Inertial focusing in two dimensional flows with sharp viscosity stratification in a microchannel

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Received 23 March 2020, revised 22 July 2020
Accepted for publication 12 August 2020
Published 28 August 2020

Abstract

Recent experimental studies have shown that lateral particle migration can be controlled passively using stratified flows of co-flowing streams. In this study, we numerically analyze particle migration in a stratified Poiseuille flow of two liquids of different viscosities. A novel numerical approach using immersed boundary method is employed to perform 2D simulations in moving frame of reference. The effect of viscosity ratio, flowrate ratio, Reynolds number and particle size on focusing position is analyzed to identify conditions under which particle migration occurs from one fluid to the other. It is shown that the particle migrates to the low viscous fluid beyond a critical flowrate ratio which increases with particle size. The results of the present study can be used to select suitable flowrate ratio to enable separation of particles of different sizes in membrane less separators.

Keywords: inertial focusing, stratified flow, particle migration and immersed boundary method

Some figures may appear in colour only in the online journal

Nomenclature

Symbols

- $d$: Diameter of the particle (m)
- $D_p$: Dimensionless diameter of the particle
- $f(x,y,t)$: External body force on the fluid domain
- $f_i$: Dimensionless force in y-direction (lateral direction)
- $F$: Force on the particle surface
- $F_i$: Dimensionless lift force
- $h$: Holdup of liquid-1 (m)
- $H$: Height of the channel (m)
- $L$: Dimensionless height of the channel
- $\tilde{Ip}$: Moment inertia of the particle
- $L'$: Length of the periodic unit cell (m)
- $L_b$: Perimeter of the particle (m)
- $m_p$: Mass of the particle (kg)
- $N_c$: Total number of grid in the Coarse region
- $N_f$: Total number of grid in the fine region
- $p':$ Pressure (Pa)
- $P'$: Periodic pressure (Pa)
- $Q_1$: Flowrate of liquid-1 per unit width (m$^2$s$^{-1}$)
- $Q_2$: Flowrate of liquid-2 per unit width (m$^2$s$^{-1}$)
- $Q_r$: Flowrate ratio ($Q_1/Q_2$)
- $Q_{cr}$: Critical flowrate ratio
- $s$: Arc length parameter
- $t':$ Dimensionless time
- $\tilde{t}$: Time (s)
- $\tilde{t}'$: Dimensionless time
- $\tilde{u}$: Initial fully developed velocity (m s$^{-1}$)
- $\tilde{u}':$ Velocity field in the stationary reference frame (m s$^{-1}$)
- $\tilde{u}$: Dimensionless velocity field in the particle reference frame
- $\tilde{u}':$ Dimensionless velocity field in the particle reference frame
- $\tilde{U}_c$: Translation velocity of the particle (m s$^{-1}$)
- $\tilde{U}_c$: Dimensionless particle translation velocity
- $\tilde{U}_p$: Particle velocity (m s$^{-1}$)
- $\tilde{V}_p$: Volume of the particle (m$^3$)
- $\tilde{X}_k$: Velocity of the particle at Lagrangian grid $\tilde{X}_k$ at $n+1$
- $\tilde{u},\tilde{u}**,\tilde{u}^{**}$: Intermediate velocity components
\[ x', y' \text{ Coordinates in the stationary frame of reference} \]

\[ x, y \text{ Coordinates in the particle frame of reference} \]

\[ \dot{x}_c(t) \text{ Center of the particle} \]

\[ \dot{x}_k \text{ Eulerian fixed grid for fluid domain} \]

\[ \dot{x}_h \text{ Lagrangian grid on the particle} \]

\[ \Delta s \text{ Grid size on the particle surface} \]

\[ \Delta \tau \text{ Time step length} \]

\[ \Delta x \text{ Grid size in x-directions} \]

\[ \Delta y \text{ Grid size in y-directions} \]

\textbf{Greek letters}

\[ \alpha' \text{ Applied pressure gradient (Pa m}^{-1}) \]

\[ \alpha \text{ Dimensionless applied pressure gradient} \]

\[ \nabla^* \text{ Del operator in stationary reference frame} \]

\[ \nabla \text{ Dimensionless del operator} \]

\[ \delta \text{ Dirac delta function} \]

\[ \rho_l \text{ Density of liquid (kg m}^{-3}) \]

\[ \rho_p \text{ Density of the particle (kg m}^{-3}) \]

\[ \mathcal{F} \text{ Hydrodynamic stress tensor (Pa)} \]

\[ \mu_1 \text{ Viscosity of liquid-1 (kg m}^{-1} \text{s}^{-1}) \]

\[ \mu_2 \text{ Viscosity of liquid-2 (kg m}^{-1} \text{s}^{-1}) \]

\[ \alpha \text{ Viscosity ratio} (\mu_1/\mu_2) \]

\[ \bar{\omega} \text{ Dimensionless viscosity} \]

\[ \dot{\omega} \text{ Angular velocity of the particle (rad s}^{-1}) \]

\[ \bar{\omega} \text{ Dimensionless angular velocity of the particle} \]

\[ \Omega \text{ Fluid domain} \]

\textbf{Dimensionless groups}

\[ \text{Re} \text{ Reynolds number} \]

1. Introduction

Separation and sorting of micron-sized particles has important applications in diagnostics, chemical and biological analysis, food and chemical processing [1, 2]. Specifically, in diagnostics, it is often necessary to separate dead cells from living cells and infected cells from normal cells. Towards this, a variety of separation techniques have been developed which can be classified as active and passive methods [3]. Amongst the separation methods, techniques based on inertial focusing, which is a passive method, are widely used, as their operation is elegant and throughput is high [4].

