NUMERICAL STUDY OF EFFECT OF THERMOPHORESIS ON PARTICLES TRAJECTORY IN A RECTANGULAR MICRO-CHANNEL

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ABSTRACT

A numerical study has been presented in this paper to predict the micro motion of particles under the action of thermophoresis. A two-dimensional, incompressible and viscous fluid flow model is proposed to simulate the fluid flow and particle trajectory in rectangular micro-channel with a length of 2000 µm and a height of 500 µm. The governing equations are discretized by using finite volume method using second order upwind scheme. The coupling of velocity and pressure terms of momentum equations are solved by using SIMPLE algorithm. The effect of thermophoretic force on particles is calculated using Discrete Phase Model which works on lagrangian approach. The objective of this study is to examine the effects of particle size and temperature difference between bottom side and top side on particle trajectories in a micro-channel. It is found that thermophoretic force increases with the increase of temperature gradient in micro-channel. The results also show that particle with smaller diameter and smaller gravity acceleration can pass through the micro-channel more easily and thermophoretic force plays vital role in capturing such small particles.

Keywords: *Thermophoresis, Particle Trajectory, DPM, Particles, ANSYS FLUENT.*

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1. INTRODUCTION

Nanoparticles play a major role in many industrial processes and natural phenomena in a variety of fields including chemical engineering, chemistry, physics, public health and biology. Nanoparticles are suspended in fluids during production, handling, processing, and by unintentional and/or undesired release to the environment. In many cases the suspending fluid is a gas. From the dusts produced by the daily cleaning and the waste gas discharged from cars and motorbikes, which deposit on the alveolus and do harm to human health, to the semiconductor quality control, the dust-collecting in the clean room, the air-pollution control and the human respiratory system protection, its importance can be seen everywhere. At present, pollutants in the atmosphere which come from industry, transportation, or agriculture, have caused kinds of environmental problems. Especially, fine particulate matter (PM) less than 10 μm such as nitrogen dioxide and monoxide, directly affects environmental quality and human health. One of the important mechanisms, usually contributed in the deposition of ultrafine particles, is thermophoresis.

Thermophoresis phenomenon refers to the behavior that small micron sized particles suspended in a non-isothermal gas will acquire a velocity in the direction of decreasing temperature. The velocity acquired by the particles is called the thermophoretic velocity and the force experienced by the suspended particles due to the temperature gradient is known as the thermophoretic force. The magnitudes of the thermophoretic force and velocity are proportional to the temperature gradient, thermal conductivity of aerosol particles and the carrier gas, thermophoretic coefficient, heat capacity of the gas and the Knudsen number. Thermophoresis causes small particles to deposit on cold surfaces. It has many engineering applications in removing small particles from gas streams, in determining exhaust gas particle trajectories from combustion devices, prevention of fouling and corrosion in heat exchangers and turbines, semiconductor manufacture and ceramic powder production.

This phenomena has been extensively studied in the literature. Brock [1,2] and Talbot et al. [3] have developed expressions for the thermophoretic force for continuum, transition and Knudsen regimes.

Goren [4] studied the thermophoretic behavior of aerosol particles in the laminar boundary layer on a flat plate. Batchelor and Shen [5] and Shen [6] predicted thermophoretic deposition of particles onto cold surfaces in two-dimensional and axisymmetric flows. Homsy et al. [7] and Walker et al. [8] have developed analytical expressions for the thermophoretic deposition rates in laminar tube and other boundary layer flows. Montassier et al. [9,10] and Stratmann et al. [11] studied the thermophoretic deposition in laminar flows and the experimental results agreed reasonably well with theoretical models when the thermophoretic coefficient expression of Talbot et al. was used. Nishio et al. [12] and Romay et al. [13] studied the thermophoretic deposition in turbulent flows and they focused on both theory and experiments. They found the thermophoretic deposition efficiency predicted was lower than the experimental results. Thakurtal et al. [14], Lo lacono and Reynolds [15] and A. Dehbi [16] studied the turbulent particle dispersion in the presence of thermophoresis using the computational fluid dynamics (CFD) and their results agreed reasonably well with the experimental results in the literature. Garg and Jayaraj [17] studied the thermop-horetic transport of aerosol particles through a forced convection laminar boundary layer in cross flow over a cylinder for hot, cold and adiabatic wall conditions. Oostra et al. [18] studied the influence of gravity on deposition of particles with thermophoresis through numerical calculations and experiments under gravity and microgravity conditions. Z. Liu et al. [24] have done the theoretical analysis of micro motion of particles under the action of thermophoresis in aqueous electrolyte solution.

