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CFD based investigation of ‘Microfluidic thermophoresis’

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Microfluidics is an emerging area of research where fluid flow through microchannel is studied and it has wide range of applications in the areas of microscale reactor technologies, process intensification, lab-on-chip devices etc. Particularly, in biomedical and biochemical applications of lab-on-chip devices, such microscale transport phenomena offers a number of advantages related to heat and mass transfer, controlled mixing etc. In the present study, particle laden flow inside such a microchannel was considered along with a thermal gradient and the whole phenomenon was investigated though the route of computational fluid dynamics (CFD). Main objective of the study was to understand the phenomenon of ‘thermophoresis’ inside such a microchannel. Thermophoresis is basically the motion of the particles under the influence of a temperature gradient. Thermophoresis inside a microchannel has lot of application in biomedical and other sectors. Although, a number of earlier works reported different aspects of thermophoresis at macroscale, its application in microfluidic system was not explored in detail. In the present work, microfluidic thermophoresis was simulated on a COMSOL based CFD platform where a three dimensional microchannel was constructed and a fluid flow inside this channel was simulated considering a low flow rate. For determining the velocity field, incompressible flow Navier-Stokes equation was solved along with the continuity equation. No slip boundary condition was adopted at the channel wall. After evaluating the velocity field, the same system was again simulated with a temperature gradient along the perpendicular direction to the flow. Next, particle tracing module was imposed on this system to study the particle dynamics inside such a channel. The particle trajectories clearly reveal the thermophoresis process inside the microchannel and it was found that particles motion is significantly influenced by the presence of thermal field. Effect of the temperature difference, particle concentration, flow rates on the particle motion was thoroughly investigated and presented in details. Fig. 1 shows the schematic diagram of the thermophoresis process inside a microchannel to briefly depict the system of investigation.

Keywords: Thermophoresis, temperature gradient, movement of microparticle, microchannel, CFD.

Introduction

Microfluidics is a subject where fluid flow through microchannel is studied in details and it explores the possibility of application of such micro-scale transport process in different areas like micro-reactors, lab-on-chip devices etc. Microchannel flow offers a number of advantages related to heat and mass transfer, controlled mixing etc. For manipulating the liquid flow inside such microchannel, external forces like electric field, magnetic field becomes very effective. Applications of such forces in microfluidic applications have been widely explored and significant number of scientific reports have shown the phenomena of electrophoresis or magnetophoresis inside microchannels. In most of these works, movement of particles or biological species under the influence of external electric or magnetic forces have been investigated. Very few papers are available which shows the effect of thermal field on the particle movement inside microchannel. Such movement of particles through the effect of fluid flow velocity in the presence of temperature gradient is known as thermophoresis and generally studied in the context of gas/solid flow.

However, the same phenomena can be applied in the laminar flow field inside microchannel and using this thermophoretic movement, isolation of rare cells, chemical species can be achieved which can be applied in different lab-on-chip devices. Thermophoretic force is defined as the force that a particle experience due to the temperature gradient and thermophoretic velocity is defined as the velocity with which the particle moves through the fluid due to thermophoretic force. Thermophoresis was first observed by Ludwig and Soret[1] in liquid and they observed that when a tube filled with salt solution kept under temperature gradient, the concentration of salt solution becomes higher at the cold end of the tube and it was also found that a flux of salt was established due to temperature gradient. Following the work of Ludwig and Soret[1], different research papers have been reported on this subject[1–20]. The present work attempts to reveal certain new aspects of thermophoresis inside microfluidic environment.

Methodology:

A three-dimensional microchannel of 800 μm width, 400 μm depth, and 40 mm length was constructed as shown in Fig. 1 in the CAD platform of COMSOL Multiphysics 4.3a. The hydraulic diameter of the channel was found to be 600 μm and a liquid flow rate of 428.568 μL/min inside the channel was considered for all the cases of simulations.

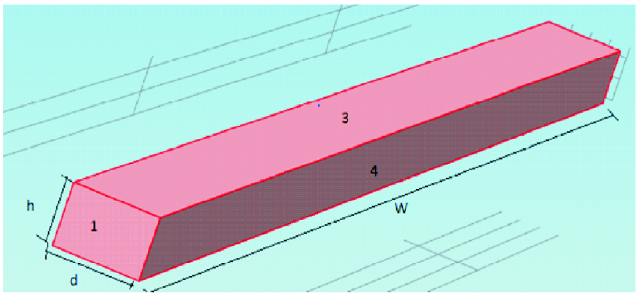

Fig. 1. 3D geometry of straight rectangular microchannels.