Inertial focusing is the cross-stream migration of particles in the presence of finite inertia. This phenomenon of lateral migration of rigid, neutrally buoyant particles, in a cylindrical channel was first observed by Segre–Silberberg [5] in a pressure driven flow. Their experiments showed that the particles focused at a radial position of \( \sim 0.6 R \), where \( R \) is the channel radius. The focusing locations are determined by a balance between the wall lift force and the shear gradient lift force [6]. The wall lift force arises as a result of the pressure difference between the wall side of the particle (high pressure) and the side of the particle facing the center (low pressure), and always acts away from the wall. The shear gradient lift force is experienced by the particle due to the curvature of the velocity profile which leads to a difference in velocity between the two sides of the particle. This force acts in the direction of higher relative velocity between the particle and the fluid and hence is directed towards the regions of higher shear rate i.e. towards the wall. These lift forces depend on the particle properties such as size, density and deformability, channel dimension and flowrate. One of the major application of the phenomenon of inertial focusing is in particle separation based on size, shape and deformability [6]. Some of the examples include filtration of bacteria from blood, isolation of platelets, isolation of circulating tumor cells from blood cells, separation of cancer cells and separation of fungal cells. To enhance particle separation, different channel geometries like serpentine channel, expansion channel and curved channel have been used [4]. However, fabrication of microchannels of such geometries may be difficult.

An alternate way to control particle separation is to use two co-flowing fluids in a microchannel [7]. In this method, particles enter the channel in one of the fluid and migrate to the other depending on the operating conditions. Of the two forces which determine the focusing position, the shear gradient force has been shown to be proportional to \( \alpha \beta \), where \( \alpha \) and \( \beta \) are the shear and shear gradient respectively [8]. By sending the two fluids parallely in a microchannel, the shear and shear gradient, and hence the shear gradient lift force can be manipulated by suitable choice of operating conditions [9]. In this way the focusing position can be controlled so that better separation can be achieved.

A few experimental works have been conducted in which separation of particles has been studied between two fluids flowing parallel to each other in a microchannel. Gossett et al [7] conducted experiments on particle migration in a co-flow of two fluids comprising of a suspension and a transfer solution. They demonstrated that the particles could migrate across the fluid streamlines from the suspension to the transfer solution and attain focusing positions in the transfer solution. Xu et al [10] and Deng et al [11] experimentally showed size based separation of particles from a suspension by inducing large velocity gradients. Here, the velocity gradient was controlled using two sheath fluids of different viscosities one each above and below the suspension fluid. Large particles got separated from the suspension and focused in the less viscous sheath fluid, whereas small particles remained in the suspension. Lee et al [12] studied particle separation in a co-flow system of two miscible liquids with different viscosities in a rectangular microchannel. They observed two kinds of focusing depending on the operating conditions: stable equilibrium focusing (because of the balance of wall and shear gradient forces) and inflection point focusing. They reported inflection point focusing for the first time, where the sign of the shear gradient force changes. Ha et al [13] and Tian et al [14] studied the particle separation in a co-flow of Newtonian fluid and non-Newtonian fluid where the particles migrate from the non-Newtonian fluid to the Newtonian fluid.

In addition to experimental studies, inertial focusing has also been studied analytically and computationally. The analytical studies focus on understanding the phenomenon of inertial focusing and the different contributions to the lift force. These studies have considered the influence of different parameters on inertial focusing, namely the particle to be neutrally or non-neutrally buoyant, in Newtonian or non-Newtonian fluid, in the absence or presence of walls, without

J. Micromech. Microeng. 30 (2020) 115009

T Krishnaveni et al

T Krishnaveni et al
or with electrical field [15]. To enable an analytical or semi-analytical solution, these studies generally limit the scope to low particle Reynolds number so that a perturbation series expansion method can be applied. Further, these studies may not be able to capture the near wall migration behavior accurately.

The limitations of the analytical approach can be overcome through computational studies which involve numerical simulations. The advantages of numerical simulations are that, the lift force, lateral particle velocity, and equilibrium positions can be obtained for a wide range of particle Reynolds number. Further, the effect of wall on the particle dynamics can also be captured. Several computational studies have been carried out to analyze inertial focusing in single phase flow. These studies have considered Couette or Poiseuille flow between parallel plates [16] or in a pipe of circular cross section [17] or duct of square cross section [18]. The particle considered is either a circle [19] or a sphere [20] depending on the dimensionality of the problem solved. Both Newtonian [21] and non-Newtonian [22] fluids have been considered. These studies have analyzed the dependence of equilibrium position, number of equilibrium positions and their stability on Reynolds number and particle size.

The literature survey reveals that, many experimental studies have been carried out on inertial focusing in single phase flow and few have been conducted with two co-flowing fluids. All the analytical and numerical simulation studies are limited to inertial focusing in a single fluid. To the best of our knowledge, no modeling study has been reported on particle separation using inertial focusing in stratified flows. Hence, the primary objective of our work is to obtain physical insights on particle migration in viscosity stratified flows through simulation. This helps cover a wide range of operating parameters without limiting to low Reynolds numbers or asymptotic conditions.

Different numerical techniques have been used to solve the equations governing the fluid flow and particle motion in fluid-particle flows [23]. Among these the immersed boundary method (IBM) has the advantage that a uniform non-body conformal grid can be used which requires less number of grids compared to a non-uniform body conformal unstructured grid. In IBM, the effect of the immersed boundary (particle presence) is incorporated as an external force field in the fluid flow equations. IBM, first proposed by Peskin [24], employs a combination of Eulerian variables and Lagrangian variables. The immersed boundary is represented as a set of discrete Lagrangian markers embedded in an Eulerian flow field. The force is determined on the Lagrangian markers and then interpolated to the Eulerian field using a Dirac delta function [25]. Different forcing methods have been proposed in the literature to simulate flow over rigid bodies, including the direct forcing method [26] and implicit direct forcing method [27]. The latter method accurately calculates the force on the particle surface such that it satisfies the no-slip condition on the surface of the particle and hence this method is adopted in the present work.

The IBM has so far been used to solve problems on a fixed reference frame. However, when analyzing particle migration in inertial focusing, it is advantageous to use a moving reference frame, since this allows a fine grid to be used near the particle and a coarse grid away from the particle and avoids remeshing when the particle is under motion. Hence, to combine the advantages of IBM and moving reference frame, for the first time in the literature, we solve the equations governing fluid and particle motion in a moving reference frame using IBM. This allows us to use a structured fine and coarse mesh simultaneously and hence is computationally efficient.

We numerically simulate the migration of a single particle in stratified Poiseuille flow. The system analyzed consists of two Newtonian fluids with different viscosities flowing parallel to each other forming a viscosity stratified flow. An IBM is used to analyze the motion of the particle. We numerically study the effect of viscosity ratio, flowrate ratio, Reynolds number and the particle size and identify the conditions under which particle migration occurs from one fluid to the other. Design of a size based particle separator based on the simulation results is also illustrated.

