International Journal of Multiphase Flow 72 (2015) 39–52

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

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

Forces on micron-sized particles randomly distributed on the surface of larger particles and possibility of detachment

Yan Cui, Martin Sommerfeld *

Mechanische Verfahrenstechnik, Zentrum für Ingenieurwissenschaften, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany

ARTICLE INFO

Article history:
Received 21 August 2014
Received in revised form 20 January 2015
Accepted 22 January 2015
Available online 31 January 2015

Keywords:
Dry powder inhaler
Carrier particles
Carrier covered with drug powder
Flow about the particle cluster
Lattice-Boltzmann Method
Fluid forces on drug particles
Probability of drug detachment

ABSTRACT

Numerical calculations based on the Lattice-Boltzmann method were performed for a particle cluster consisting of a large carrier particle covered with small spherical drug particles which were exposed to a constant velocity air flow. Prior to these studies, the simulations were validated based on a test case where a single particle is situated on a plane wall and exposed to a linear shear flow. The present simulations were compared with analytical results and other simulations. Moreover, the required small particle resolution and the domain size were properly selected based on an extensive numerical study. The diameter of the carrier particles was 100 μm, while the fine particles had diameters of 3 μm and 5 μm, respectively. The range of Reynolds numbers considered was between 1 and 200. Moreover, the coverage degree of the carrier by the small particles was varied in the simulations between 10% and 50%, and this influence on the detachment was determined. From these simulations the fluid dynamic forces on the drug particles were extracted in dependence of the angular position in order to estimate the possibility of drug particle detachment. Detachment might occur through lift-off, sliding or rolling. Lift-off was found to be not possible due to the acting small normal forces even at $Re = 200$. The probability of sliding and rolling detachment in dependence of the angular position was estimated based on measured adhesion properties, i.e. van der Waals force, adhesion surface energy and friction coefficient. With these studies it is aimed to understand drug particle detachment from carrier particles in an inhaler device as a basis of modelling and optimising dry powder inhalation.

Introduction

The detachment or re-suspension of particles from surfaces is quite a very old problem since it is related to numerous natural, technical and industrial applications. The earlier work is mainly affiliated to soil transport by wind and in rivers. Industry related applications include the wide area of powder handling processes where deposited powders need to be re-suspended from walls (e.g. pneumatic conveying, electrostatic precipitators or filtration), cleaning of electronic devices, silicon wafers and computer hard disks. The present work concerns a problem in pharmaceutics where dry powder inhalers (DPI) for pulmonary drug delivery are being increasingly utilised in medical treatment, as for example in asthma therapy. In that case however, the powder particles should be in the size range between 1 and 5 μm in order to ensure their transport up to the pulmonary alveoli during a breathing period. Due to their inertia, larger particles would already deposit in the upper parts of the respiratory system (Kleinstreuer and Zhang, 2010). Unfortunately, the required fine powders are very cohesive and consequently hardly dispersed in an air stream. Therefore, the fine drug powder is blended with larger carrier particles (typically in the size range of 50–100 μm) in a mixer for producing carrier particles coated with the fine drug particles. Accordingly, this larger powder can be much easier dispersed from the reservoir of an inhaler by the breathing air-stream. For achieving high drug delivery efficiency, the drug particles have to be again detached from the carrier within the inhaler device through the stresses in the air flow or collisions with the device walls or a grid which is quite often used (Telko and Hickey, 2005). As a result, the dispersed fine drug particles can be easily transported deep into the lung while the carrier particles remain in the inhaler or are deposited in the upper airways and thereafter naturally cleared. The detachment of the drug powder in the rather complex airflow of an inhaler is brought about by acceleration and deceleration of the carrier (i.e. inertial force), shear gradients in the flow and turbulent stresses (Frijlink and de Boer, 2004). Therefore, delivering a high

* Corresponding author.
E-mail address: martin.sommerfeld@iw.uni-halle.de (M. Sommerfeld).

http://dx.doi.org/10.1016/j.ijmultiphaseflow.2015.01.006
0301-9322/

drug particle fraction requires a proper balancing between the adhesive forces and the removal forces during the inhalation process. The strength of the van der Waals forces may be adapted by modification of the carrier surface, for example through surface roughness (Flament et al., 2004). However, the strength of the detachment forces in an inhaler is very difficult to evaluate experimentally. Normally, the integral drug delivery efficiency by the inhaler is obtained only as a basis to optimize inhaler design (Telko and Hickey, 2005). Hence, the detachment of fine drug powder from a carrier particle by fluid dynamic stresses is a special problem of particle detachment from surfaces.

Because of its huge importance, the detachment of fine particles from surfaces, especially in turbulent flows, was already examined for many years, mainly theoretically and experimentally (e.g. Reeks et al., 1988; Wen and Kasper, 1989; Soltani and Ahmadi, 1994; Phares et al., 2000; Ibrahim et al., 2008). Since several years also fully resolved direct numerical simulations (DNS) are being used for determining lift and drag forces acting on single particles attached to a wall (Sweeney and Finlay, 2007; Zeng et al., 2009; Larsen et al., 2010). In these studies laminar shear or boundary layer flows are considered mostly. From their simulations Sweeney and Finlay (2007) proposed complex fitting curves for the drag (C_D) and lift (C_L) coefficients in dependence of the particle Reynolds number (determined with the centre velocity impinging the sphere). In the work of Zeng et al. (2009) also the situation of a sphere touching the wall was considered and they presented the non-dimensional lift force as a function of the particle Reynolds number determined with the particle radius and the friction velocity. Their own simulations as well as a proposed correlation were compared with several analytical results and also experiments for Reynolds numbers between 1 and 10. More recently Derksen and Larsen (2011) calculated the fluid dynamic forces on random assemblies of particles attached to a plane wall using the Lattice-Boltzmann Method (LBM) combined with an immersed boundary method. These studies were performed for a plane shear flow at low Reynolds numbers. One important finding of this study is the drastic reduction of the drag and lift force with increasing occupancy of the wall with particles. The reason for that is the tendency of the flow to pass over all the fine particles at high surface occupancy. The values for the lift actually become close to zero for coverage degrees of more than 40%.

