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Effect of correcting near-wall forces on nanoparticle transport in a microchannel

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ABSTRACT

This paper studies the importance of corrections that account for the presence of walls on the forces acting on nanoparticles during their transport in microchannels. Theoretical and experimental investigations have reported anisotropic and hindered motion of nanoparticles near a microchannel wall. To investigate the influence of the near-wall effects, various conditions were examined. In particular, computer simulations were performed with and without the near-wall correction of forces. The corresponding capture efficiency and the average penetration of the captured nanoparticles were compared, and the importance of the near-wall corrections was assessed. Effects were evaluated for the nanoparticle diameter, the channel width, the channel length, and the pressure gradient. The results indicate that the inclusion of wall effects is crucial for the analysis of nanoparticle transport in microchannels.

1. Introduction

Since the introduction of the first microfluidic devices, these miniaturized fluidic manipulation systems have been regarded as one of the most promising technologies of the late twentieth century. Studies of microfluidic devices have attracted many researchers from a variety of disciplines.

Two-phase gas–solid flows have been studied extensively in macro-sized systems due to their numerous industrial applications. Generally, computational modeling of gas–particle flows can be performed in either Eulerian or Lagrangian frameworks. Implementation of these methods generally depends on the particle concentration and the importance or the simplicity of the particle tracking. It is obvious that the size of the particles can be one of the most important parameters for the physics of such flow. Ahmadi (2009a, 2009b) and Tu, Inthavong, and Ahmadi (2013) have provided an extensive review on nanoparticle transport flow in a macroscopic geometry.

Analytical investigation indicates a variation in the flow patterns near particles, depending on whether they are in the bulk or wall region of a channel, resulting in a non-homogenous drag force and the diffusion of nanoparticles near a wall. These effects result in the enhancement of the drag coefficient and a hindering of diffusion. The fundamental theories of these processes were established a long time ago (see Brenner, 1961; Goldman, Cox, & Brenner, 1967a, 1967b). Recently, this non-homogenous effect has been explored experimentally via different particle-tracking methods, such as evanescent wave microscopy, 3-D R-TIRFM (total internal reflection fluorescence microscope; see Banerjee & Kihm, 2005; Huang, Guasto, & Breuer, 2009; Kihm, Banerjee, Choi, & Takagi, 2004).

Some researchers have investigated the wall effects on flow characteristics in macrochannels. Ounis, Ahmadi, and McLaughlin (1993) analyzed the transport and the deposition of Brownian particles in a turbulent channel flow. Fukagata, Zahrai, Bark, and Kondo (1999) considered turbulent channel flow with 70-μm copper particles. They indicated that wall effects have a strong influence on the particle statistics. Zhang and Ahmadi (2000) simulated particle deposition in a vertical duct in the turbulent flow regime using a one-coupling assumption. In addition, Arcen, Tanière, and Oesterlé (2006) undertook the computation of turbulent dilute gas–solid channel flow. They studied the influence of using wall-corrected drag coefficients and a lift force on the dispersed phase characteristics. Their results indicated that the lift and the drag force corrections do not lead to significant changes in the statistical properties of the solid phase, with the exception of some statistics for the high-inertia particles. Nasr, Ahmadi, and McLaughlin (2009) studied four-way-coupled two-phase flows, including the effects of particle collisions in turbulent duct flows. They included the

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wall-correction effects on the drag and the lift forces acting on the particles, in addition to the damping effects of particles on turbulence. Tian and Ahmadi (2007) discussed the limitations of the commercial code for analyzing the nano- and microparticles in duct flows.

The transport of nanoparticles in micro-sized channels has many applications, such as the flow in pulmonary passages, micro-sized fluidized bed, micro-reactors, micro mixers, and filters (Tu et al., 2013). Generation and handling of nanoparticles is, in principle, feasible for microchannels (Kockmann, Dreher, Engler, & Woias, 2008). Kockmann et al. (2008) investigated the application of T-shaped micromixers for the generation of nanoscale aerosols by mixing hot vapor–gas mixtures with cold gas. Huang, Lai, and Lin (2006) conducted an experiment by developing a microfluidic chip that is capable of generating relatively uniform micro-droplets. The device can actively control the droplet diameter in addition to being a low-cost process with high throughput. Kwon et al. (2009) and Kim, Park, Hwang, and Kim (2008) proposed a size classification system for airborne particles for air-based labs-on-a-chip using a micro-machined electrical mobility analyzer. Luo, Du, Wang, Lu, and Xu (2011) provided an extensive review on the controllable preparation of nanoparticles in a microchannel. In addition, one potential attraction for industrial applications of aerosol processing in micro-reactors is the necessity to minimize the internal particle deposition. The large surface-to-volume ratio that is advantageous in many applications demands special attention for controlling unwanted particle deposition on the microchannel walls (Heim, Wengeler, Nirschl, & Kasper, 2006). Increasing the deposition can also be desired for certain applications such as filtration.