This paper is organized as follows: the geometry of the system and mathematical model are described in section 2. The IBM is detailed in section 3. Simulation results on particle migration in stratified Poiseuille flow are discussed in section 4. The key conclusions are summarized in section 5.

2. Mathematical modeling

2.1. Geometry of the system

Experiments on inertial focusing in co-flowing liquids have been performed in rectangular microchannels driven by a pressure drop. Though these channels are 3D, in the present analysis, we consider a 2D domain. A 3D domain can be approximated as a 2D domain, if the aspect ratio (width/height) is greater than 3 [28]. Such an approximation enables us to obtain physical insights on inertial focusing in co-flowing liquids in a computationally efficient way.

The two-dimensional domain chosen for the present analysis is shown in figure 1, which depicts stratified flow of two fluids between two infinite parallel plates. The distance between the two parallel plates is \( H' \) and length is \( L' \). The two fluids with different viscosities \((\mu_1, \mu_2)\) flow parallel to each other at flowrates \( Q_1 \) and \( Q_2 \) respectively. The volume fraction occupied by the bottom fluid \((h' / H')\) is the holdup. In the absence of the particle, the fluid flow is fully developed and the undisturbed velocity profile \((\vec{u}_0(y'))\) is parabolic since the flow is driven by a constant pressure gradient. A freely suspended circular particle of diameter \(d'\) located at \( x' (t) \) is also depicted in figure 1.

2.2. Assumptions

The model is based on the following assumptions:

1. the flow field in the absence of the particle is fully developed;
2. the two fluids are Newtonian;
3. densities of the two fluids and the particle density are same i.e. the particle is neutrally buoyant;
Consider an undisturbed fully developed flow $\mathbf{u}'(y')$. Introduction of a rigid solid particle of diameter $d'$ located at $\mathbf{x'}_c(t)$ modifies the flow field to $\mathbf{u}(y')$. This flow field in a stationary reference frame is governed by

$$\nabla' \cdot \mathbf{u}' = 0, \quad (1)$$

$$\rho_f \left( \frac{\partial \mathbf{u}'}{\partial t} + \mathbf{u}' \cdot \nabla' \mathbf{u}' \right) = -\nabla' P' + \nabla' \left( \mu(\nabla' \mathbf{u}' + (\nabla' \mathbf{u}')^T) \right), \quad (2)$$

where $\rho_f$ is the density of the fluid, and $\mu$ is the viscosity given as

$$\mu = \begin{cases} \mu_1 & y' \leq h' \\ \mu_2 & y' > h' \end{cases}. \quad (3)$$

Here, $\mu_1$ and $\mu_2$ are the viscosity of the two fluids and $h'$ is the interface location as shown in figure 1.

The boundary conditions imposed are

(i) No-slip and no penetration for velocity and Neumann condition on pressure at the channel walls ($y' = 0$ and $y' = H'$).

$$u'(y' = 0) = 0, \quad u'(y' = H') = 0,$$

$$v'(y' = 0) = 0, \quad v'(y' = H') = 0,$$

$$\frac{\partial P'}{\partial y'} (y' = 0) = 0, \quad \frac{\partial P'}{\partial y'} (y' = H') = 0. \quad (4)$$

(ii) Periodic boundary conditions are applied at the upstream and downstream ends of the channel ($x' = 0$ and $x' = L'$).

We incorporate this condition as described in Patankar et al. [31], where the total pressure gradient is divided into two components, i.e. pressure drop per unit length ($\alpha'$) responsible for the fluid flow and the pressure gradient ($\frac{\partial P'}{\partial x'}$) in which pressure ($P'$) is spatially periodic. This is written as

$$\frac{\partial P'}{\partial x'} = \alpha' + \frac{\partial P'}{\partial x'}. \quad (5)$$

This modifies the x-momentum equation as

$$\rho_f \left( \frac{\partial u'}{\partial t} + u' \frac{\partial u'}{\partial x'} + v' \frac{\partial u'}{\partial y'} \right) = -\alpha' - \frac{\partial P'}{\partial x'} + \frac{\partial}{\partial x'} \left( 2\mu \frac{\partial u'}{\partial x'} \right) + \frac{\partial}{\partial y'} \left( \mu \left( \frac{\partial u'}{\partial x'} + \frac{\partial u'}{\partial y'} \right) \right). \quad (6)$$

The periodic boundary conditions imposed are

$$u'(x' = 0) = u'(x' = L'), \quad (7)$$

$$v'(x' = 0) = v'(x' = L'),$$

$$P'(x' = 0) = P'(x' = L').$$

The pressure gradient responsible for the fluid flow is explicitly accounted using $\alpha'$ as a source term in the x-component Navier–Stokes equation.

(iii) We use the single fluid formulation, and hence do not explicitly impose boundary conditions at the interface.

(iv) The boundary condition on the particle surface is

$$\mathbf{U}_p' = \mathbf{U}'_c + \mathbf{\omega}'_c \times (\mathbf{x} - \mathbf{x'}_c), \quad (8)$$

where $\mathbf{U}'_c$, $\mathbf{\omega}'_c$, and $\mathbf{x'}_c$ are the translation velocity, the angular velocity and the location of the center of mass of the particle, respectively in a stationary reference frame, and $\mathbf{U}_p$ is the particle velocity.

The equations of motion for the particle are given by the Newton–Euler equations [32]. The translation velocity of the
The resultant dimensionless equations are
\[ \nabla \cdot \vec{u} = 0, \]
\[ \frac{\partial \vec{u}}{\partial t} + \vec{u} \nabla \vec{u} = \left( -\frac{d\vec{U}_c}{dt} \right) - \frac{\alpha}{\tau} - \nabla P + \frac{1}{Re} \nabla \left( \vec{u}(\nabla \vec{u} + (\nabla \vec{u})^T) \right), \]
\[ \vec{u} = \vec{u}_0 - \vec{U}_c \text{ as } |\vec{x}| \to \infty. \] (18)

Here, \( Re \) is the Reynolds number, \( \rho U_c H' / \mu_2; D_p \) is the dimensionless particle size, \( d/H' \); and dimensionless viscosity is defined as
\[ \tau = \begin{cases} \mu_1 / \mu_2 & y \leq h \\ 1 & y > h, \end{cases} \] (19)

where, \( h \) is the dimensionless interface location, specifically holdup of fluid 1.