2. MATHEMATICAL MODEL

To study the thermophoresis phenomena a two-dimensional rectangle micro-channel with a length of 2000 μm and a height of 500 μm is selected in this study as shown in Fig. 1.

2.1. Fluid flow model

The fluid flow in micro-channel is assumed to be two-dimensional, continuous incompressible and laminar flow for which the continuity, momentum and energy equations can be written as:

$$\begin{cases} \dfrac{\partial(\rho u)}{\partial x} + \dfrac{\partial(\rho v)}{\partial y} = 0 \\ \rho\left(u\dfrac{\partial u}{\partial x} + v\dfrac{\partial u}{\partial y}\right) = \rho F_x + \mu\left(\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}\right) \\ \rho\left(u\dfrac{\partial v}{\partial x} + v\dfrac{\partial v}{\partial y}\right) = \rho F_y + \mu\left(\dfrac{\partial^2 v}{\partial x^2} + \dfrac{\partial^2 v}{\partial y^2}\right) \\ \rho c_p\left(u\dfrac{\partial T}{\partial x} + v\dfrac{\partial T}{\partial y}\right) = k\left(\dfrac{\partial^2 T}{\partial x^2} + \dfrac{\partial^2 T}{\partial y^2}\right) \end{cases} \quad (1)$$

Boundary conditions for the model are as follows:

$$\begin{cases} x = 0, 0 < y < d, u = u_0, v = 0, T = T_0 \\ x = L, 0 < y < d, P_d = 0, \dfrac{\partial T}{\partial x} = 0 \\ 0 \le x \le L, y = d, u = 0, v = 0, T = T_1 \\ 0 \le x \le L, y = 0, u = 0, v = 0, T = T_2 \end{cases} \quad (2)$$

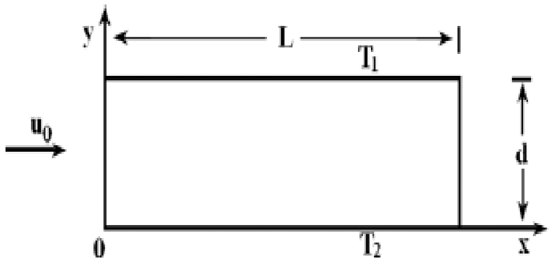

Fig.1. **A Schematic of Micro-Channel.**

2.2. Thermophoretic force and particle motion

In the gas or liquid medium with a temperature gradient, a particle might move from hot region to cold region because it receives more hits from molecules in hot side than that in cold side and the molecular in hot side have more kinetic energy. The macroscopical force which makes the particle moving towards cold region is called thermophoretic force.

Early in 1909 Knudsen had finished primary experiment work of rare gas dynamics and defined Knudsen number. Momentum, heat, and mass transfer between a particle and the surrounding gas molecules depend on the Knudsen number (Kn) which is the ratio of the mean free path of the gas molecules (λ_{gas}) and the particle diameter:

$$Kn = \frac{2\lambda_{gas}}{d_p} \quad (3)$$

Further, he divided the gas flow in pipe into several regions:

(1) Kn→0 (Re→∞): Eular Equation (molecular diffusion is neglected);

(2) $Kn < 10^{-3}$: Navier–Stokes Equation (Boundary conditions without slip);

(3) $10^{-3} < Kn < 10^{-1}$: Navier–Stokes Equation (Boundary conditions with slip);

(4) $10^{-1} < Kn < 10$: Transition region;

(5) $Kn > 10$: Free molecular stream.

