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Modeling and simulation of particle–wall adhesion of aerosol particles in particle-laden turbulent flows

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ABSTRACT

The present study is concerned with the development of a computational model for predicting particle–wall adhesion (deposition) of aerosol particles in turbulent particle-laden flows. Particularly, the standard hard-sphere model is extended to include the adhesion during sticking or sliding particle–wall collisions. For both impact types the deposition condition of a particle on bounding walls is determined. The strategy of the proposed model is based on the momentum-based agglomeration model by Breuer and Almohammed (2015). The main advantage of the proposed model compared to the state-of-the-art in the literature is that the adhesive impulse is determined more reasonably taking the time intervals of the compression and the restitution phase into account. Furthermore, if the deposition condition is not satisfied, the treatment of the particle motion after the impact including adhesion depends on the particle–wall type (sticking or sliding). To examine the effect of the particle–wall adhesion, the developed model is first evaluated using simple test cases including oblique particle–wall collisions with friction. In the second step, the performance of the adhesion model is validated based on a horizontal turbulent channel flow against existing experimental data of Kvasnak et al. (1993) and numerical results by Fan and Ahmadi (1993)based on an energy-based deposition model. The predictions of the present model agree very well with the experiments and the numerical results chosen for the validation study as well as the empirical relation by Wood (1981). Third, the adhesion model is employed to investigate the influence of different simulation parameters (normal restitution coefficient for particle–wall collisions and particle diameter) on the particle–wall adhesion and deposition process in a vertical turbulent channel flow laden with a huge number of primary particles. The results show that the inclusion of the adhesion significantly reduces the number of particle–wall collisions, whereas the number of particle–particle collisions is only slightly reduced. Furthermore, the number of deposited particles is higher for small particles than for large particles, since the adhesive impulse is inversely proportional to the diameter of the primary particles. The proposed adhesion model is developed and tested in the context of large-eddy simulation, but it can also be applied in DNS or RANS predictions.

1. Introduction

Turbulent flows laden with adhesive aerosol particles occur in a wide range of industrial and environmental applications as well as natural phenomena. Therefore, substantial effort has been made in the past decades to understand the complex behavior of these flow systems. An accurate prediction of the kinetics of particle deposition leads to an improved design of engineering flow systems. Particle–wall adhesion is an important mechanism, since it influences the interaction between the particles and the wall and hence the volume fraction in the near-wall region. The importance of particle–wall and particle–particle collisions increases with increasing mass loading.

The flux of the particles towards the wall is typically characterized by the dimensionless deposition velocity $v_d^+ = v_d/u_\tau = (N_d/t_d^+)/(N_0/h_0^+)$. Here, N_0 is the initial number of primary particles uniformly distributed in a region within a dimensionless distance of $h_0^+ = h_0 u_\tau/\nu_f$ from the wall. N_d stands for the number of deposited particles during the dimensionless time $t_d^+ = t\, u_\tau^2/\nu_f$.

Previous studies on particle deposition have a long history. For example, Liu and Agarwal (1974) experimentally investigated the deposition of aerosol particles in a turbulent vertical pipe flow. The particles were assumed to be spherical droplets of olive oil. The results show that the dimensionless deposition velocity increases linearly with the square of the dimensionless relaxation time for $\tau_p^+ < 10$. The observations are in good agreement with the theory

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based on the "diffusion free-flight" model of Friedlander and Johnstone (1957) and Beal (1970). Furthermore, Liu and Agarwal (1974) found that the particle deposition velocity increases until about $\tau_p^+ = 30$ and then slightly decreases beyond this value.

Wood (1981) proposed an empirical relation for the dimensionless particle deposition velocity as a function of the dimensionless particle relaxation time $v_d^+ = 0.057\,\mathrm{Sc}^{-2/3} + 0.00045\,\tau_p^{+2}$. Here, Sc stands for the Schmidt number. This relation is in good agreement with experimental data for the case of smooth walls, but it is less accurate in the case of rough walls due to its high sensitivity to any kind of wall roughness. Kvasnak et al. (1993) experimentally studied the wall deposition rate in a horizontal turbulent channel flow. The particles deposited on a flat gold plate covered with a thin film coating corresponding to a reduction of the restitution coefficient. They concluded that the deposition velocity increases with increasing diameter. The measured deposition velocities agreed well with the experimental results of Papavergos and Hedley (1984). In addition, they modified the empirical model by Wood (1981) taking the effect of gravity into account such that the deposition velocity reads $v_d^+ = 0.057\,\mathrm{Sc}^{-2/3} + 0.00045\,\tau_p^{+2} + g^+\tau_p^+$, where $g^+ = g\,\nu_f/u_\tau^3$ denotes the dimensionless gravitational acceleration. This correlation leads to good agreement with their experimental data. This experimental test case will be used in Section 4 for the validation of the developed adhesion model.

Numerical simulations were also carried out to investigate the particle deposition using different approaches. McLaughlin (1989) performed direct numerical simulations (DNS) to study the particle deposition in a vertical channel flow. He did not use any particle–wall deposition model, rather assuming that a particle deposits on the wall if the gap between the particle and the closest wall is smaller than the particle size. Thus, particle–wall collisions were not considered. The predicted deposition rate was lower than the one measured by Liu and Agarwal (1974) for $\tau_p^+ < 2$ and higher outside this range.

