürgens (2012) and Alletto (2014) first generalized the agglomeration model towards oblique collisions allowing relative tangential velocities at the contact point. Later on, the friction at the contact point was also accounted for by Alletto (2014), whose extended model incorporates both the translational kinetic energy and the rotational kinetic energy of the particles into the energy balance and the resulting agglomeration condition. Furthermore, sticking and sliding collisions are distinguished within this model. In Alletto (2014), first an a priori analysis and then an a posteriori evaluation with application to a downward pipe flow at low Reynolds number were carried out yielding reasonable results but missing a profound validation procedure.

Besides the energy-based agglomeration criteria, momentum-based conditions were derived. These are the natural choice in the context of Newton's second law, which represents a momentum equation solved for the description of the motion of the particles. For the collision process itself, so-called hard-sphere (see, e.g., Hoomans et al., 1996; Crowe et al., 1998) and soft-sphere models (see, e.g., Cundall and Strack, 1979; Tsuji et al., 1993) have to be distinguished. In soft-sphere models, also known as the discrete element method (DEM), the deformation of the particles is explicitly taken into account during the collision allowing the penetration of particles. The procedure is more accurate than the momentum-based hard-sphere model, but it renders impracticable in many cases especially at high mass loadings. Thus, in the following the focus will be on the hard-sphere approach and the corresponding agglomeration models.

Within the context of rapid granular flows, Weber et al. (2004) incorporated attractive inter-particle forces into hard-sphere (molecular dynamics) simulations using a square-well potential. In contrast to other models, in which the van-der-Waals force is a continuous function of the inter-particle distance, the square-well potential treats cohesive forces as they arise from impulsive events. Thus, this model represents a possible mean of incorporating cohesive effects into continuum (kinetic-theory) models as well as discrete particle (hard-sphere) models. For the latter, the inter-particle attraction can be applied directly to each binary particle–particle collision. Using the square-well model, the particles experience an instantaneous, attractive force of dirac-delta type at a pre-defined inter-particle distance. An agglomeration process denoted capture-cohesive interaction (Weber et al., 2004) is characterized by a normal relative velocity, which for a given coefficient of restitution is too small to overcome the cohesive well. In Weber and Hrenya (2006), the square-well model is applied to discrete particle fluidized-bed simulations and compared with the Hamaker description of van-der-Waals forces. To convert material-specific Hamaker constants into equivalent square-well parameters, a mapping method is developed. Qualitatively and quantitatively similar results are found for both models.

Kosinski and Hoffmann (2010) partially overtook general ideas of Weber et al. (2004) and Weber and Hrenya (2006) for the derivation of an impulse-type hard-sphere particle collision model. Based on the momentum equations for the collision of two particles including a repulsive impulse due to mechanical deformation, the classical hard-sphere model is extended by a cohesive impulse to study agglomeration. Similar to the standard collision model without attractive forces (see, e.g., Crowe et al., 1998) two cases have to be distinguished: (i) the particles stop sliding during the collision and (ii) the particles continue to slide throughout the entire collision. Considering solely the repulsive impulse, the particles will bounce off after collision although they lose mechanical energy due to various dissipative processes involved in the collision. However, including the cohesive force changes the situation completely, since the particles enter a potential well and may not manage to escape from this potential well after the collision. That leads to the corresponding agglomeration conditions, which will be given in more details in Section 'Agglomeration model'. Furthermore, also the translational and angular velocities of the formed agglomerate can be determined. The critical issue is the derivation of a reasonable approximation for the cohesive impulse due to the attractive forces.

Cohesive forces due to the Hamaker interaction are known functions of the separation between particle surfaces. For the determination of the impulse, however, an expression for the force as a function of time is required. Thus, a change of variables is necessary. As a first rather simple model Kosinski and Hoffmann (2010) estimated the actual period of contact (sum of the compression and recovery period) from a relation in the literature (see, e.g., Hertz, 1882; Johnson, 1985; Stronge, 2000). Hence, the periods before and after the collision during which the cohesive force is also effective, are suspended. Furthermore, assuming Hamaker interaction between two perfect spheres in contact acting during this period only, the unknown cohesive impulse can be determined since the force is constant for a constant separation between the particles.

Kosinski and Hoffmann (2010) carried out first tests for their extended hard-sphere model in a laminar two-dimensional channel flow showing the formation of agglomerates but no detailed validation process. Balakin et al. (2012) studied the agglomeration efficiency of particles in a turbulent but nevertheless two-dimensional shear flow under varying conditions (inter-particle friction, stiffness, density and volume fraction). The agreement with theoretical investigations is undifferentiated, since the theories also broadly scatter. Kosinski and Hoffmann (2011) extended the analysis and determined the cohesive impulse by combining the soft-sphere approach based on a dimensional analysis. Unfortunately, they did not compare the new outcome with their previous model (Kosinski and Hoffmann, 2010). Note that in all previous studies the agglomerates are modeled as volume-equivalent spheres.

The objectives of the present paper are set as follows:

- (i) Improvement of the agglomeration model by Kosinski and Hoffmann (2010) regarding the collision time.
- (ii) Further improvement of the agglomeration model based on different concepts for modeling the structure of the arising agglomerate.
- (iii) Extension of the application area of the improved agglomeration model towards fully three-dimensional turbulent flows simulated by the large-eddy simulation technique combined with a deterministic hard-sphere collision approach.
- (iv) Analysis and evaluation of the resulting entire simulation strategy for a wide parameter range.