The mean free path of the gas molecules (λ_{gas}) is the average distance a molecule travels before it changes its direction. The change in direction takes place when a gas molecule collides with another. The transfer processes follow continuum relationships at small Kn (large particles), but transfers to the free molecule regime at large Kn (small particles) [22]. The mean free path of the gas molecules depends on pressure and temperature of the gas. The Knudsen number for a given particle can change significantly in non-isothermal environments such as aerosol reactors. The pressure and temperature dependence of the gas mean free path can be calculated as follows [19]:

$$\lambda_{gas} = \lambda_{gas,0} \left(\frac{T}{T_0}\right) \left(\frac{p_0}{p}\right) \left(\frac{1+\frac{S}{T_0}}{1+\frac{S}{T}}\right) \quad (4)$$

where $\lambda_{gas,0}$ = 65.3 nm is the mean free path of the gas molecules at conditions (T_0 = 296 K, p_0 = 1 atm) and S is the Sutherland constant (S = 113 K for air) which accounts for the attractive potential between the molecules [20].

For particles that are larger than the mean free path of the gas, the motion in a temperature gradient is rather difficult to describe theoretically. The explanation is based on a creep velocity directed towards the high temperature side, propelling the particle towards the low temperature side. Brock [1] derived the thermophoretic velocity in the continuum regime using a fluid mechanics approach with slip-corrected boundary conditions. The thermophoretic force given by Brock [1] is a function of thermal (C_t) and momentum (C_m) exchange coefficients which can be expressed by the accommodation coefficient (α) [3]:

$$F_{th} = -\frac{9}{2}\pi \frac{\mu^2}{\rho_g} d_p \left(\frac{1}{1+3\,C_m Kn}\right)\left(\frac{\frac{k_g}{k_p}+C_t Kn}{1+2\frac{k_g}{k_p}+2\,C_t Kn}\right)\frac{\nabla T}{T_0} \quad (5)$$

Best agreement with experimental data was obtained with C_t = 2.48 and C_m = 1.00 for pure diffuse reflection of molecules. Equating the thermophoretic force with the particle drag force results in the thermophoretic velocity [1]:

$$V_{th} = -\frac{3}{2}\frac{\mu}{\rho_g} C_c \left(\frac{1}{1+3C_m Kn}\right)\left(\frac{\frac{k_g}{k_p}+C_t Kn}{1+2\frac{k_g}{k_p}+2\,C_t Kn}\right)\frac{\nabla T}{T_0} \quad (6)$$

where, C_c is the thermal-slip coefficient, C_t is the thermal jump coefficient and C_m is the momentum exchange coefficient. Kn is the Knudsen number, T_0 is the mean medium temperature in the vicinity of the particle, d_p is the particle diameter, μ and ρ_g are the molecular viscosity and density of medium, ∇T is the temperature gradient, k_g and k_p are the thermal conductivity coefficient of medium and particle, respectively.

Brock's theory was amended and developed by many researchers, and the formula also changed continually But all the different formulas of thermophoresis theories can briefly be expressed as:

$$V_{th} = -K\frac{\upsilon}{T_0}\nabla T \quad (7)$$

where, K is the thermophoretic coefficient or the reduced thermophoretic velocity V_{th} , υ is the kinematic viscosity of the medium.

The motion of an individual particle in a micro-channel obeys Newton's second law:

$$F_i = ma_i = m\frac{du_{pi}}{dt} \quad (8)$$

where, F_i is all external forces exerted on the particle in the i direction, m is the mass of the particle, a_i is the acceleration in the i direction, u_{pi} is the particle velocity in the i direction.

Also F_i can be written as:

$$F_i = ma_i = F_{mi} + F_{bi} - F_{gi} - F_{vdwi} + F_{ai} \quad (9)$$

where F_{mi}, F_{bi}, F_{gi} and F_{vdwi} are the drag force (the friction force), the buoyancy force, the gravity force and the van der Waals force in the i direction, respectively; F_{ai} is the other additional force exerted on particles.

F_{mi} can be written as [21]:

$$F_{mi} = 6\pi r\mu\frac{Re_{pi}C_{Di}}{24}\left(u_i - u_{pi}\right) \quad (10)$$

where, d_p and r are the particle diameter and radius; μ is the molecular viscosity of fluid; Re_{pi} is the particle Reynolds number, C_{Di} is the drag coefficient; u_i and u_{pi} are the velocity of fluid and particle, respectively.