Other studies were performed using the large-eddy simulation (LES) technique. For instance, Wang and Squires (1996) carried out LES of particle deposition in a vertical channel flow using two different Reynolds numbers. In their study, deposition is assumed to take place if a particle is within a distance of one radius of the spherical particle from the wall. The dimensionless deposition velocity predicted by LES exhibits the same dependency on the dimensionless relaxation time and the density ratio ρ_p/ρ_f as found by McLaughlin (1989), but they underpredict the DNS results. However, their predictions are still in fair agreement with the empirical relation of Liu and Agarwal (1974). Furthermore, they found that the dimensionless deposition velocity increases with increasing τ_p^+ or decreasing density ratio, and it was only slightly affected by the Reynolds number. When including the subgrid-scale velocity fluctuations in the particle motion, the wall-normal deposition velocity increases by about 30% for small particles, while there is virtually no influence of the SGS velocities for $\tau_p^+ = 6$. Wang and Squires (1996) also concluded that the consideration of particle–particle collisions further improves the agreement between predictions and experiments. Winkler et al. (2006) used LES to investigate the effects of the two- and four-way coupling on the deposition velocity in a square duct flow. Again, no deposition model was employed, but rather the same criterion as applied in the latter numerical studies was used. They concluded that the one-way coupled approach is sufficient for volume fractions less than 10^{-4}, since at low volume fractions the inclusion of the two-way coupling and the particle collisions does not significantly alter the deposition trends. For large particles the deposition rates are in good agreement with the experiment by McCoy and Hanratty (1977), while for small particles they are two orders of magnitude higher. Furthermore, the deposition rate of the low Stokes number particles increases significantly by considering the subgrid-scale velocity fluctuations for the particles. The inclusion of the two- and four-way coupling were found to enhance the deposition rates.

It is important to note that the deposition condition employed in the above mentioned numerical studies is reasonable when studying, for example, the deposition of inhaled particles on the wetted airway walls (see e.g., Breuer et al., 2006). However, in engineering applications this is typically not the case and thus an adhesion model has to be developed which also allows that particles bounce back from the wall under certain conditions. In this context, Li and Ahmadi (1993) carried out channel flow simulations for different materials of the particles, while the walls were assumed to be made of gold. For the deposition of the particles a simple energy-based model proposed by Dahneke (1971) was applied (see Section 2.5.2). In this model, it is assumed that a particle adheres to the wall if its wall-normal velocity is lower than a critical approach velocity $v_{p,n}^{*,D}$. The latter depends on the surface potential energy E_s, the restitution coefficient $e_{n,\,w}$ and the mass of the particle m_p. Their numerical results were compared with the experimental data of Papavergos and Hedley (1984) and with the analytic relation by Wood (1981). A good agreement between the results and the experimental data was observed. For $d_p > 10\,\mu\mathrm{m}$ the effect of particle rebound becomes noticeable when using different values of the restitution coefficient. Additionally, for particles larger than $10\,\mu\mathrm{m}$ a lower deposition velocity was observed when increasing the restitution coefficient.

In the framework of the present study the hard-sphere model is employed. However, this approach originally does not include the particle–wall adhesion. Kosinski and Hoffmann (2009) extended the standard hard-sphere model taking the particle–wall adhesive force into account. In their model, they distinguished between the repulsive and the adhesive impulse during a collision. For the determination of the adhesive impulse they did not estimate the times of the compression and the restitution phase during which the adhesive force acts. Instead, they assumed a constant force acting over a certain range of surface separation, namely from a surface separation δ_1, at which the van-der-Waals interaction can be neglected, to a minimum separation distance δ_0. The force corresponds to a spatially averaged mean value of the van-der-Waals force over these surface separations. Based on the Hamaker constant, the restitution coefficient and the above mentioned variables the maximum initial velocity $v_{p,n}^{*,KH}$ leading to deposition was estimated. It should be also noted that analog to the energy-based model by Dahneke (1971) the limiting velocity $v_{p,n}^{*,KH}$ is proportional to $1/d_p$ and is constant for a given material and size of the particles. Kosinski and Hoffmann (2009) carried out a simple test using their model with one particle colliding with a wall to show the influence of the adhesion on the collision process. However, their predictions were not validated at all.

Breuer and Almohammed (2015) and Almohammed and Breuer (2016) developed two techniques (momentum-based and energy-based model) for the prediction of the agglomeration process due to particle–particle collisions in turbulent flows. Both models were validated in a simple shear flow and a particle-laden turbulent vertical channel flow. However, in both studies the influence of the particle–wall adhesion was not taken into account.

The aim of this work is therefore to develop a methodology for modeling the adhesion of dry, electrostatically neutral particles on the walls (i.e., by the van-der-Waals force). The developed momentum-based model is borrowed from the corresponding agglomeration model. Thus, the main difference between the model of Kosinski and Hoffmann (2009) and the approach presented in this study is the modeling strategy of the adhesive impulse and the deposition condition. In the new model the adhesive impulse is determined by taking the compression and the restitution phase separately into account leading to different effects on