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Direct numerical simulation of deformable droplets motion with uncertain physical properties in macro and micro channels

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ABSTRACT

The lateral migration rate, equilibrium position of droplets and their final distribution determine the main characteristics of multiphase flows within channels such as total flow rate and pressure drop. Since the performance of inertial microfluidics in the context of classification and sorting of cells relies deeply on migration rate as well as the distribution of particles suspended in the carrier fluid moving within a micro-channel, the subject becomes more critical when we move toward micro-scale problems . The main parameters dominate the flow field are viscosity ratio, density ratio, drops deformability, Reynolds number (Re) and the ratio of drops diameter to channel height. Changes in these parameters result in new and different flow conditions, and therefore lead to different migration rates and particle distribution patterns. In order to understand the effect of uncertainty in material properties such as viscosity, we conduct numerical simulations on deformable droplets motion within two-dimensional macro and micro-scale channels using combination of front tracking method and a newly proposed Uncertainty Quantification (UQ) model. The deformable droplet motion in both macro and micro-scale channels are studied in two separate sections of this paper. In each section, the deterministic case is investigated using front tracking method and the accuracy of the results is verified by comparison with the available data in the literature. Next, along with Monte–Carlo methods, the proposed stochastic particle tracking (SPT) approach is applied to propagate the uncertainties associated with droplet physical properties to flow variables. Numerical experiments indicate a faster convergence rate for this approach with respect to the number of samples in comparison with Monte Carlo and Quasi-Monte Carlo simulations.

1. Introduction

The motion of deformable droplets and bubbles suspended in an ambient fluid has been an active area of research in the recent decades as its outcomes can be used in different branches of science and technology such as microfluidics for cell sorting and separation [1,2] and pumping of slurries and crude oil in pipelines and refinery plants [3,4]. The equilibrium position of drops and their final distribution in the channel is of significant importance as it determines the total flow rate, pressure drop as well as the performance of inertial microfluidics in classification and enrichment of particles and cells [2,5]. Experiments and numerical simulations ranging from macro-scale to micro-scale have been done so far in order to investigate the migration and behaviors of bubbles and droplets in different channel flow conditions [6–10]. Depending on the flow conditions, the main parameters affecting the lateral migration of deformable droplets and bubble and consequently their equilibrium position are viscosity ratio, density ratio, drops deformability, Reynolds number (inertia) and the ratio of drops diameter to channel height [6,8]. Hiller and Kowalewski [11] experimentally showed that drops with a viscosity ratio (ratio of droplet viscosity to ambient viscosity) in the order of 0.1 accumulate around the channel axis. Moreover, at a high viscosity ratio of 1, drops reach their equilibrium positions somewhere between channel centerline and its wall. Karnis et al. [12] observed that in low Reynolds Poiseuille flow with negligible inertial force, highly deformable drops move toward the centerline of the channel when the viscosity ratio of the droplet and the ambient fluid is low. When the viscosity is large, droplets behave like solid spherical particles and concentrate at a distance halfway between channel wall and its axis. Matas et al [13] conducted an experimental study to investigate the effect of inertia on the motion of suspended particles. They examined the migration of suspended spherical

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particles in Poiseuille flow at a wide range of Reynolds numbers (Re) from 67 to 2400 and showed that particles move toward the channel wall as the inertia effect (Re) gets larger.

Chan and Leal [14] used theoretical approach to investigate the lateral migration of small spherical droplets in Poiseuille flow and considered the effects of both inertia and drops deformability. They obtained the final shape of the drop at the equilibrium position as well as the axial velocity of the deformed drop. They predicted that drops move toward the channel wall when the viscosity ratio varies between 0.5 and 10, but for the ratio less than 0.5 or greater than 10, the drop tends to migrate toward centerline. Mortazavi and Tryggvason [6] numerically studied the lateral migration of a neutrally buoyant deformable droplet in a two-dimensional Poiseuille flow. Regarding the effect of viscosity ratio, in agreement with Chan and Leal [14], they found out that at low inertia limit (small Reynolds number; Re <1), the motion of the droplets depends strongly on the ratio of the drop viscosity to carrier fluid. For viscosity ratio equal to 0.125, the droplet tends to migrate toward the centerline, while it approaches the channel wall for viscosity ratio of 1.0. Their results showed that the rate of drop migration increases as it becomes more deformable. For higher Reynolds numbers in the range of 5 to 50, droplet shows two different behaviors, based on flow conditions. It either settles down at a distance halfway between channel axis and its wall, or shows oscillatory motion. The amplitude of this transient oscillation in drop position gets larger as the Reynolds number or drop density increases, or the viscosity of the drop decreases. They also determined that drops with higher density tend to move away further from the channel wall in comparison with lighter drops and show oscillatory behaviors as the Reynolds number is raised. Chen et al. [7] conducted a numerical and experimental study on migration of droplets in micro-channels due to inertial force. In their work, simultaneous effects of inertia and drop deformability were studied. They determined that droplets larger than half of the channel height settle down at the centerline in the height direction, while two other equilibrium positions were observed between the centerline and the wall in the width direction. As the Reynolds number is increased, the equilibrium position of micro-scale drops shifts toward channel centerline. This phenomenon is a result of changing in lift force acting on drops due to high deformation in their shapes. Dabiri et al. [15] showed that deformable bubbles accumulate around the centerline of the vertical channel in bubbly upflows and the flow rate is close to the single phase flow rate. However, with less deformable bubbles concentrating near channel walls, the flow rate deviates significantly from single phase flow trend and gets much smaller.