Re is the relative Reynolds number, which is defined as [21]:

$$Re_{pi} = \frac{(u_i - u_{pi})d_p\rho_l}{\mu} \quad (11)$$

where, ρ_l is the density of fluid.

The drag coefficient C_{Di} is defined according to the Stokes law:

$$C_{Di} = \frac{24}{Re_{pi}} \quad \left(Re_{pi} < 1\right) \quad (12)$$

The gravity and buoyancy forces are given by the following equations:

$$F_{gi} = \frac{4}{3}\pi r^3 g_i \rho_p \quad (13)$$

$$F_{bi} = \frac{4}{3}\pi r^3 g_i \rho_l \quad (14)$$

where, g_i is the gravity acceleration in the i direction.

2.3. Main assumptions

In order to simply the calculation, the following assumptions are made:

(1) Two-dimensional, continuous, incompressible and laminar flow;

(2) Heat and mass transfer between fluid and particles are neglected;

(3) No particle rebounds on walls;

(4) All particles are spherical;

(5) Pressure gradient force, Basset force, virtual mass force, Brownian force and Saffman's lift force are neglected.

2.4. Numerical Simulation

A finite volume method is used to discretize the flow and energy equations. The discretization form of density, momentum and energy is a second-order upwind scheme and ''SIMPLE'' algorithm is adopted for pressure-velocity coupling. Spherical particles with density of 2.5 gm/cm^3 and of four sizes of 1 μm, 2.5 μm, 5 μm and 25 μm are employed for simulation in the numerical model. The initial fluid flow velocity u_0 in x-direction is assumed to be 5 mm/s and initial temperature T_0 is assumed to be 400 K. The value of acceleration due to gravity is taken as 9.8 m/s^2.

Simulations were performed using intel core 2 duo processor (1.73 GHz CPU, 2 GB RAM processor) on ANSYS FLUENT 12 software. Meshing is done over the two dimensional domain using 1139 quadrilateral cells with maximum cell squish of 3.9936×10^{-3} and maximum aspect ratio of 1.90058. Particle trajectory is calculated using Discrete Phase Model (DPM) which uses the Lagrangian approach to solve the particle's equation of motion. The solution is considered to be converged when the normalized residual of the algebraic equation is less than a prescribed value of 1×10^{-5}. Under-relaxation is required to secure convergence of the iterative procedure. The values of the under-relaxation factors adopted here are 0.3, 0.7 and 1 for pressure, momentum, and energy equations, respectively.

3. RESULTS AND DISCUSSIONS

The temperature distribution of the fluid with the inlet fluid velocity of 5 mm/s and the wall temperature is assumed to be 300 K in top side and 300 K, 310 K, 320 K and 350 K in bottom side respectively are showed in Fig.2.When the fluid flows through the rectangular micro-channel, the velocity decreases because of the viscous force. The effect of thermophoresis on particle motion and trajectory are obtained by changing the temperature field and the relations between particle trajectory and fluid flow are studied.

Fig. 3 shows the 2.5 μm diameter particle's trajectory when the particles with temperature of 400 K are injected from inlet surface and with the inlet fluid velocity of 5 mm/s and top side wall temperature is assumed to be 300 K which is kept constant throughout while temperature in bottom side is assumed to be 300 K, 310 K, 320 K and 350 K, respectively. As shown in figure for same wall temperature of 300 K, maximum particles are trapped on bottom side because of gravity force. When the bottom wall temperature is increased to 310 K then the particle trajectory gets diverted to top side wall. As shown, with the increase of temperature difference between bottom side and upper side, the thermophoretic force becomes bigger, due to which the particle flow trajectory moves away from the bottom side. When the bottom wall temperature is increased further to 320 K then maximum amount of particles are trapped on top side wall. This happens because thermophoretic force increases and becomes big enough to overcome the gravity force. When the bottom wall temperature is further increased to 350 K, then almost all particles are trapped by top wall with minimum particle residence time.