At first, Navier-Stokes equation for incompressible flow system was solved along with the energy equation to get the velocity and temperature field of the flow domain considering water as the liquid phase. Eqs. (1) and (2) show the forms of the continuity and Navier-Stoke's eqs.:

$$\Delta.\rho_f u = 0 \tag{1}$$

$$\rho_f u\,(\Delta.u) = -\Delta p + \Delta\mu_f[\Delta u + (\Delta u)^T] \tag{2}$$

where, μ is the velocity (m/s), ρ is the static pressure; ρ_f and μ_f are the fluid density and viscosity, respectively. After getting the velocity and temperature field, particle tracing module was added which considers drag force (F_D), gravity force (F_g), thermophoretic force (F_T) etc. and particle trajectory was determined under the influence of these forces using Newton's second law (time dependent governing equation) as shown in eq. (6).

$$F_D = \frac{m_p(u - v)}{\tau_p},\ \tau_p = \frac{\rho_p d_p^2}{18\mu} \tag{3}$$

$$F_g = \frac{m_p g\,(\rho_p - \rho)}{\rho_f} \tag{4}$$

$$F_T = \frac{6\pi d_p \mu^2 C_S \Lambda \Delta T}{\rho(2\Lambda + 1)T},\ \Lambda = \frac{K_f}{K_p} \tag{5}$$

$$\frac{d}{d_t}(m_p v) = F_D + F_g + F_T \tag{6}$$

where, F_D is the drag force, F_T is thermophoretic force, and F_g is the gravitational force. Other symbols used in the above equations have the following meaning:

m_p = particle mass,
τ_p = particle velocity response time,
v = velocity of particle,
u = fluid velocity,
ρ_p = particle density,
K_f = thermal conductivity of the fluid,
K_p = thermal conductivity of particle,
ρ = density of the fluid ,
T = temperature,
μ = dynamic viscosity of fluid,
d_p = particle diameter,
C_s = thermophoretic correction factor,
g = acceleration due to gravity.

In the fluid flow analysis, incompressible Newtonian fluid was considered along with no slip boundary conditions at the wall. This is to be noted that expression for thermophoretic force (eq. (5)) shows that the intensity of the force is proportional to the temperature gradient and similar type of expression was also used in earlier studies[21].

Initially, temperatures of the upper wall and lower walls were kept same to neglect the effect of thermophoretic force on the particle movement and then temperature gradient is applied gradually from lower value to higher value. During application of thermal gradient, the upper wall was considered as hot wall and lower wall was kept as cold wall. Polystyrene particles of 10 micron diameter were considered for the present study. This is noteworthy to mention here that polymeric particles (like polystyrene particles) are frequently used in particle based microfluidic applications[22–26]. Generally, to model the biological cells, such type of particles have wide spread applications. In the present study, density of the polymeric particles was considered to be 1040 kg/m^3 and thermal conductivity (kp) of the particles was considered to be 033 [$w/(m - k)$].

All the equations were solved using finite element based solver of COMSOL Multiphysics 4.3a. For analysing the results, the flow domain was divided into 8 cells along the length of the channel and 2 cells along the height of the channel. Particle number of each sub-cell was counted after completion of each simulation and to check the effect of thermophoresis only the cells of the intermediate section (4th and 5 th cells along the length) was considered.

Result and discussions

In the present study, an attempt was made to know about the effect of thermophoresis inside three dimensional straight rectangular microchannels using CFD. Effect of temperature gradient on the intensity of thermophoresis has been studied in details.

Navier-Stokes and continuity equation at steady state were solved considering laminar flow throughout the channel at isothermal condition by applying suitable boundary conditions and it gives the velocity and temperature field of the entire flow domain. After that particle tracing algorithm was implemented to know the particle trajectory which is time dependent and it was computed for 10 s. After the computation with particle tracing, particle trajectory was obtained along with the velocities of the particles. In the following section, results of the simulation are presented where 100 numbers of particles were considered.

Temperature difference (ΔT) in this study means the temperature difference between the upper and lower wall of the considered microchannel. Here temperature of the lower face is always kept at constant (300 K) and the temperature of the upper face changes from 302.5 K to 307.5 K, 315 K, 330 K, 350 K and 400 K.

