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Novel thermophoretic particle separators: Numerical analysis and simulation

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HIGHLIGHTS

- A novel technique and design is proposed for the separation of particles with different characteristics.
- Transport equations in a microchannel are solved numerically taking into account the thermophoresis force.
- Differences between thermophoresis in gases and liquids are demonstrated.

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ABSTRACT

In this paper, it is shown that thermophoresis is a viable method for precise particle separation (sieving) and manipulation in microchannels. To do so, thermophoresis force acting on particles suspended in air and water flowing in a microchannel heated from below are simulated and relative magnitude and difference of thermophoresis force acting on a particle in a gas and liquid is discussed, discerned and elucidated. To show the potential of thermophoresis to serve as a sieve, transport equations for suspension of polystyrene in water and gold particles in air are solved numerically, both in the absence and presence of gravity. In simulations, particles are considered as a discrete phase and their trajectories are tracked using a Lagrangian approach. It is shown that thermophoresis can be used to separate macromolecules and particles from a water stream in a microchannel with one inlet and two outlets. Also, it is demonstrated that thermophoresis can be used as a means to separate multiple particle streams with different characteristics such as size and density from a gas flowing in a microchannel. Two microchannel geometries were numerically analyzed and it is shown that in both cases particles with different sizes are forced to exit through a different outlets. This effect can be used to separate, concentrate, manipulate, trap, target and transfer macromolecules such as bio-molecules and DNA in a microchannel. The correct application of thermophoresis theory in a gas and liquid is elucidated throughout the simulations.

1. Introduction

Thermophoresis is a phenomenon that occurs in a non-isothermal mixture and during which suspended (non-Brownian) particles experience a force pushing them, usually, in the direction of the temperature drop. The carrier fluid could be a gas or liquid, although the effect is more profound in gases owing to the presence of weaker cohesive intermolecular forces. While the suspended particles could be micron or sub-micron sized, the effect has been studied extensively on micron sized particles. As particle size decreases, the Brownian forces become noticeable as well. In the limit when the size of the suspended phase approaches the molecular sizes, this phase simply mixes or dissolves in the carrier fluid and the phenomenon becomes similar to thermodiffusion, which is separation of two Brownian species as a result of a temperature gradient [1].

Thermophoresis in stagnant gases and liquids is a classic and fundamental physics problem, and has been extensively studied. It is also present in flowing fluids that experience a temperature gradient. Recently, nanofluids have been used for heat transfer augmentation in thermal systems, and thermophoresis has a significant role in such cases. We are investigating the contribution of thermophoresis in natural convection in nanofluids, which will be published in a separate paper. This work is focused on the dynamics and kinematics of fluid flow (gas and liquid) with suspended

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particles of the order of 1 μm in microchannels in the presence of a temperature gradient. A review of thermophoresis in stagnant gases and liquids and analytical derivation of an expression for thermophoresis velocity is found in Ref. [2]. While the general theory of thermophoresis as a fundamental and classic research area is established rather well, its effect in fluid flow and combined with convection in applied and engineering research has been overlooked resulting in contradicting, or redundant studies with misleading conclusions. In an attempt to identify the significance of thermophoresis and other forces in flowing systems, Buongiorno [3] studied the relative effect of seven phenomena that cause a slip motion between the main fluid and particles. These effects include inertia (drag), Brownian diffusion, thermophoresis, diffusiophoresis, Magnus effect, fluid drainage, and gravity. These forces may potentially impel the particles to move with velocities different from the velocity of the main flow. Based on a time scale analysis, it was concluded that in nanofluids, only thermophoresis and Brownian diffusion can cause slip. In the case of micron-sized particles, Brownian diffusion is less important, but gravity (weight and buoyancy) is an important force as well. The inertia effect is also the main force carrying the particles in the direction of the flow. Other forces may be present as well depending on the nature and condition of the flow and particles.

As stated above, this work is focused on the effect of thermophoresis in forced convection in flowing systems. Numerical and theoretical works on forced convection of particle-laden flows in conventional and microchannels are abundant, e.g., Refs. [4–21]. However, thermophoresis effect has been considered in very few works, and often inadequately. Tahir and Mital [11] used the correlation developed by McNub and Meisen [22] to account for thermophoresis, and the Stokes–Einstein formula for the Brownian diffusion of particles in a fluid flow. We have recently shown that the McNub and Meisen formula significantly overestimates the thermophoresis effect [23]. Application of this expression obscures the real contribution of thermophoresis. Bayat and Nikseresht [9] performed a numerical study on turbulent forced convection in nanofluids, assuming a single phase model linked with effective physical properties of nanofluids, neglecting slip effects such as thermophoresis. Duangthongsuk and Wongwises [10] developed an analytical expression for the estimation of heat transfer coefficient in a laminar flow. In their model, Brownian diffusion is considered but thermophoresis is neglected. Their results overestimate the experimental data. In an experimental and numerical work, He et al. [5], studied forced convection of a nanofluid in laminar flow in a miniature channel. In their numerical analysis, several effects such as thermophoresis was considered; however, the Talbot et al. [24] expression for thermophoretic force, which is applicable to gases only, was used to model thermophoresis of liquid nanofluids.