In order to assess the fluid forces on fine drug particles attached to a larger carrier the Lattice-Boltzmann Method (LBM) is applied for simulating flows about the particle cluster (i.e. carrier particle and hundreds of drug particles) fully resolved by the numerical grid. The present work is restricted to laminar plug flow only. From these simulations the flow conditions required to detach the drug particles are evaluated.

The present article is organised in the following way. First the principles of the LBM are briefly outlined including the methods employed for enhancing the spatial resolution of the LBM, namely curved wall boundary condition and local grid refinement. Special emphasis is put on calculating the fluid dynamic forces on two particles separately which are in close contact. Then the present simulations are validated by comparing simulated lift and drag coefficients for a particle in contact with a plane wall with analytic results, experiments as well as other simulations. For the special case of a larger carrier covered with hundreds of micron-sized particles studies on the required domain size and the necessary resolution of the fine particles are introduced. Then the calculated fluid dynamic forces acting on the drug particles are analysed and discussed in detail for a range of relevant properties of the particle cluster and the flow. Finally, the possibility of drug particle detachment is evaluated on the basis of experimental information for particle-particle interaction mechanisms.

Numerical method

For the present flow simulations the Lattice-Boltzmann Method (LBM) is adopted and further developed (Dietzel et al., 2011). Instead of solving conservation equations for macroscopic properties as done by using the Navier-Stokes equations, the discrete Boltzmann equation is solved, describing the fluid behaviour on a mesoscopic scale. Thereby the change of the probability distribution function, which describes the number of fluid elements having the velocity v at the location x and at time t, is solved to simulate the flow of a Newtonian fluid. Hence, besides the spatial discretization realised by the numerical grid, time and particle velocities are discretized as well. Information is allowed to propagate to a neighbouring lattice node in one of the discrete lattice directions only at one time step, followed by a collision step.

Lattice-Boltzmann method

In the following a brief outline of the applied LBM is given. The discretized Lattice Boltzmann equation combined with a single relaxation time collision operator approximated by the BGK (Bhatnagar–Gross–Krook, Bhatnagar et al., 1954) approach is given below:

$$f_{\sigma i}(\mathbf{x}+\boldsymbol{\xi}_{\sigma i}\Delta t, t+\Delta t) - f_{\sigma i}(\mathbf{x},t) = -\frac{\Delta t}{\tau}\left(f_{\sigma t}(\mathbf{x},t) - f^{(0)}_{\sigma i}(\mathbf{x},t)\right) \tag{1}$$

where $\Delta x = \boldsymbol{\xi}_{\sigma i}\Delta t$ is the width of the spatial discretization, Δt the duration of one time step and τ the relaxation time. The discrete equilibrium distribution function is given by:

$$f^{(0)}_{\sigma i}(\mathbf{x},t) = \omega_{\sigma i}\rho\left(1 + \frac{3\xi_{\sigma i}\mathbf{u}}{c^2} + \frac{9(\xi_{\sigma i}\mathbf{u})^2}{2c^4} - \frac{3\mathbf{u}^2}{2c^2}\right) \tag{2}$$

In this work the D3Q19 model for 3 dimensions and 19 discrete velocity directions is used as shown in Fig. 1. Hence, $\omega_{\sigma i}$ are the weighing factors of this model, $c = \Delta x/\Delta t$ is the grid constant and $\boldsymbol{u}$ is the velocity vector.

Fluid density ρ and momentum can be obtained from moments of the discrete distribution functions in the following way:

$$\rho(\mathbf{x},t) = \sum_{\sigma}\sum_{i} f_{\sigma i}(\mathbf{x},t) \tag{3}$$

$$\rho(\mathbf{x},t)\mathbf{u}(\mathbf{x},t) = \sum_{\sigma}\sum_{i} \boldsymbol{\xi}_{\sigma i} f_{\sigma i}(\mathbf{x},t) \tag{4}$$

For allowing a proper resolution of all relevant scales, a multigrid method is integrated into the numerical code as illustrated in Fig. 2 (Dietzel and Sommerfeld, 2010, 2013). The purpose is to

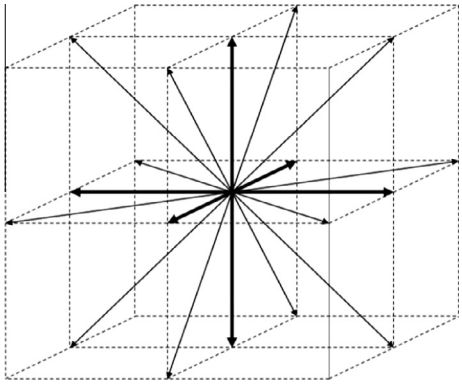

Fig. 1. Discrete velocity directions of the D3Q19 model.