Fig. 2 shows some contour profiles obtained from the CFD simulation of a particular case when the number of particle is 100 and temperature difference between lower and upper surface is only 1 K. This is a representative result and Fig. 2(a) shows the cross-section wise velocity contour along the length of the channel. It shows zero velocity at the wall and maximum velocity at the centre of the channel which is expected at the laminar flow condition. Fig. 2(b) shows the temperature distribution along an XZ plane. It shows that from upper wall to lower wall, temperature gradually increases. Fig. 2(c) shows the particle velocity contour along a cross sectional plane and Fig. 2(d) shows the cross sectional planes along with particles in each quadrant or subcells. In order to understand the effect of thermophoresis, particle number of each sub-cell is calculated and particle number of upper half of the channel and lower half of the channel was plotted against time and such plots at different temperature differences are shown in Fig. 3.

Each plot of Fig. 3 shows temporal variation of two particle numbers, upper half particle numbers and lower half particle numbers. Difference of particle numbers between both these portions of the channel is an indicator of the effect of thermophoresis. Fig. 3(a) shows the temporal variation of the particle numbers when there exist no temperature gradient across the channel cross section. The plot reveals that there is no significant difference in particle numbers between the upper and lower portion of the channel and it was found that after the initial few seconds, the particle numbers of both the phases are almost same. Fig. 3(b) and 3(c) show the similar type of particle distribution when very small thermal gradient (temperature difference 1 K and 2.5 K respectively) have been applied across the cross section of the channel. In comparison to Fig. 3(a), Fig. 3(b) and 3(c) show slight difference between the particles numbers of upper and lower section of the channel. However, the difference is not so significant since the applied thermal gradient is too small. To enhance the effect of thermal gradient, in Fig. 3(d) to 3(h), the temperature difference is gradually increased from 7.5 K to 15 K, 30 K, 50 K and 100 K respectively. The results clearly show that as the temperature difference increases, the difference in particle numbers between the upper and lower section of the channel is gradually increased and from 7.5 K onwards, this difference becomes prominent. It was also observed that with higher degree of temperature difference, the attainment of equilibrium particle concentration in each half of the channel becomes faster. For example, when the temperature difference is as high as 100 K (as shown in Fig.