The IBM is used to solve the fluid flow equations (18) along with the particle motion equations (9) and (10). In the next Section, the implementation of IBM is discussed in detail.

3. Immersed boundary method

The IBM captures the interaction of moving solid boundaries with fluid flow [26]. This method uses a non-body conformal grid where two separate grids are used in a domain \( \Omega \) as shown in figure 2. An Eulerian-fixed grid (\( \bar{x} \)) is used for the fluid flow and a Lagrangian grid (\( \hat{x} \)) is used on the particle surface to capture the particle dynamics. Here \( i \) and \( k \) represent the Eulerian and Lagrangian grid numbers, respectively. The lowercase and uppercase letters are used to represent the Eulerian fluid domain and Lagrangian grid respectively.

The immersed boundary is represented as a simple closed curve \( \Gamma' \) of length \( L_b \) by the parametric representation \( \bar{x}(s) \), \( 0 \leq s \leq L_b \). Here, \( s \) is the arc length parameter representing the solid boundary. The presence of a solid boundary is represented as an external body force in the Navier–Stokes equations (20).

The dimensionless equations governing the fluid flow field with immersed boundary, in the moving reference frame are given by
\[ \nabla \cdot \vec{u} = 0, \]
\[ \frac{\partial \vec{u}}{\partial t} + \vec{u} \nabla \vec{u} = \left( -\frac{d\vec{U}_c}{dt} \right) - \frac{\alpha}{\tau} - \nabla P + \frac{1}{Re} \nabla \left( \vec{u}(\nabla \vec{u} + (\nabla \vec{u})^T) \right) + \vec{f}(\bar{x}, t), \] (20)

where \( \vec{f}(\bar{x}, t) \) is the external body force on the fluid domain \( \Omega \) which arises due to the presence of the solid particle. This force is calculated such that it satisfies the no-slip condition on the surface of the particle. First, the force \( \left( \vec{F}(\hat{x}_k, t) \right) \) is found on the particle surface (on the Lagrangian grid), and then interpolated to the Eulerian grid \( \bar{x} \) using
\[ \vec{f}(\bar{x}, t) = \sum_k \vec{F}(\hat{x}_k, t) \delta(\bar{x} - \hat{x}_k) \Delta s, \] (21)
where $\delta (\vec{x} - \vec{X})$ is the Dirac delta function and $\Delta s$ is the Lagrangian step length.

To satisfy the no-slip condition on the particle surface, the velocity field needs to be interpolated from the fluid domain (Eulerian grid) to the particle surface. This is done using

$$
\hat{U}(\vec{X}_k, t) = \sum_i \sum_j \hat{U}(\vec{x}, t) \delta(\vec{x} - \vec{X}_k) \Delta x \Delta y,
$$

where $\hat{U}(\vec{x}, t)$ is the interpolated velocity on the particle surface. The Eulerian and Lagrangian variables are related by the Dirac delta function as shown in equations (21) and (22), which is approximated as

$$
\delta(\vec{x} - \vec{X}) = d1(x_i - X_k) d1(y_j - Y_k),
$$

where,

$$
d1(r) = \begin{cases} 
\frac{(1 - |r|/\Delta r)}{\Delta r} & \text{if } |r| \leq \Delta r \\
0 & \text{otherwise,}
\end{cases}
$$

$k$ is the Lagrangian grid number, $r = \vec{x} - \vec{X}_k$ and $\Delta r$ is the grid size. This representation is equivalent to a bilinear interpolation between the Eulerian and the Lagrangian variables.

$$
\int_{\Gamma} (-p\vec{T} + \vec{r}) \cdot d\vec{S} \text{ in equations (9) in terms of the immersed boundary force is given by equation (25) as derived in [32]}
$$

$$
\int_{\Gamma} (-p\vec{T} + \vec{r}) \cdot d\vec{S} = -\rho_f \int_{V_p} \vec{f} dV + \rho_f V_p \frac{d\vec{U}_f}{dt}.
$$

The type of the grid and the numerical scheme used to solve fluid flow and particle motion equations using IBM are discussed in the next Section.

### 3.1. Numerical scheme

The fluid flow equations are solved in the reference frame that moves with the particle. This facilitates employing a finer grid near the particle and a coarser grid away from the particle as shown in figure 3. Here $N_f$ is the total number of grids in the fine region and $N_c = N_{c1} + N_{c2}$ is the total number of grids in the coarse region. $l$ is the length of finer grid region and is dependent on the particle size. The step size in coarse grid region is $(H - l)/(N_c - 1)$ and in finer grid region is $l/(N_f - 1)$. Such non-uniform gridding is computationally efficient as it captures the rapidly varying flow field near the particle. Re-meshing or use of adaptive mesh near the particle is avoided here since we work in the moving reference frame. As we calculate the lift force curves to determine the equilibrium positions, the moving reference frame is elegant, since the position of the particle is fixed at different locations in the direction transverse to the flow.

A staggered grid is used to solve the Navier–Stokes equations using pressure projection approach [34]. Equation (20) is solved using a projection method where the fractional step approach is used. The non-linear advection and diffusion terms are discretized using a second order central difference scheme and the semi implicit Crank–Nicolson method respectively. At the beginning of each time step, the solution $\vec{u}^{n-1}$, $\vec{u}^n$ is used to calculate $\vec{u}^{n+1}$.

The time advancement and spatial discretization is described next. As a first step, the first predictor velocity
\[ \vec{u}^* \text{ is calculated without the body force as} \]
\[
\frac{\vec{u} - \vec{u}^p}{\Delta t} = -\alpha - \nabla P^p + \frac{1}{2\rho_c} \left( \nabla \left( \mu_c (\nabla \vec{u}^p + (\nabla \vec{u}^p)^T) \right) + \nabla \left( \mu_r (\nabla \vec{u} + (\nabla \vec{u})^T) \right) \right) \quad (26)
\]
\[
\vec{u}^* = \vec{u} + \Delta t \vec{u}^p. \quad (27)
\]

Here, \( \vec{u}^* \) is the second predictor velocity that includes the body force \( \vec{f} \) due to the presence of the solid particle and its evaluation is given in section 3.2.

