TRANSPORT AND DEPOSITION OF SPHERICAL MICROPARTICLES WITH SINGLE-SHELL IN A 90 DEGREE BEND

by

Zhen-Hua CHEN[a]***, Kai ZHANG***[b*]***, Xiao-Fei LV***[c]***,***
Yan-Hua XING[b]***, and Hong JIANG***[b]

[a] Zhejiang-California International NanoSystems Institute, Zhejiang University, Hangzhou, China
[b] Department of Mechanics, China Jiliang University, Hangzhou, China
[c] China REACH Solution Center, Hangzhou CIRS Co. Ltd., Hangzhou, China

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Theoretical investigation on particle transport in a 90 degree bend was carried out. The finite volume method was used to simulate the flow field in the bend pipe, and one-way coupled Lagrangian method was used to calculate the trajectory and deposition efficiency of microparticles. The unique relationship between the irreversible deposition efficiency and radius ratio of single-shell microparticle was given finally.

Key words: *single-shell model, radius ratio, cm factor, deposition efficiency, dielectrophoresis*

Introduction

Large number of microparticles used in various industries always exists with one shell. For example, some kinds of particles which are used in dry electrophotographic marking are specially dealt with different compounds to improve flow ability, and many microparticles used in granular bed filters are covered with the material that they are filtered to show their changes of electric and dielectric properties [1]. In other cases, bioparticles always have mutiple structures [2], for example, cell consists of outer cell wall, membrane, and cytoplasm layer, *etc*. Therefore, single-shell model based on the effective moment method was proposed to solve those problems, which can be easily adapted to computational modeling comparing to effective moment method [3]. In a microchannel, when particles are transported by electrokinetic flow, under the effect of both the hydrodynamic and electric forces, a large number of microparticles will deposit in the bend and separated [4]. Microparticle's deposition efficiency (*DE*) is a crucial factor for its relevance to sample handling [5], such as separation of particles and surface fouling. Unlike the classic dipole moment method, the single-shell model is more suitable for the study of transport and deposition of particles with multiple layers.

Computational model

Microparticle with single-shell is shown in figure 1(a) in a 90 degree bend, which is filled with aqueous solution as shown in fig 1(b). The effective moment method is usually

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[*] Corresponding author; e-mail: zkzb3026@cjlu.edu.cn

used for transport of spherical particles without shell in the dielectrophoresis (DEP). However, for microparticles with shells the DEP model should be modified.

As shown in fig. 1(a), r_1 and r_2 are the radius of the outer and inner layers of the microparticle, respectively, and single-shell microparticle's radius ratio $\beta = r_1/r_2$. σ_1 and σ_2 are the outer and inner conductivity of the microparticle, and σ_m is the conductivity of the electrolyte solution.

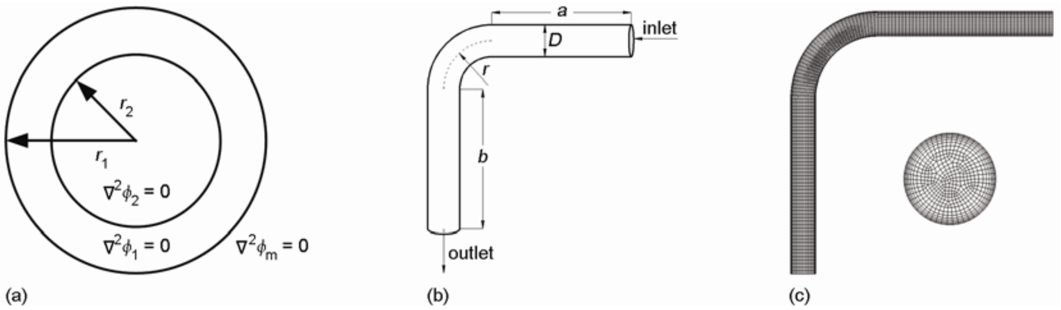

Figure 1. (a) Schematic of the single-shell model, (b) geometry, (c) mesh of the 90 degree bend pipe

The density of the microparticle $\rho_p = 1550$ kg/m^3, particle zeta potential $\zeta_p = 0.032$ V. In addition, it is assumed that specified water is used as the electrolyte solution, and its physical properties are given by relative permittivity $\varepsilon = 80$, permittivity of the vacuum $\varepsilon_0 = 8.85\cdot10^{-12}$ CV^{-1}m^{-1}, viscosity of the solution $\mu = 1.003\cdot10^{-3}$ kgm^{-1}s^{-1}, wall zeta potential $\zeta_w = -0.02$ V, density of the electrolyte solution $\rho = 998.2$ kg/m^3.

For steady and incompressible flow, those dimensional governing equations are [6]:

$$\rho(\vec{V}\nabla)\vec{V} = -\nabla p + \mu\nabla^2\vec{V} + 2n_\infty ze\sinh\frac{ze\varphi}{k_bT}\nabla\phi \tag{1}$$

$$\nabla^2\varphi = -\rho_e/\varepsilon\varepsilon_0, \quad \nabla^2\phi = 0, \quad \rho_e = -2n_\infty ze\sinh\frac{ze\varphi}{k_bT} \tag{2}$$

Particle transport equation can be written as:

$$\frac{d\bar{u}^p}{dt} = \vec{F}_{DEP} + \vec{F}_{EP} + \vec{F}_w + \vec{F}_D + \vec{F}_g$$