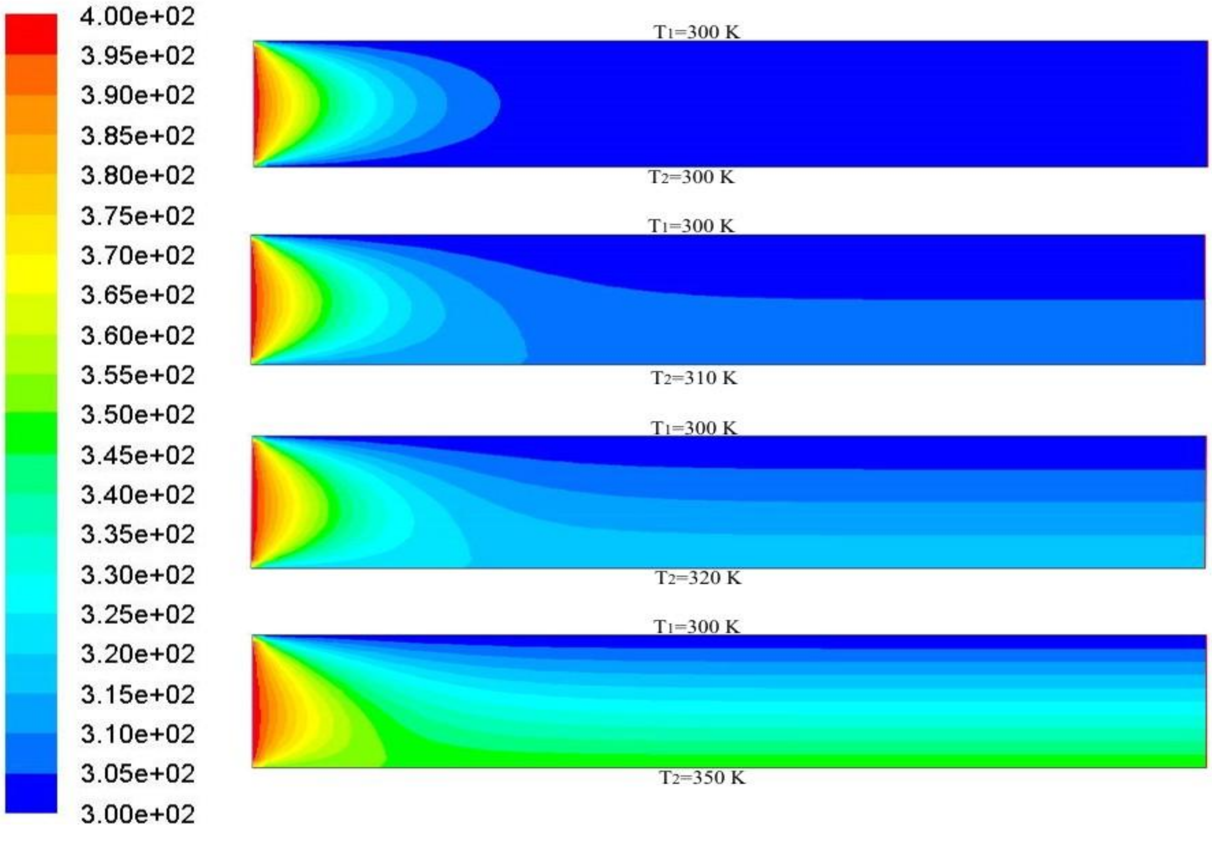

Fig.2. Contours of Static Temperature distribution in micro-channel with inlet fluid velocity of 5mm/s and different values of wall temperature T_1 and T_2 at top and bottom side respectively.