The third predictor velocity, \( \vec{u}^{**} \), which includes the pressure correction is calculated as
\[
\vec{u}^{**} = \vec{u}^* + \Delta t \nabla P^p. \quad (28)
\]

The pressure is determined using the pressure Poisson equation (29)
\[
\nabla^2 P^{n+1} = \frac{(\nabla \vec{u}^{**})}{\Delta t}. \quad (29)
\]

The pressure is calculated such that the obtained velocity profile is divergence free, resulting in
\[
\vec{u}^{n+1} = \vec{u}^{**} - \Delta t \nabla P^{n+1}. \quad (30)
\]

In the above equations, \( \vec{u}, \vec{u}^*, \vec{u}^{**} \) are the intermediate velocity components between the steps \( n \) and \( n + 1 \), and \( \Delta t \) is the computational time step.

3.2. Boundary force evaluation

The procedure to find the Lagrangian force is given, so that the second predictor velocity \( \vec{u}^* \) satisfies the boundary values \( \tilde{U}^* \). First, \( \tilde{U} \) is obtained from equation (26) and interpolated to the Lagrangian grid to obtain the velocity \( \tilde{U}(\tilde{x}_k) \), as
\[
\tilde{U}(\tilde{x}_k) = \sum_x \sum_y \tilde{u}(\tilde{x}) \delta(\tilde{x} - \tilde{x}_k) \Delta x \Delta y. \quad (31)
\]

The above interpolation procedure is applied to equation (27) directly, to yield
\[
\sum_x \sum_y \tilde{f}^e(\tilde{x}) \delta(\tilde{x} - \tilde{x}_k) \Delta x \Delta y = \frac{\tilde{U}^*(\tilde{x}_k) - \tilde{U}(\tilde{x}_k)}{\Delta t} \quad (32)
\]
where \( \tilde{U}^*(\tilde{x}_k) \) is the interpolated velocity of \( \vec{u}^* \) at the Lagrangian grid \( k \). By setting \( \tilde{U}^*(\tilde{x}_k) = \tilde{U}_p^{n+1}(\tilde{x}_k) \), the force field \( \tilde{f}^e \) is determined such that \( \vec{u}^* \) satisfies the boundary condition on the particle surface.

Substituting equations (21) in (32), we obtain
\[
\sum_m \sum_x \sum_y \tilde{f}^m(\tilde{x}_m) \delta(\tilde{x} - \tilde{x}_k) \delta(\tilde{x} - \tilde{x}_m) \Delta x \Delta y \Delta \]
\[
s = \frac{\tilde{U}_p^{n+1}(\tilde{x}_k) - \tilde{U}(\tilde{x}_k)}{\Delta t}. \quad (33)
\]

Here \( \tilde{U}_p^{n+1}(\tilde{x}_k) \) is the velocity of the rigid particle at the Lagrangian grid \( k \) at time instant \( 'n + 1' \), which is given by Newton-Euler equations. This results in a system of linear equations, which are solved to obtain \( \tilde{f}^e(\tilde{x}_k) \) at the Lagrangian markers. Equation (21) is used to interpolate the body force on the Eulerian grid. The Newton-Euler equations are discretized as [32]
\[
\tilde{U}_p^{n+1} = \tilde{U}_p^{n+1} \times \tilde{\vec{x}} \quad (34)
\]
\[
\tilde{U}_c^{n+1} = \left( 1 + \frac{\rho_f}{\rho_p} \right) \tilde{U}_c - \frac{\rho_f}{\rho_p} \tilde{U}_c^{n-1} - \frac{\rho_f}{\nu_p \rho_p} \sum_{x,y} \tilde{f}^e \Delta x \Delta y \Delta t \quad (35)
\]
\[
\tilde{\omega}_c^{n+1} = \left( 1 + \frac{\rho_f}{\rho_p} \right) \tilde{\omega}_c - \frac{\rho_f}{\rho_p} \tilde{\omega}_c^{n-1} - \frac{\rho_f}{I_p \rho_p} \sum_{x,y} (\tilde{x} \times \tilde{\vec{f}}) \Delta x \Delta y \Delta t \quad (36)
\]
and the particle path is calculated using
\[
\left( \frac{d\tilde{x}}{dt} \right)^{n+1} = \tilde{U}_c^{n+1}. \quad (37)
\]

3.3. Algorithm

The algorithm to solve the fluid flow and the particle migration in each time step is summarized below:

1. Solve equation (26) to obtain the intermediate velocity \( \tilde{u} \)
2. Calculate \( \tilde{U} \) at the particle surface using equation (31)
3. Calculate the Lagrangian body force \( \tilde{f}^e(\tilde{x}_m) \) using equation (33)
4. Distribute the Lagrangian body force to the Eulerian grid using equation (21)
5. Calculate \( \tilde{u}^* \) and \( \tilde{u}^{**} \) using equations (27) and (28)
6. Calculate the pressure using the pressure Poisson equation (29)
7. Update the fluid velocity \( \tilde{v}^{n+1} \) using equation (30)
8. Transform \( \tilde{v}^{n+1} \) to the Lagrangian grid using equation (22) and calculate the body force acting on particle surface using equation (33)
9. Calculate the particle velocity and rotation at \( n + 1 \) using the Newton-Euler equations (34)–(36)

Steps (1)–(9) are repeated over each time step to solve for the fluid flow and the particle motion. The direction of the migration of the particle is obtained from the lift force, which is discussed next.
3.4. Lift force calculation

The lift force is exerted on the particle in the lateral direction (y-direction). This force shows the direction in which the particle migrates. The point at which the lift force is zero represents the equilibrium position, where the particle focuses. To calculate the lateral force exerted on the particle due to inertia, we assume that the particle translates freely in the flow direction and rotates freely and it does not move in the lateral direction [18]. The algorithm given above is followed with the particle translation velocity in the y-direction \( (U_{c,y} = 0) \) set to zero. The force on the particle surface is calculated as given by Step (8) of the algorithm and this force is transformed to the Eulerian grid as given in Step (4) of the algorithm. Since this represents the force per unit area acting on the fluid, the lift force acting on the particle is calculated using

\[
F_j = - \sum_{x,y} f_j \Delta x \Delta y \tag{38}
\]

where the lift force has been non-dimensionalized using \( \rho \gamma U^2 / \Delta H \). The lift force thus calculated includes contributions from both the wall and shear gradient lift forces.

