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Simulation of bubble dynamics in a microchannel using a front-tracking method

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ABSTRACT

By using a front-tracking approach for moving boundaries, whose surface properties are solved in terms of an immersed-boundary method, the dynamics of bubble transport in a microchannel is computationally studied. This methodology allows the simulation of a liquid–gas system with a realistically large density ratio. In accordance with the pressure-driven inlet/outlet condition generally encountered in experiments, a projection method enforcing incompressibility is implemented as the solution scheme. The approach is then applied to two unique problems of bubble dynamics in microchannels. The first is concerned with bubble transport in a channel with sudden contraction. A bubble slug is placed in the microchannel embedded with a pair of side blocks. In the flow driven by pressure difference, the bubble slug would pass through or be stuck by the blocks, depending on the variations of Reynolds number and Weber number. With such variations of key parameters, furthermore, the bubble slug may deform in different manners. In the second part, the ascending dynamics of multiple bubbles is investigated, specifically regarding their interactions. It is found that in the confined space of small scale, the behaviors of bubbles are constrained by the walls, and not much interaction between bubbles is observable particularly when the flow is dominated by an imposed pressure difference. If the channel is sufficiently wide, for a pair of rising bubbles which are lined in a row, substantial interactions between the bubbles and the walls are observed. By changing the dimensionless parameters of rising bubbles and the channel width, variations in bubble shape, rising trajectory, and the wakes behind bubbles are discussed based on such essential mechanisms as the interplay of vortices and nonuniform pressure field. Moreover, a third bubble is inserted at the center and the flow structure is analyzed.

1. Introduction

Transportation of bubbles is critical in various technologies such as mechanical fabrication, processes in chemical engineering, and applications of micro/nano fluidic devices that are being largely extended to biological and medical treatments. Examples of specific interest are given by the removal issue of CO_2 bubbles that are created at the anode of micro direct methanol fuel cells (μDMFC) and migrated to the diffusion layer, and transport of fluids in microreactors used in chemical industry. Although the motion of a bubble has been studied broadly in a large domain where buoyancy provides a key driving force both by experiment [1–3] and simulation [4–6], it is not considered to a similar extent in confined systems where the surface-to-volume ratio is essentially large and interfacial tension becomes dominant. In this regard, the work is purported to simulate and analyze the transport of bubbles in a small channel, which is an elemental geometry generically observed in micro devices.

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The front-tracking method adopted for the simulation was originally developed by Unverdi and Tryggvason [7] for multiphase flows and has been applied also to other moving boundary problems such as solidification [8] and flame propagation [9,10]. In view of its effective treatment and handling for the front which may accurately track the motions of interfaces without significant loss of mass conservation of different phases, the method has been applied successfully for simulation of multiphase flows with substantial deformation of interfaces [11–13]. The surface properties are treated by means of the immersed-boundary method [14], by which the singular sources of interfaces are spread to neighboring volumetric grid points. This methodology allows simulation of a liquid–gas system with realistically large density ratio. In the two-dimensional (2D) Cartesian coordinates, multiple bubbles or droplets can be simulated in the same domain without substantially increasing effort. The tool is thus preferable for numerical analysis of two-phase flow dynamics in a channel where multiple bubbles are considered. The solution scheme is based on the projection method [15]; but since it is generically fit for a Dirichlet boundary condition of velocity, a special treatment for pressure-driven inlet condition needs to be implemented, to account for the operation usually encountered in real situations.

The methodology is then used to analyze two crucial problems of bubble transport in microchannels that have not been well understood, i.e., passage of a bubble through obstructed areas and interactions between bubbles in confined space. The former is concerned with bubble transport in a microchannel with sudden contraction when the Reynolds number is not very large. The second problem regards the dynamics of multiple bubbles rising in parallel; understanding of their interactions is limited not only for confined space but also in an open domain that is usually considered. Through the studies based on the simple configurations, the behaviors of bubbles carried in devices of small scale shall be further comprehended and controlled.