Akhatov, Hoey, Swenson, and Schulz (2008a, 2008b) conducted a combined theoretical and experimental study and illustrated the focusing influence of the Saffman lift force in the fluid dynamics of aerosol flows through micro-capillaries. They concluded that, under the proper conditions, the lift force causes the migration of nanoparticles toward the centerline of the capillary and should be considered for the design of an effective aerosol-focusing apparatus. Tavakoli, Mitra, and Olfert (2011) studied the aerosol penetration in a microchannel using the Eulerian framework. They investigated the effect of a non-zero concentration of nanoparticles at the wall, which was reported by Gallis, Torczynski, and Rader (2008). They concluded that the nanoparticles will stick to the wall and that a zero-concentration boundary condition is sufficiently accurate. Furthermore, they reported that the aerosol penetration decreases in the slip flow regime. Sinha, Ganguly, De, and Puri (2007) theoretically and experimentally tracked a magnetic particle in a microchannel in distilled water by considering the magnetic and the drag forces. Sbrizzai, Faraldi, and Soldati (2005) investigated the behavior of diesel soot particles in the microchannels of a porous-ceramic particulate filter. They included the Knudsen number and the Brownian force effect in their simulation on the deposition of particles. Zheng and Silber-Li (2009) experimentally studied the lift force acting on nanoparticles near a wall in a microchannel. They concluded that the lift force is significant in the range of two to six times the diameter of the nanoparticles from the wall. Afshar, Shams, Nainian, and Ahmadi (2009) studied the dispersion of nanoparticles under the Saffman lift, Brownian, drag, and gravity forces in a microchannel. They evaluated the nanoparticle deposition as a function of the pressure drop and the nanoparticle diameter. Using an Eulerian approach, Chatterjee, Bhattacharjee, and Mitra (2012) analyzed the particle transport and deposition on the microchannel walls under the effects of surface chemical heterogeneity. Perry and Kandlikar (2006) investigated the process of particulate fouling in microchannels. They considered particles with diameters of 3–10 μm. Wu, Kuznetsov, and Jasper (2010) analyzed the filtration efficiency in electrically charged monolith filters using the slip flow regime. Moreover, Basirat Tabrizi, Kamyar, Mansoori, and Saffar-Avval (2010) investigated the slip effect on particle transport in a minichannel by considering only the drag force.

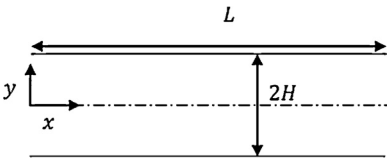

Fig. 1. Schematic of the geometry and the parameters of a microchannel.

The presented literature survey indicates that the wall effects on the transport and the deposition of nanoparticles in microchannels are not fully understood. Because of the importance of wall effects at the microscale, it appears likely that the wall corrections for forces are even more important in nanoparticle transport in microchannels. Therefore, in this study, the effects of wall presence on the drag force and consequently the Brownian force acting on nanoparticles were examined. A series of numerical computer simulations were performed with and without the near-wall force corrections. The corresponding capture efficiencies and the average penetrations of nanoparticles were compared.

2. Analysis

For the investigation of the wall effects, we only consider a simple geometry and flow to reduce the computational error. Therefore, we consider an incompressible, fully developed 2-D flow between two parallel plates with a channel width of 2H, as shown in Fig. 1. The Eulerian–Lagrangian approach is used for modeling the carrier fluid and the dispersed phase. For a dilute particle concentration, a one-way coupling assumption is made, indicating that the fluid carries the particle, but the effect of the particles on the fluid flow is negligible.

Two Knudsen numbers characterize the physics of the nanoparticle transport in microchannels. The channel Knudsen number is defined as $Kn_{\mathrm{ch}} = \lambda/(2H)$, where λ is the gas mean free path, which reflects rarefaction effect of the gas flow in the microchannel, and the particle Knudsen number is defined as $Kn_{\mathrm{p}} = 2\lambda/d_{\mathrm{p}}$, where d_{p} is the particle diameter, which accounts for rarefaction of the flow around the nanoparticles. Generally $Kn_{\mathrm{ch}} < 0.001$ and $0.001 < Kn_{\mathrm{ch}} < 0.1$ correspond to the continuum and the slip regimes, respectively (Kandlikar, Garimella, Li, Colin, & King, 2006).

Considering rarefaction in a microchannel in the slip regime, the velocity profile is given as (Kandlikar et al., 2006):

$$U_{\mathrm{f}}^{x} = \frac{-1}{2\mu_{\mathrm{f}}}\frac{dP}{dx}H^2\left(1-\left(\frac{y}{H}\right)^2+4Kn_{\mathrm{ch}}\left(\frac{2-\sigma}{\sigma}\right)\right), \qquad (1)$$
$$U_{\mathrm{f}}^{y} = 0.$$

Here, μ_{f} is the gas viscosity, P is the pressure, and σ is the tangential momentum accommodation coefficient. It is assumed that $\sigma = 1$ for the diffusive-like reflection approximation.

2.1. Forces acting on the nanoparticles

The important forces that act on nanoparticles are the drag, Saffman lift, Brownian, van der Waals (vdW), and gravity forces.