An alternative method to determine the equilibrium position is to track the trajectory of the particle. The simulations performed by us showed that the equilibrium position determined from particle trajectory and lift force curve are identical. We however use the lift force curve to determine the equilibrium position in this work as it is computationally elegant. The model equations and the numerical procedure to determine the flow field and the lift force have been discussed so far. We discuss the results of particle migration in a stratified Poiseuille flow in the next Section.

4. Particle focusing in a stratified Poiseuille flow

The interface location/holdup for the Poiseuille flow is dependent on the flowrate ratio \( (Q_2 / Q_1) \) and the viscosity ratio \( (\mu_t / \mu_p) \). This relationship of the interface location/holdup on flowrate ratio and viscosity ratio is given in the appendix. The non-dimensional variables governing the system are the Reynolds number \( (Re) \), flowrate ratio \( (Q_r) \) viscosity ratio \( (\mu_r) \) dimensionless particle size \( (D_p) \) and holdup \( (h) \). The viscosity ratio less than one is considered in analysis. Here, the more viscous fluid is on top of the less viscous fluid and the particle enters the channel in the more viscous fluid.

4.1. Grid independence analysis

The flow profile is solved on a non-uniform grid. A finer grid is used near the particle and a coarser grid elsewhere. The variation of lift force along the channel height is shown in figure 4 for different grid sizes. We observe that the lift force primarily depends on the number of grids near the particle. We conclude that \( N_c = 100 \) and \( N_f = 80 \) are sufficient to obtain a grid independent solution for the parameters used in figure 4. The number of grids needed to get a grid independent solution depends on the operating parameters such as viscosity ratio and diameter of the particle. The maximum number of grids required for \( \mu_r = 0.25 \) were \( N_c = 300 \) and \( N_f = 160 \). Grid independence is established for all the results presented in this work.

4.2. Particle migration in single phase Poiseuille flow

The numerical implementation of the IBM in the moving reference frame is validated with the results reported by Feng et al [16]. Here, the Reynolds number is 40 (defined with the maximum velocity) and \( D_p = 0.25 \). The lift force curve obtained in the present work is shown in figure 5. There exist three equilibrium positions to which the particle can migrate. The equilibrium position between the center of the channel and the bottom (top) wall arises from the balance between the wall repulsion lift force and the shear gradient lift force and is obtained as \( 0.252 (0.748) \). These two equilibrium positions represented by solid circles are stable. There exists an equilibrium position at the center because of the symmetry of the flow profile. This focusing position is unstable and is represented by an open circle. Particle entering the channel above (below) the unstable equilibrium position moves towards the top (bottom) equilibrium position. The locations of these points are the same as those reported by Feng et al [16].

4.3. Effect of flowrate ratio

The particle has three equilibrium positions in Poiseuille flow. When two fluids of different viscosities flow parallel to each other, the equilibrium positions change based on the flowrate ratio and the viscosity ratio for a given particle and \( \text{Re} \). Variation of the equilibrium positions with the flowrate ratio is shown in figure 6 for \( \text{Re} = 10 \), \( \mu_r = 0.5 \), and \( D_p = 0.2 \). Here, the interface location depends on the flowrate ratio and is depicted as a solid line in figure 6. The more viscous fluid lies above the interface. The value of \( Q_2 \) is fixed in our simulation, and
the flowrate ratio is varied by changing $Q_1$. As the flowrate ratio increases the total flowrate in the channel increases which requires a higher driving force to pump the fluids across the channel. This results in an increase in the pressure drop which is shown in figure 6 as a dashed line. The shape of the velocity profile changes with the flowrate ratio in stratified flows. This alters the particle equilibrium positions.

There exist three equilibrium positions for each flowrate ratio as shown in figure 6. Two of these are stable positions, represented by the solid circles and one is unstable, represented by the open circle. The equilibrium positions are not symmetric about the center of the channel as the velocity profile is not symmetric due to viscosity stratification. This asymmetry in equilibrium positions can be explained by constructing the lift force curve. Variation of the total lift force for $Re = 10$, $\mu_r = 0.5$, $D_p = 0.2$, $Q_r = 1$ and $Q_r = 9$ is shown in figures 7(a) and (b) respectively. The interface location is represented by the dashed line and the stable and unstable equilibrium positions are represented by the solid and open circles, respectively. The particles entering above (below) the unstable equilibrium position migrate towards the top (bottom) equilibrium position. For $Q_r = 1$, one stable equilibrium position (top) exists in the high viscous fluid and the unstable and the other stable (bottom) equilibrium positions exist in the low viscous fluid. It is seen that the particles present in the high viscous fluid will focus only at the equilibrium position in the high viscous fluid since it enters above the unstable equilibrium position. The migration of the particles from high viscous fluid to low viscous fluid is not possible for $Q_r = 1$. As depicted in figure 7(b), all three equilibrium positions exist in the low viscous fluid for $Q_r = 9$. The particles in the high viscous fluid will cross the interface and migrate to the equilibrium position in the low viscous fluid.

It is observed that as the flowrate ratio increases, the upper focusing position shifts downward and the particle migrates away from the top wall. This equilibrium position crosses the interface beyond a certain flowrate ratio as shown in figure 6. The migration of the particles from the more viscous fluid to the less viscous fluid is governed by the top equilibrium position. So, hereafter we focus only on the top equilibrium position as its location determines the migration of the particle from the more viscous fluid to the less viscous fluid. Specifically, if this lies in the lower fluid then we are assured that all particles entering the channel with the more viscous fluid will migrate to the low viscous fluid.

4.4. Effect of viscosity ratio

Another parameter which influences the particle migration is the viscosity ratio. The shape of the velocity profile changes with the viscosity ratio in stratified flows. This alters the particle equilibrium positions. Variation of the top stable equilibrium position with the flowrate ratio for different viscosity ratios is shown in figure 8. As discussed earlier, as the flowrate ratio increases, the particle migrates from the more viscous fluid to the less viscous fluid. There exists a critical flowrate ratio beyond which this occurs and this depends on the viscosity ratio.