2. Numerical methodology

The approach of front tracking [7] and its application in microfluidics are described in the following.

2.1. Front tracking method

The Navier–Stokes equations are solved for both gas and liquid phases in a unified domain:

$$\frac{\partial(\rho\mathbf{V})}{\partial t}+\nabla\cdot(\rho\mathbf{V}\mathbf{V})=-\nabla P+\rho\mathbf{g}+\nabla\cdot\mu_{\mathrm{eff}}\left(\nabla\mathbf{V}+\nabla\mathbf{V}^{T}\right)+\int_{\Delta s}\sigma_{\mathrm{eff}}\kappa\,\mathbf{n}\delta(\mathbf{r}-\mathbf{r}_f)da \tag{1}$$

where $\mathbf{V}$, ρ, and P are the velocity, density, and pressure respectively normalized by the characteristic bubble velocity V_c, liquid density ρ_ℓ, and the dynamic pressure $\rho_\ell V_c^2$, and t is time normalized by L_c/V_c, where L_c is the characteristic length. The effective viscosity μ_{eff} is the reciprocal of Reynolds number, $Re=\rho_\ell V_c L_c/\mu_\ell$, where μ_ℓ is the liquid viscosity. The effective surface tension coefficient σ_{eff} is the reciprocal of Weber number, $We=\rho_\ell V_c^2 L_c/\sigma$, where σ is the surface tension of liquid. In Eq. (1) the surface tension is added as a delta function integrated locally over the interface separating immiscible fluids within unit volume in order to render a singular force exerted by the interface, and is calculated over the entire bubble surface. The notations for volume and surface are for 3D systems but we have used their 2D versions, *i.e.* surface and line. Here κ is twice the mean curvature, $\mathbf{n}$ the outwardly directed unit normal vector at the bubble surface, and $\mathbf{r}$ the space vector with the subscript f designating the interface.

The procedure to solve the Navier–Stokes equations follows the projection method described in [15], with

$$\frac{(\rho\mathbf{V})^{n+1}-(\rho\mathbf{V})^{*}}{\Delta t}=-\nabla_h P^{n+1} \tag{2}$$

where the unprojected mass flux is defined as

$$(\rho\mathbf{V})^{*}=(\rho\mathbf{V})^{n}-\Delta t\left(\nabla_h\cdot(\rho\mathbf{V}\mathbf{V})+\rho\mathbf{g}+\nabla_h\cdot\mu_{\mathrm{eff}}\left(\nabla\mathbf{V}+\nabla\mathbf{V}^{T}\right)+\int_{\Delta s}\sigma_{\mathrm{eff}}\kappa\,\mathbf{n}\delta(\mathbf{r}-\mathbf{r}_f)da\right)^{n}. \tag{3}$$

Taking divergence on both sides (divided by ρ) yields the Poisson equation for pressure,

$$\nabla_h\cdot\left(\frac{1}{\rho^{n+1}}\nabla_h P^{n+1}\right)=\frac{\nabla_h\cdot\mathbf{V}^{*}-\nabla_h\cdot\mathbf{V}^{n+1}}{\Delta t}. \tag{4}$$

Here the subscript h and the superscript n respectively refer to the discretizations in space and time. The divergence of velocity at $n+1$ in Eq. (4) is taken as zero in order to ensure the condition of incompressibility. Furthermore, the singular term due to a surface force in Eq. (3) is smeared out of the interface onto finite neighboring grid points by using the immersed-boundary method of Peskin [14]. A cosine weighting function is used to spread the interfacial properties toward surrounding cells, based on a Lagrangian–Eulerian treatment of moving front markers and stationary grid points. To carry out the geometric conservation of the Dirac delta function, i.e., $\int_{-\infty}^{+\infty}\delta(x-x_f)dx=1$, a discrete form is established to satisfy