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Numerical study of aerosol particle deposition in simple and converging–diverging micro-channels with a slip boundary condition at the wall

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ABSTRACT

The design of micro-devices involving aerosol transport requires the study of the deposition of aerosols in micro-channels. In this study, the slip and no-slip boundary conditions for the gas flow regime were applied to the Navier–Stokes equations to obtain the particle deposition in simple and converging–diverging micro-channels. The equation of particle motion included inertial, viscous, Brownian, and gravity terms. It was found that the ratio of gravity to inertial effects controls the deposition of particles with diameters of 0.1–1 μm, and the ratio of diffusion to inertial effects controls the deposition of particles with diameters of 0.01–0.001 μm. Comparison between the no-slip and slip flow regimes showed that the deposition of 0.1- to 1-μm-diameter particles was less and the deposition of 0.01- to 0.001-μm-diameter particles was greater for the slip flow regime. There was no significant difference between slip and no-slip flow regimes for the deposition of 0.01- to 0.1-μm-diameter particles. Finally, it was shown that the stagnated gas in the corners of the converging–diverging micro-channel produced similar gas velocity profiles under the slip and no-slip flow regimes.

1. Introduction

Micro-devices can produce, separate, or analyze aerosol particles since the size of micro-channels is on the order of that of aerosol particles (Gawad, Schild, & Renaud, 2001; Khan, Gunther, Schmidt, & Jensen, 2004; McClain, Culbertson, Jacobson, & Ramsey, 2001; Nisisako, Torii, & Higuchi, 2004; Pamme, Koyama, & Manz, 2003; Sugiura, Nakajima, Itou, & Seki, 2001). Additionally, there are new medical and industrial processes that include aerosol transport and demand investigation of the penetration of aerosols in micro-channels. Interest in micro-scale penetration of aerosols has thus increased.

Various aerosol penetrations have been studied, but there have been few studies relating to micro-channels. Heim, Wengeler, Nirschl, and Kasper (2006) used a T-shaped micro-mixer to mix aerosols and a gas stream to determine particle penetration inside walls under various conditions. Yamada, Nakashima, and Seki (2004) proposed an empirical method with which to separate particles by size in a pinched micro-channel and a micro-channel with a rectangular cross-section. Takagi, Yamada, Yasuda, and Seki (2005) presented another method with which to separate particles using an asymmetrically arranged multiple-branch micro-device. This method can separate nonspherical biological substances, such as blood cells. Another medical investigation was carried out by Leslie, Domansky, Hamilton, Bahinski, and Ingber (2011) in aerosol drug delivery for the lung on a chip.

Liu and Nazaroff (2001) modeled the proportion of particles and reactive gases penetrating through building envelopes, as air enters through cracks and wall cavities. This model was developed for steady-state air flow penetrating idealized rectangular smooth surface cracks. In another work, they experimentally measured the particle penetration through surrogates of cracks in building envelopes (Liu & Nazaroff, 2003). Xu, Liu, and Zhu (2010) obtained the particle penetration as a ratio of the downstream to upstream ultrafine particle concentrations across seven idealized cracks. They concluded that the crack length and height and the pressure drop across the cracks affected the particle penetration. Zhao, Chen, Yang, and Lai (2010) presented three approaches to predict coefficients of particle penetration through a single straight crack in building envelopes. Tavakoli, Mitra, and Olfert (2011) analytically studied the particle penetration through rectangular and cylindrical micro-channels. The particle penetration varied with the dimensionless deposition factor and Knudsen number (Kn) of

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List of symbols

C_C	Cunningham correction to Stokes drag law, defined as $C_C = 1 + (2\lambda/d_P)(1.257 + 0.4e^{\left(-\frac{1.1d_P}{2\lambda}\right)})$
d_{ij}, d_{ik}	deformation tensors
d_P	particle diameter (m)
EC	Eckert number
F_B	Brownian force (N)
F_D	drag force (N)
F_L	lift force (N)
g_y	acceleration due to gravity (m/s^2)
k	constant ($k = 2.594$)
k_B	Boltzmann constant
n	direction normal to the flow direction near the wall
P	pressure (Pa)
S_0	spectral intensity defined as $S_0 = (216\nu k_B T)/(\rho\pi^2 d_P^2 C_C(\rho_P/\rho)^2)$
s	flow direction near the wall
T	temperature (K)
t	time (s)
U	gas velocity in the x direction (m/s)
U_{in}	inlet gas velocity in the x direction (m/s)
U_P	particle velocity in the x direction (m/s)
U_s	tangential gas velocity in the flow direction (m/s)
U_w	wall velocity (m/s)
V	gas velocity in the y direction (m/s)
V_P	particle velocity in the y direction (m/s)
μ	gas viscosity (kg/m^2 s)
ρ	fluid density (kg/m^3)
ρ_P	density of the particle (kg/m^3)
γ	the ratio of specific heats of fluid
ν	gas kinematic viscosity (m^2 s)
ξ_0	zero-mean, unit-variance-independent Gaussian random number
σ_v	cumulative momentum coefficient

the gas. They used the Navier–Stokes standard theory for the continuous regime of gas flow with $Kn = 0.01$–0.1.