The formula described here involves electrokinetic and hydrodynamic forces. The DEP force $\vec{F}_{DEP}$ that exerted on a spherical for homogeneous body suspended in a local electric field is expressed as:

$$\vec{F}_{DEP} = \frac{2\pi r_p^3\varepsilon_m Re[K(w)]\nabla\vec{E}^2}{m_p} \tag{3}$$

where r_p is the particle radius, m_p – the particle mass, ε_m – the permittivity of the suspending medium, ∇ – the Del vector (gradient) operator, $\vec{E}$ – the electric field, $Re[K(w)]$ – the real part of the Clausius-Mossotti (CM) factor, for direct-current DEP, CM can be given by:

$$K(w=0)=\frac{(1-\chi)\beta^3+\alpha(2+\chi)}{(1+2\chi)\beta^3+2\alpha(1-\chi)} \tag{4}$$

where $\alpha=(\sigma_2-\sigma_1)/(\sigma_2+2\sigma_1)$, $\chi=\sigma_\mathrm{m}/\sigma_1$. Other expressions for electrophoretic force $\vec{\mathrm{F}}_\mathrm{EP}$, drag force $\vec{\mathrm{F}}_\mathrm{D}$, gravity force $\vec{\mathrm{F}}_\mathrm{g}$, and repulsive force $\vec{\mathrm{F}}_\mathrm{w}$ have been listed in our group's previous research paper [6]. In addition, to ensure statistical independence, the mesh convergence and particle number independence tests are performed, fig. 1(c). The number of mesh used in numerical simulation shows that the discrepancy in velocity profiles is less than 1% when the mesh was further refined. The particle number of 20,000 could produce particle number independent simulation results.

Results and discussion

The CM factor $K(w)$ has relation with radius ratio of the microparticle, then the electric properties and the magnitude of DEP force depend on radius ratio of the microparticle. As shown in fig. 2, for a direct current electric field, the CM factor $K(w)$ varies from 0.7 to –0.4, as radius ratio β ranges from 1.01 to 1.64. When radius ratio β is less than 1.13, positive DEP (pDEP) makes the particle move towards the higher electric field because of $K(w) > 0$; When radius ratio β is more than 1.13, negative DEP (nDEP) makes the particle move towards the region with lower electric field because of $K(w) < 0$.

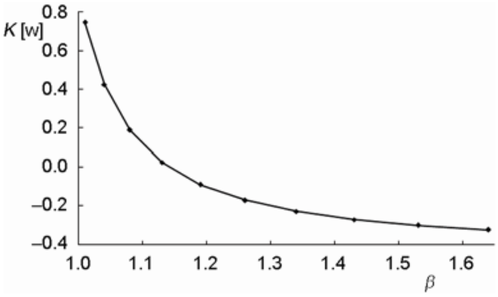

Figure 2. Schematic of the *K*(*w*)-*β* curves

In order to understand the regional particle deposition, *DE* in the bend is defined as $DE=N_\mathrm{d}/N_\mathrm{o}$, here N_0 is the number of particles entering and depositing in the 90 degree bend region, and N_d is the number of particles released from the inlet. As shown in fig. 3, the tendency of all *DE*–*β* curves seems similar. When β approaches 1.0, both $K(w)$ and *DE* have their maximum values, which causes a high pDEP force to make a large number of particles deposit in the inner of bend. Because the DEP force of the inner particle and DEP force of the outer particle have the same direction, the total DEP force reaches its maximum value and performs a maximum pDEP. After experiencing the maximum value, the *DE*–*β* curve decreases rapidly and reaches the minimum value. When β approaches 1.1 $K(w)$ decreases to zero, that causes the DEP force to become weak rapidly until it almost disappeared, and only few particles deposited in the bend. At the same time, the DEP force of the inner particle almost completely offsets the outer one, and then it shows a weak DEP force which causes a lower *DE* in the microchannel. However, as the radius ratio β grows continuously, the DEP force shows up again and increases until the curve develops to a middle value, because one of the DEP force of one particle only cancels part of another's. In addition, after β

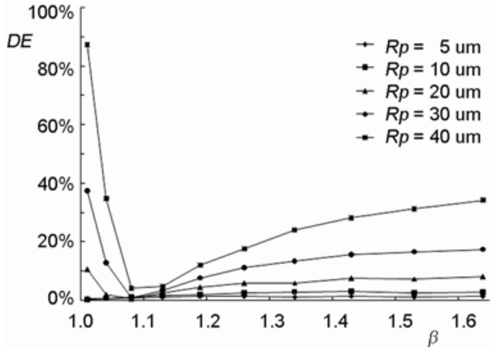

Figure 3. Schematic of the *DE*-*β* curves

gets its minimum value $K(w)$ becomes negative, and microparticles are repelled to deposit in the outer of the bend forced by the nDEP force.

As shown in fig. 3, *DE* ranges from 0.6% to 87.32% with the growth of the particle's diameter. In the microchannel flow, microparticles are usually forced to change its direction in the bend, for particles with same radius ratio but different diameters, it's difficult for larger microparticle to follow fluid and easier to deposit in the bend due to larger inertia. Furthermore, the electrokinetic forces can also change the particle's trajectory and enhance the *DE*, therefore, microparticles with the same radius ratio but different diameters perform different *DE*.

Conclusions

Modified single-shell model based theoretical and numerical investigation of electrokinetic transport and deposition of single-shell microparticles in a 90 degree bend were carried out. The finite volume method was used to simulate the flow field in the bend pipe and one-way coupled Lagrangian method was used to calculate the trajectory, and *DE* of microparticles. For specified radius ratio of microparticles, it was found that microparticles with larger diameters have higher *DE* in the microchannel due to its larger DEP force and hydrodynamic force; the DEP force ranges from positive to negative which causes the $DE–\beta$ curve experience a high-low-high process as the radius ratio of single-shell particle changes.

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