While as discussed, droplets equilibrium position in micro-channels has been the subject of different numerical studies and as a result the major contributing factors affecting it have been determined, Stan et al. [8] have also measured and calculated the equilibrium position of micro-scale buoyant and neutrally buoyant droplets in micro-channels and showed that existing analytical models [13,14,16] fail to predict the correct equilibrium position and consequently the lift forces acting on particles in micro-channels. The parametric uncertainty can be a contributing factor to this inaccuracy.

The previous studies mostly concentrate on the effect of physical parameters on migration of droplets and their equilibrium distribution patterns and hence the effects of uncertainty in physical properties of suspended particles as well as ambient fluids on the flow condition have not been discussed so far in the literature. The parameters such as viscosity ratio, density ratio, Reynolds number, particle size and deformability can change the balance between the inertial lift force, deformation-induced lift force and wall confinement effect and therefore influence the distribution of suspended particles in the flow. Any uncertainties in droplet or the carrier fluid properties propagates into the whole flow domain and disturbs the balance between lift, inertial and drag forces acting on suspended particle resulting in a new equilibrium position and migration rate. In the present study, the flow regime is assumed to be laminar as the flow field in most applications in the micro-scale area, ranging from cell separation to heat sinks and heat pipes for space application, is the laminar flow regime [7,17–23]. Also, transition to turbulent flow can impose a pressure drop as high as 20–25 bars in the device [24,25] which makes the use of micro-scale devices for certain applications almost impossible. Here, we first investigate the transient motion of different droplets and bubbles in two-dimensional macro and micro-scale channels using front tracking method separately in two different sections. In each section after confirming the accuracy and validity of our numerical model for deterministic cases by comparing its results with the available data in the literature, the effects of uncertainties in specific physical properties are studied. A novel Uncertainty Quantification (UQ) method is proposed for this purpose. Comparison of our results with Quasi-Monte Carlo (with Sobol quasi-random sequence generator [26]) and Monte Carlo simulations for two canonical problems of two phase flows in macro/micro channels indicates both its accuracy and computational efficiency. Consequently, the required number of samples for obtaining statistics of the flow with a reasonable accuracy reduces considerably, when the proposed UQ approach is used. As such, computational superiority of this novel method with respect to the number of expensive deterministic CFD evaluations leads to a significant gain regarding the saving in computational resources.

2. Theoretical foundation for deterministic model

2.1. Governing equations

Consider the motion of a suspended deformable viscous particle carried by an ambient flow in a two-dimensional rectangular channel as shown in Fig. 1. The incompressible Navier–Stokes equations can be applied to analyze the flow motion within droplet and the surrounding fluid. In one-fluid approach [27,28], a single set of governing equations, Eq. (1), can be solved for the whole computational domain, as long as sharp changes in material properties such as viscosity and density are allowed and the effect of surface tension is included by adding an appropriate source term at the interface between two phases [27,28].

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla P + \nabla \cdot \mu\left(\nabla u + \nabla u^T\right) + \int_s \sigma \kappa n \delta\left(x - x_f\right) ds. \tag{1}$$

Here, u, P, ρ and μ are velocity, pressure, the density and viscosity fields, respectively. The last term in the right hand side of Eq. (1) represents the effect of surface tension (σ) which acts on the interface between two fluids. Here, the mean curvature for three and two-dimensional flows is dented by κ. Also, n is the unit vector normal to the interface. The surface tension acts only on the interface between phases and therefore is represented by the Dirac delta function (δ). The variables x and x_f are the point at which Eq. (1) is solved and a point at the interface of the two phases, respectively. Here, we consider the fluids to be incompressible as well as immiscible with constant physical properties. Therefore, the following set of equations is derived from the continuity equation for this two-phase flow system:

$$\nabla \cdot u = 0, \quad \frac{\mathrm{D}\rho}{\mathrm{D}t} = 0, \quad \frac{\mathrm{D}\mu}{\mathrm{D}t} = 0. \tag{2}$$