Liu et al. [13] studied the effect of thermophoresis on particle trajectory and sedimentation of nanoparticles in the flow in a microchannel, using a discrete phase model in the Fluent® software. They showed that applying a temperature gradient across the walls of a channel can balance the effect of the gravitational force on nanoparticles, thus preventing particle sedimentation within the channel. In their analysis, however, the Talbot et al. [24] expression was used, which is only valid for thermophoresis in gases and overestimates thermophoresis effect in liquids. Recently, Singh et al. [14] reported results, which are very similar or identical to those of Liu et al. [13]. In another study, flow and migration of alumina–water nanofluids in a channel was studied, considering all forces including thermophoresis; however, the Talbot expression was used again, which introduces errors to the calculations [16]. In a similar study, Coleman and Nnanna [17] studied nanoparticle deposition in nanofluid transport in a microchannel taking into account thermophoresis, Brownian motion, etc.

Application of temperature gradient in separation and manipulation of biological molecules and particles has been reported as well. Thamdrup et al. [18] worked on manipulation, movement and stretching of DNA molecules in microchannels by light-induced local heating of the carrier fluid. Maeda et al. [19] studied DNA manipulation, accumulation, folding and separation by thermophoresis. Geelhoed et al. [20] fabricated a thermophoretic separator in the form of a silicon microchannel. It was observed that 1.5 K temperature difference between the walls can effectively separate particles from the main stream. Vigolo et al. [21] also fabricated a microfluidic device in which polystyrene submicron spheres in NaCl were separated from the solution by thermophoretic forces. They also discussed various means such as varying the properties of the carrier liquid as well as temperature gradient for better control of the separation process. Thermal Field-Flow Fractionation (ThFFF), which is a well established technique for the separation of various macromolecules and particles such as polymers and living bacteria is another example of the application of a temperature gradient in particle or species separation. For instance, Janča et al. [25,26] have studied the role of shape of living bacteria in their separation, and Schimpf and Giddings [27] studied separation of polymer solutions all using the ThFFF.

In the light of above literature review and discussion, the objective of this work is defined as follows: First, given that erroneous expressions for thermophoresis have been used in the numerical simulations of convective liquid flows in channels, the best available expression or experimental data is introduced and used to perform numerical simulations to investigate the correct contribution of thermophoresis in microchannels. Second, owing to the capability of the temperature gradient in particle separation and the lack of numerical simulations, transport equations are solved numerically for several microchannel geometries to investigate separation of particles in gas and liquid flows.

2. Thermophoresis in gases and liquids

When a temperature field is maintained in a mixture, thermophoretic forces are exerted on all molecules including suspended particles; loosely speaking particles experience a force similar to the gravitation force, although the nature of thermophoretic force is different and complex. Thermophoresis in gases has been extensively studied, e.g., Brock [28], Epstein [29] and Talbot et al. [24]. After discovering the thermophoresis by Maxwell, Epstein was the first who derived an equation for the thermophoretic force exerted on a spherical particle in a gas. To improve the Epstein expression's prediction power and to account for various slip conditions, Brock performed a hydrodynamic analysis in near continuum regime and for small Knudsen numbers (Kn) and developed a general equation for the thermophoretic force, which has three matching coefficients, such as the thermal slip and momentum exchange coefficients. Others have attempted to modify the coefficients for various Kn numbers. For the entire range of the Kn number, Talbot et al. [24] proposed values for the matching coefficients in the Brock's expression. This equation has been widely used in many applications that involve a temperature gradient in *gases* and is given as follows:

$$F_T = -\frac{12\pi\eta\nu R C_s\left(\frac{k}{k_p}+C_t\frac{\lambda}{R}\right)\ \frac{\nabla T}{T}}{\left(1+3C_m\frac{\lambda}{R}\right)\left(1+2\frac{k}{k_p}+2C_t\frac{\lambda}{R}\right)} \tag{1}$$

where the matching parameters Cs is 1.17, Cm is 1.14 and Ct is 2.18, η and ν are dynamic and kinematic viscosities of the gas, k and k_p are thermal conductivities of the gas and particle, respectively, R is the particle radius, and λ is the mean free path of the gas molecules.