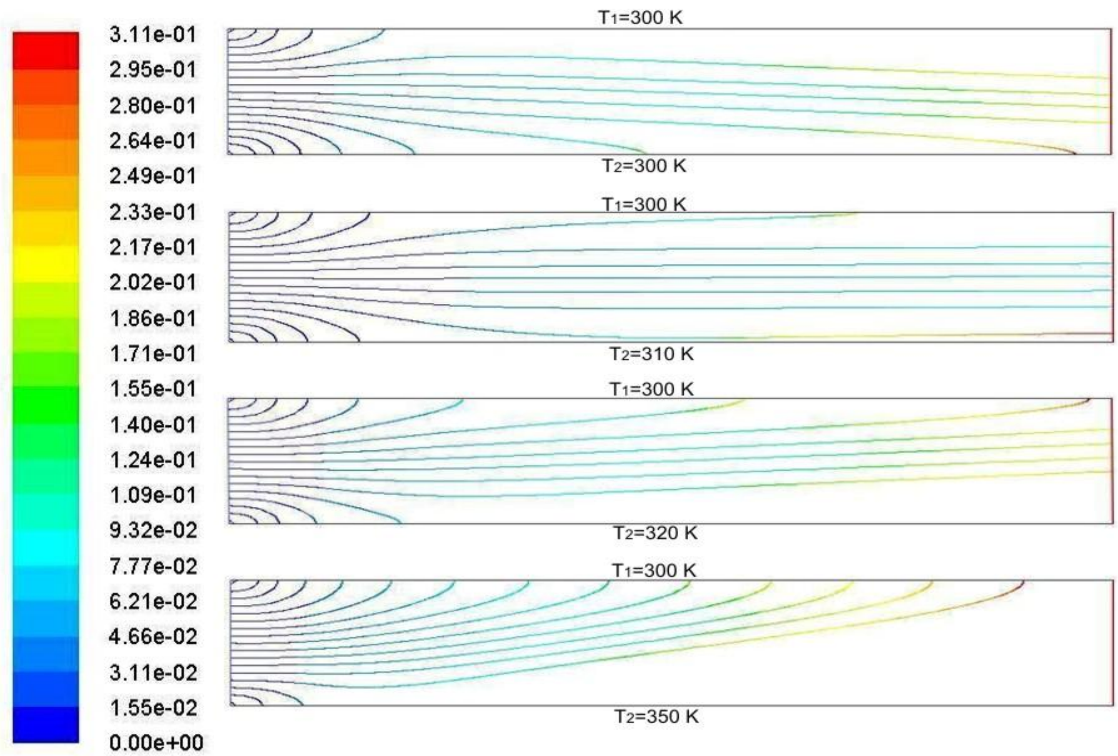

Fig.3. Particle (d_p =2.5 μm) traces coloured by Particle residence time (in sec) in channel with inlet fluid velocity of 5mm/s.