The gas flow regimes for each range of the Knudsen number are defined as continuous for $Kn = 0$–0.001, slipping for $Kn = 0.001$–0.1, transition for $Kn = 0.1$–1, and molecular free transfer for $Kn = 1$–∞ (Karniadakis, Beskok, & Aluru, 2005). Therefore, the gas velocity distribution must be calculated by the Navier–Stokes equation with the Maxwell equation as the slip boundary condition (non-zero gas velocity) at the walls, in the 0.01–0.1 Knudsen number range. In the present study, this modeling procedure for aerosol deposition in a simple micro-channel and a converging–diverging micro-channel is described. The converging–diverging micro-channel is modeled for its likeness to the pores of porous solids.

2. Modeling

A finite volume method of computational fluid dynamics based on the SIMPLE algorithm was used for two-dimensional modeling of the flow field in micro-channels with smooth walls. The simple and converging–diverging micro-channels were meshed using rectangular elements and the corners of the converging–diverging micro-channel were meshed using a combination of rectangular and triangular elements. A smaller mesh size was used near the walls for greater accuracy. The mentioned mesh comprised approximately 30,000 nodes that were checked for grid independency. The motion of aerosol particles in micro-channels was modeled using the Lagrangian method. Spherical aerosol particles with diameters of 0.001–1 μm were injected through simple and converging–diverging two-dimensional micro-channels having hydraulic diameters of 50 μm and lengths of 2500 μm. The inlet velocity of the air flow was considered to be 0.006 m/s ($Re = 0.02$). Fig. 1 schematically shows the simple and converging–diverging micro-channels. The aerosol particle fraction in the air flow varied with position and time. Gravitational, Brownian, and lifting forces acted on the aerosol particles in each micro-channel.

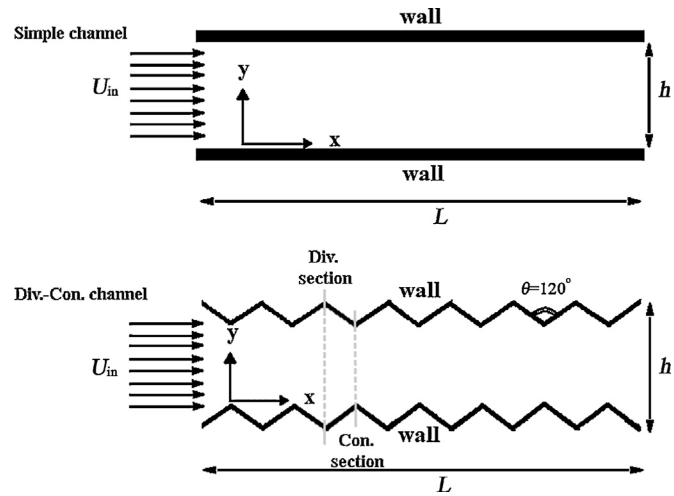

Fig. 1. Schematic diagrams of simple and converging–diverging micro-channels.

The gas velocity at the wall was considered to be nonzero because the gas flow in the micro-channel was in a slip regime ($Kn = 0.001$–0.1). The entrance length was neglected in the micro-channel. Therefore, it was assumed that flow in the channels was incompressible and fully developed (Duan & Muzychka, 2010). The steady-state continuity and Navier–Stokes momentum equations were needed to simulate the flow field. These equations for incompressible flows are (Batchelor, 1967)

$$\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0, \tag{1}$$

$$\rho\left(U\frac{\partial U}{\partial x} + V\frac{\partial U}{\partial y}\right) = -\frac{\partial P}{\partial x} + \mu\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right), \tag{2}$$

$$\rho\left(U\frac{\partial V}{\partial x} + V\frac{\partial V}{\partial y}\right) = -\frac{\partial P}{\partial y} + \mu\left(\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2}\right) + \rho g_y. \tag{3}$$

The boundary condition applied to the micro-channel wall was a first-order slip condition, which was presented by Maxwell as (Karniadakis et al., 2005)

$$U_s - U_w = \frac{Kn(2-\sigma_v)}{\sigma_v}\frac{\partial U_s}{\partial n} + \frac{3Kn^2 Re(1-\gamma)}{EC}\frac{\partial T}{\partial s}. \tag{4}$$

The cumulative momentum coefficient (σ_v) indicates the fluid–surface interplay. The second term of this equation relates to the fluid creepage on the wall. This term is zero for incompressible fluids under the isothermal condition. The particles were uniformly dispersed at the inlet of the channel ($x = 0$) and entered the channel with the inlet gas velocity. It was assumed that a particle was deposited if its distance from the wall was equal to its radius. The force balance on the aerosols in the Lagrangian method is defined as (Torby, 1984)

$$\frac{dU_P}{dt} = g_y\frac{\rho_P - \rho}{\rho} + F_D(U - U_P) + F_B + F_L. \tag{5}$$