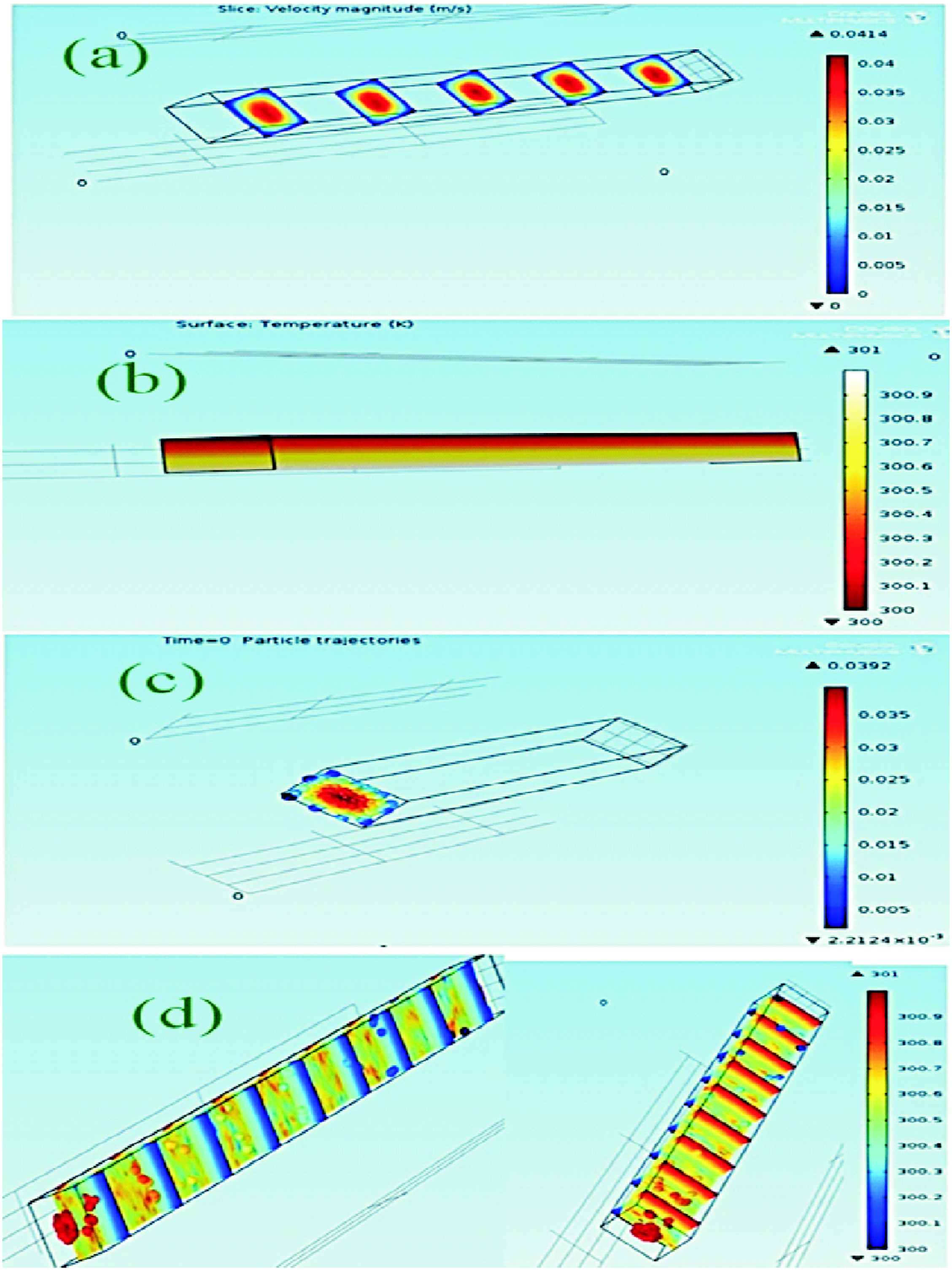

Fig. 2. For T = 1 K (a) cross sectional planes showing the velocity contours at different locations, (b) surface temperature distribution shown along XZ plane of the channel, (c) contour of particle velocities along YZ direction, (d) represents all the upper and lower quadrants of the channel along with particles.