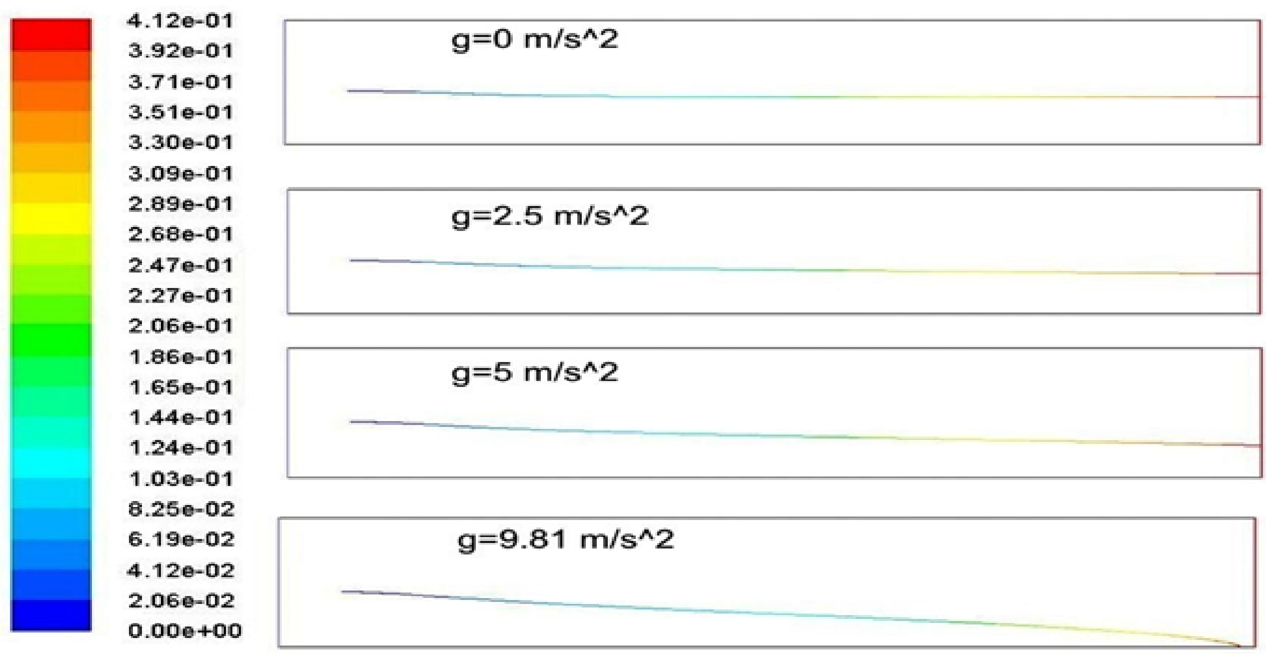

Fig.4. Particle (d_p =2.5 μm) flow trajectory coloured by Particle residence time (sec) v/s gravity acceleration with the inlet fluid flow velocity of 5 mm/s and wall temperature of 300 K for both top and bottom wall.

Fig.4. shows particle (2.5 μm) motion trajectory with initial position of 100 μm in x-direction and 200 μm in y-direction vs. gravity acceleration with the fluid inlet velocity of 5 mm/s and the wall temperature of 300 K for both top and bottom wall. As shown, the particle can easily pass through the micro-channel with small gravity acceleration. With the increase of gravity acceleration, the particle motion trajectory moves towards the bottom side. The density of particle is bigger than that of fluid, which leads to a rapid increase of the gravity force to the buoyancy force.

Fig.5. shows the effect of particle's diameter (1 μm, 2.5 μm, 5 μm and 25 μm) with initial position of 100 μm in x-direction and 200 μm in y-direction on the particle motion trajectory with the fluid inlet velocity of 5 mm/s and the top wall temperature of 300 K and bottom wall temperature of 310 K. The drag force of fluid per unit particle mass mainly depends on particle's diameter d_p. As shown, particle motion trajectory moves towards the nether side with the increase of particle diameter, the particle (1 μm) and the particle (2.5 μm) escapes while the particle (5 μm), the particle (25 μm) and the particle (250 μm) are trapped.

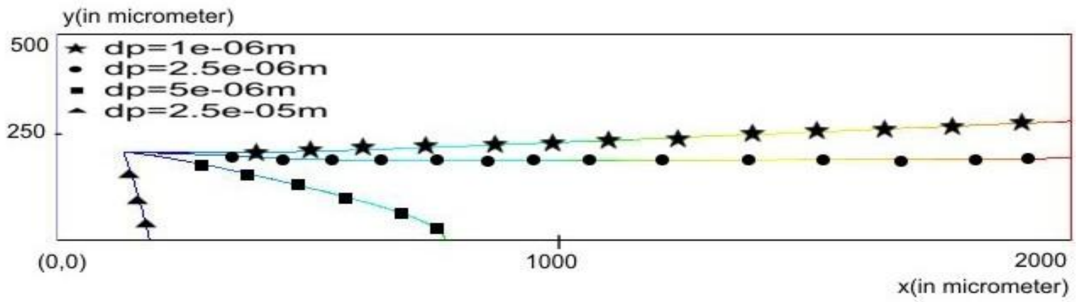

Fig.5. Particle's flow trajectory v/s particle's diameter with inlet fluid velocity of 5mm/s and having top wall temperature of 300 K and bottom wall temperature of 310 K.

5. CONCLUSIONS

A two-dimensional, incompressible and viscous fluid flow model is established using Discrete Phase Model of ANSYS FLUENT to simulate the fluid flow and particle motion trajectory in a rectangular micro-channel. The effect of thermophoretic force on sepration motion of particles in micro-channel is analyzed. The particle motion trajectories considering the effects of particle's size and temperature difference between bottom side and top side in micro-channel is simulated. The following conclusions can be drawn: (1) Thermophoretic force increases with the increase of temperature gradient in micro-channel. (2) With increase in wall temperature of bottom side, the particle's trajectory, which was earlier trapped by bottom side gets diverted to upper cooler side wall. (3) The smaller the gravity acceleration, the more easily the particle passes the channel. (4) Particles with smaller diameter can pass through the channel more easily. Therefore, thermophoretic force plays a vital role in trapping these small particles.

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