For a given flowrate ratio, as the viscosity ratio decreases the velocity gradient increases and shear gradient decreases in the more viscous fluid. As a result the wall lift force increases and the shear gradient lift force decreases in the more viscous fluid. Hence the particle migrates away from the top wall as the viscosity ratio decreases. So a lower flowrate ratio is required for the particle separation from the more viscous to the less viscous fluid as viscosity ratio decreases as shown in figure 8. To conclude, as the viscosity ratio decreases (viscosity of the less viscous fluid is decreased), the critical flowrate ratio above which particle transfer across the two phases is ensured also decreases.

4.5. Effect of particle size

The dependence of the equilibrium position for two different particle diameters is shown in figure 9 for $Re = 10$ and $\mu_r = 0.667$. For $Q_r = 1$, the small particle focuses near the top wall as compared with the large particle. As the flowrate ratio increases, the large particle focuses towards the wall and the small particle focuses towards the center. This implies that the smaller particle requires a lower flowrate for transferring from the more viscous to the less viscous fluid as shown in figure 9. This can be explored in design and operation of size-based separation of particles as the critical flowrate ratio across which particles are transferred depends on the particle size. Even though the critical flowrate ratio is less for the small particle; it requires more time for focusing as the smaller particle has low migration velocity compared to the larger particle [10].

This slow migration phenomenon of small particles can be seen in the particle path lines. Path lines of two different size particles are depicted in figure 10 for $Re = 10$, $Q_r = 9$ and $\mu_r = 0.667$. Both particles start at $H = 0.8$ and their positions
Figure 6. Variation of the equilibrium positions as a function of the flowrate ratio for $Re = 10$, $\mu_r = 0.5$ and $D_p = 0.2$ in a stratified Poiseuille flow. The solid line represents the interface location and the dashed line represents the pressure drop. As the flowrate ratio increases, the pressure drop increases and the particle migrates from more viscous to the less viscous fluid.

Figure 7. Variation of the total lift force with the channel height for $Re = 10$, $\mu_r = 0.5$, $D_p = 0.2$ (a) $Q_r = 1$ and (b) $Q_r = 9$ in a stratified Poiseuille flow. The solid and open circles represent stable and unstable equilibrium positions respectively. Interface location is represented by the dashed line.

are tracked with time. As shown in figure 10, the large particle reaches its equilibrium position much faster than the small particle. This difference arises as the smaller size particle has low migration velocity and hence it requires more time to reach the equilibrium position. While designing a particle separator based on size, the length of the microchannel is hence a design
variable and is usually chosen such that only larger particles are focused [4].

4.6. Critical flowrate ratio

It is seen from the above analysis that, there exists a critical flowrate ratio beyond which the particle migrates from one fluid to the other. Variation of the critical flowrate ratio ($Q_{cr}$) with the viscosity ratio for different particle diameters is shown in figure 11. The critical flowrate ratio decreases on reducing the viscosity ratio as discussed in section 4.4. This critical flowrate ratio strongly depends on the particle size. A smaller particle needs a lower flowrate ratio for migrating from the more viscous fluid to the less viscous fluid. This result has implication in selection of flowrate ratio to achieve particle separation in inertial focusing devices. For a given viscosity ratio (e.g. 0.5), if a flowrate ratio (e.g. 2.5) is chosen between the critical flowrates (2.3 and 3) of two different particle sizes (0.1 and 0.15), the two particles can be separated since, the smaller size (0.1) particle will migrate to the lower viscous

Figure 8. Variation of the equilibrium position with the flowrate ratio for different viscosity ratios (a) $\mu_r = 0.667$, (b) $\mu_r = 0.5$, (c) $\mu_r = 0.4$, (d) $\mu_r = 0.333$, (e) $\mu_r = 0.25$, (f) $\mu_r = 0.2$ for Re = 10 and $D_p = 0.2$; the solid line represents the interface between two fluids.
Figure 9. Variation of the equilibrium position with the flowrate ratio for different particle diameters for Re = 10 and $\mu_r = 0.667$ and the solid line represents the interface between two fluids.

Figure 10. Path lines of two different size particles in a stratified Poiseuille flow for Re = 10, $\mu_r = 0.667$ and $Q_r = 9$. The small particle migrates slowly compared with the larger one hence required more time or length to reach the equilibrium position.

Fluid and the larger particle (0.15) will remain in the high viscous fluid. If the flowrate ratio chosen is above the critical flowrate ratio of both the particles, both the particles will migrate to the low viscous fluid. However larger particles will migrate at shorter lengths compared to the smaller particles. Hence, in this case, the separation of the particles depends on the length of the channel. If the channel is very short, both the particles will remain in the high viscous liquid and if the channel is very long, both the particles would have migrated to the low viscous liquid. Hence an optimal channel length is to
be chosen to enable separation of the particles. This possibly explains the experimental observation made by Xu et al. [10] on the migration of large particles from the suspension fluid to the low viscous fluid within the channel length used in the experiments.

Based on our simulations of the dependency of the critical flowrate ratio on the viscosity ratio and the dimensionless particle size, an empirical correlation has been developed as given below

\[ Q_{cr} = 16 \mu r D_p^{0.5} \]  

(39)

The simulated data shown in figure 11 has been used to develop the above correlation. The range of validity of this correlation is \(0.2 < \mu_r < 0.7, 0.1 < D_p < 0.2\) and \( Re = 10\). This correlation predicts the simulated data within an average absolute relative error of 5%. From the correlation it can be seen that the critical flowrate ratio varies linearly with viscosity ratio and varies with the square root of particle diameter. The linear variation captured by the correlation is inline with the observation in figure 11 where the critical flowrate ratio varies almost linearly with viscosity ratio, especially for large particles. This relationship will help experimentalists choose operating conditions such as the flowrate ratio to guarantee migration of particles of a given diameter from one fluid to the other of given viscosity ratio for \(Re = 10\).