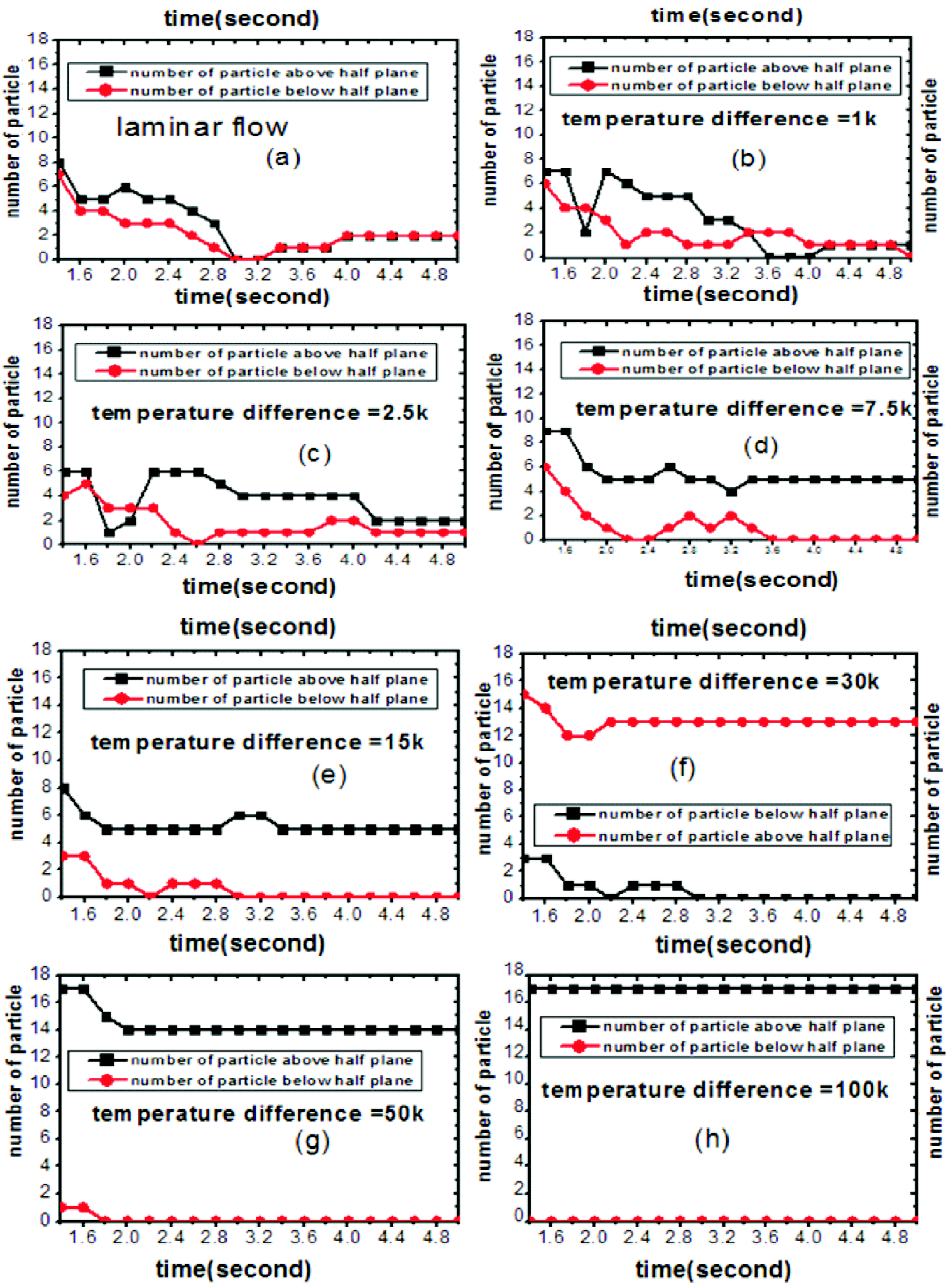

Fig. 3. (a) shows variation of number of particle with time at T = 0 K, (b) shows variation of number of particle with time at T = 1 K, (c) shows variation of number of particle with time at T = 2.5 K, (d) shows variation of number of particle with time at T = 7.5 K, (e) shows variation of number of particle with time at T = 15 K, (f) shows variation of number of particles with time at T = 30 K, (g) shows variation of number of particles with time at T = 50 K, (h) shows variation of number of particles with time at T = 100 K.

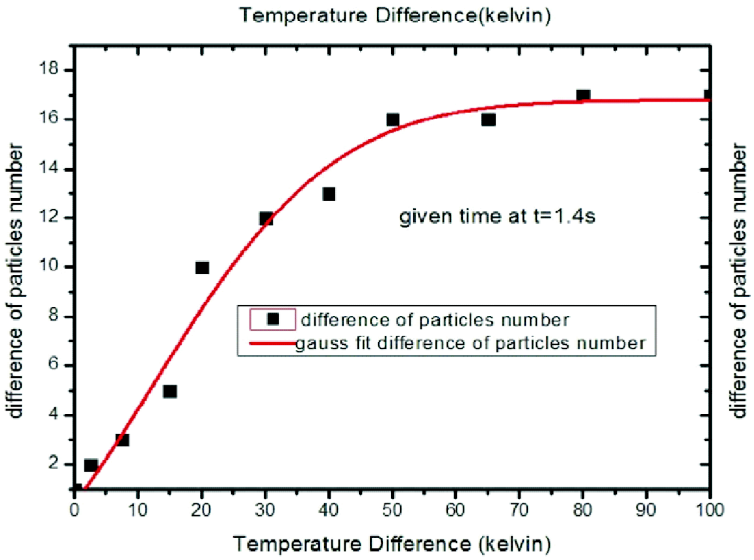

Fig. 4. Variation of the difference of particle number with respect to temperature difference at a given time at *T* = 1.4 s.

3(h), the equilibrium particle concentrations in lower and upper half of the channel are reached almost instantaneously with maximum difference in particle numbers. These results clearly show the influence of themal gradient in the movement of particles in a liquid filled microchannel.

In order to check the effect of particle migration with temperature difference at a particular instant of time, Fig. 4 is presented which basically shows the variation of particle number difference (between lower and upper half of the channel) with temperature differences. The results of the plot are calculated at a fixed point of time (1.4 s). It shows that at lower degree of temperature difference, particle number difference is very low and it gradually increases with the increasing value of temperature difference. It was found that as the temperature difference goes beyond 55 K, the value of particle number difference reaches a steady value. Further increase of temperature difference does not show any significant change in the extent of particle migration.

Conclusions

The present study shows the phenomenon of thermophoresis inside a microfluidic channel through a detail CFD based simulations. Migration of polymeric microparticles inside a liquid filled microchannel has been studied under the influence of a thermal gradient applied to the perpendicular direction of the flow. The results show that movement of particles are significantly influenced by the external thermal gradient and it shows that up to a certain value of temperature difference, the extent of particle migration shows a linear relationship and after reaching a limiting higher value, the particle migration becomes complete and further increase in temperature difference do not show any significant change. Such control of particle movement with the application of thermal gradient can be used in a number of futuristic lab-on-chip devices such as circulating tumour cell isolation inside microchannel. In this regard, Tang *et al.* showed such tumour cell isolation using magnetic field[27], whereas, Chang *et al.* achieved such separation using electric field[28]. To the best of our knowledge, no body has attempted so far to study the effect of thermal field for such applications. The present fundamental study is a primary step in that direction.

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