4.7. Design of stratified flow particle separator

The simulation results obtained in this work can be used to design a particle separator based on stratified flows. Such a design is illustrated in this section. Suppose we have a suspension of viscosity 0.0015 kg m\(^{-1}\) s and density 1000 kg m\(^{-3}\) with neutrally buoyant particles of diameter 10 \(\mu m\) and 20 \(\mu m\) and it is required to separate the particles in a microfluidic channel using stratified flow. Let the channel be of width 100 \(\mu m\) and depth 300 \(\mu m\) so that the assumption of 2D flow is satisfied. Let the exchange liquid (low viscous liquid) be chosen as water with a viscosity of 0.001 kg m\(^{-1}\) s. To achieve particle separation using stratified flow configuration, let the flowrate of high viscous liquid be set at 270 \(\mu l\ min^{-1}\). These conditions are chosen such they match the simulation conditions in figure 9. From this figure, the critical flowrate ratios for 10 \(\mu m\) and 20 \(\mu m\) particles are \(4\) and \(5\), respectively. To separate the particles of both the sizes from the high viscous liquid, flowrate of the low viscous liquid should be chosen beyond that corresponding to \(Q_r = 5\). For example, 1620 \(\mu l\ min^{-1}\) which corresponds to \(Q_r = 6\). In this case, both the 10 \(\mu m\) and 20 \(\mu m\) particles migrate to the low viscous liquid. However, if the objective is to separate the two particles based on size, then the flowrate of low viscous liquid should be chosen such that \(Q_r\) lies between 4 and 5. For example, a water flowrate of 1215 \(\mu l\ min^{-1}\) corresponding to \(Q_r\) of 4.5 can be used. In this case, particles of 10 \(\mu m\) will get separated from the high viscous liquid to the low viscous liquid and the particles of 20 \(\mu m\) will remain in the high viscous liquid, thus achieving a size based separation. Further, if it is required to separate the 20 \(\mu m\) particles also from the high viscous liquid, a second microchannel can be used in which the water flow corresponding to more than \(Q_r\) of 5 (water flowrate of more than 1350 \(\mu l\ min^{-1}\)) is used. Thus the results of this simulation study can be used for design of particle separators using stratified flow for complete separation or size based separation.

5. Summary and conclusions

Inertial focusing in co-flowing fluids has been experimentally shown recently, to have better control over equilibrium positions, compared to inertial focusing in single phase flow. In this work, we have computationally studied the migration of a particle from one fluid to another in a stratified Poiseuille flow. The two fluids have different viscosities and flow parallel to each other in a stratified flow. The governing equations have been solved numerically in a moving reference frame using the IBM, for the first time in the literature.

In the stratified Poiseuille flow, there exists a critical flowrate ratio beyond which the particle migrates from the more viscous fluid to the less viscous fluid. This critical flowrate ratio increases with viscosity ratio and increases with particle size. The results obtained in this work, can be used to obtain operating parameters to efficiently separate particles from one fluid to the other. It has been shown that separation of particles of different diameters can be achieved by suitable selection of flowrate ratio.

Our analysis shows that the equilibrium position is not very sensitive to the size of the particles. However, the difference in the migration velocity can be exploited to separate particles based on size since larger particles focus faster and require shorter channel lengths as compared to smaller particles. The approach adopted in this work can be used to design microfluidic systems for membrane less transfer of particles from one fluid to another fluid, as illustrated by the design example.
To the best knowledge of the authors, this is the first modeling work performed to study particle migration in a 2D stratified flow. This study can be extended to analyze particle migration in a 3D stratified flow. These 3D simulations would be able to capture the inflection point focusing, which was experimentally observed by Lee et al. [12]. The framework developed in this work can also be extended to deformable particles like cells and liquid drops. The deformability of the cells induces an additional lift force which changes the equilibrium position compared to a rigid particle. Although IBM can be used to simulate lateral migration of deformable particles, the simulations would require very small grid resolution and the solution can be very sensitive to the Dirac delta function stencil. Further, because of the deformation, it may be difficult to use the moving reference frame for such simulations.

Calculation of interface location in the stratified Poiseuille flow

Here, we present a 2D model for predicting the fully developed velocity profile and the interface location as a function of the flowrate ratio \( Q_1 = Q_1/Q_2 \) and the viscosity ratio \( \mu_r = \mu_1/\mu_2 \). A schematic of the co-current flow of the two fluids is shown in figure 1. Assuming the fluid flow as steady, laminar, fully developed and pressure driven, the equations governing the fluid flow in the two layers in dimensional form are

\[
\nabla \cdot \mathbf{u}_i' = 0, \quad \nabla \cdot \mathbf{u}_2' = 0, \\
\mu_1 \frac{\partial \mathbf{u}_1'}{\partial y'} = -\frac{\Delta p}{\mu_1 L}, \\
\mu_2 \frac{\partial \mathbf{u}_2' }{\partial y'} = -\frac{\Delta p}{\mu_2 L}.
\]

Subject to the boundary conditions

\[
\mathbf{u}_1' = 0 \text{ at } y' = 0, \\
\mathbf{u}_2' = 0 \text{ at } y' = H', \\
\mathbf{u}_1' = \mathbf{u}_2' \text{ at } y' = h', \\
\mu_1 \frac{\partial \mathbf{u}_1' }{\partial y'} = \mu_2 \frac{\partial \mathbf{u}_2' }{\partial y'} \text{ at } y' = h'.
\]

The solution to this system results in the following flow field is obtained

\[
\mathbf{u}_1' = \frac{\Delta p}{2\mu_1 L} y' (W_1 - y'),
\]

\[
\mathbf{u}_2' = \frac{\Delta p}{2\mu_2 L} (H' - y') (y' - W_2).
\]

The flowrates of the two fluids are given as

\[
Q_1 = \frac{\Delta p}{12\mu_1 L} a,
\]

\[
Q_2 = \frac{\Delta p}{12\mu_2 L} b.
\]

where the constants are defined as,

\[
W_1 = H' + W_2, \\
W_2 = \frac{(H' - H')}{(1 -\mu_r)} (H' - H'), \\
a = 3W_1 h' H' - 2h'^2, \\
b = H'^3 - 3W_2 H'^2 - 3H' h'^2 + 6H' h' W_2 + 2h'^3 - 3W_2 h'^2 \\
\mu_r = \mu_1/\mu_2.
\]

Now, the ratio of the flowrates is

\[
\frac{Q_1}{Q_2} = \frac{1}{\mu_r b}.
\]

Equation (A47) can be solved using non-linear solver in Wolfram Mathematica to obtain the interface location at different flowrate ratios and the viscosity ratios.

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