Computers & Fluids 107 (2015) 272–284

Contents lists available at ScienceDirect

Computers & Fluids

journal homepage: www.elsevier.com/locate/compfluid

Boundary elements method for microfluidic two-phase flows in shallow channels

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ARTICLE INFO

Article history:
Received 23 April 2014
Received in revised form 10 September 2014
Accepted 29 October 2014
Available online 21 November 2014

Keywords:
Microhydrodynamics
Lab On A Chip
Droplets
Free interface
Interface stabilization
Gauss block elimination

ABSTRACT

In the following work we apply the boundary element method to two-phase flows in shallow microchannels, where one phase is dispersed and does not wet the channel walls. These kinds of flows are often encountered in microfluidic Lab-On-A-Chip devices and characterized by low Reynolds and low capillary numbers.

Assuming that these channels are homogeneous in height and have a large aspect ratio, we use depth-averaged equations to describe these two-phase flows using the Brinkman equation, which constitutes a refinement of Darcy's law. These partial differential equations are discretized and solved numerically using the boundary element method, where a stabilization scheme is applied to the surface tension terms, allowing for a less restrictive time step at low capillary numbers. The convergence of the numerical algorithm is checked against a static analytical solution and on a dynamic test case. Finally the algorithm is applied to the non-linear development of the Saffman–Taylor instability and compared to experimental studies of droplet deformation in expanding flows.

1. Introduction

Microhydrodynamics is a branch of fluid dynamics that deals with slow viscous flows at small length scales. In recent years the research field of microfluidics investigated the possibilities that microhydrodynamics offers to perform chemistry or biology on a micrometric scale. Such efforts have led to an increasing number of Lab-On-A-Chip applications in the last ten years [1]. In this course droplet microfluidics has emerged [2], because it exploits the laminar flow in microchannels to precisely control and steer operation on droplets, which act as highly parallelizable reaction chambers.

Microfluidic length scales are in the order of tens to hundreds of micrometers. When microfluidic channels are filled with two immiscible liquids, for instance water and oil, the viscosities are in the order of $\mu \approx 10^{-3}$ Pa s and surface tension or interfacial tension in the order of $\gamma \approx 10^{-2}$ Pa m, depending on the fluid mixture and surfactants. Due to the small length scale the flow resistance in these channels is high, which is one reason why flow rates usually range between a few nl/min to hundreds of µl/min with flow velocities in the order of mm/s. The Reynolds number, $\mathrm{Re} = \frac{\rho U L}{\mu}$, is small and therefore, it is often a reasonable approximation to discard the non-linear inertial terms and to consider Stokes flow, which is described in Section 2.

However, when considering two-phase flow even in the Stokes regime, the dynamics become non-linear due to the free interface between both liquids. The non-linearity stems from domains of different viscosity separated by a mobile interface under surface tension.

Two competing effects dominate the dynamics; one comes from viscous shear and the other from surface tension. The capillary number expresses the balance between viscosity and surface tension: $Ca = \frac{\mu U}{\gamma}$, which is considered here to be between 10^{-5} and 10^{-1}.

Throughout the article we consider shallow channels that lie in a common plane. Instead of trying to resolve the full three-dimensional problem, we solve a depth-averaged problem, which is two-dimensional. For shallow channels the velocity profile in the thin direction (z-axis) is assumed to be parabolic, a hypothesis that is also used to derive Darcy's law in two-dimensions (x–y plane). Darcy's law states that the flow velocity $\mathbf{u}$ is given by the pressure gradient divided by viscosity μ and a permeability coefficient k^2, $\nabla p = -\mu \mathbf{u} k^2$.

Although there have been propositions to account for tangential surface stresses in Darcy's law [3], the inability to impose tangential stresses and velocities renders this approach incomplete.

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http://dx.doi.org/10.1016/j.compfluid.2014.10.016
0045-7930/

In this work we propose the use of the Brinkman equations instead, which include a correction to the Darcy's law in form of the depth-averaged in-plane Laplacian, a reminiscence of the 2*D* Stokes equation. For droplet flows the Brinkman equation was to our knowledge first proposed by Boos and Thess [4] and Bush [5], who treated the flow induced by a thermo-capillary effect.

The Brinkman equation is solved with a boundary element method (BEM), which eliminates one more dimension turning the problem from a 2*D* differential equation into an integral equation on a 1*D* line. While BEM approaches have been followed for 3*D* Stokes flows [6], for 2*D* Stokes flow [7] and Darcy flow [8], recall that simulations of 2*D* Stokes flow cannot account for the confinement in the *z*-direction whereas Darcy's law becomes invalid close to boundaries and interfaces. The use of the Brinkman equation requires high aspect ratios to justify depth-averaging but we will see that it might still accurately captures the dynamics for aspect ratios approaching 1. Close to boundaries or interfaces the Brinkman equation gives much better results than Darcy's law, because it captures depth averaged boundary layers even if the averaged equations become inconsistent [4].

The derivation of the depth-averaged problem is presented in Section 2 and the numerical method is described in Section 3 together with a stabilization scheme for the surface tension on the interface and an acceleration using Gauss block pre-condensation and multi-core parallelism.

The method is applied to the non-linear development of the Saffman–Taylor instability of finger formation and to the numerical modeling of two recent experimental studies of droplet deformation in Section 4. Section 5 concludes with a brief discussion of the method and its results.

2. Governing equations

Throughout the article vectors and tensors are written in bold face unless they are represented by a Greek character. Scalars or components of vectors and matrices are written in normal face. All field variables are non-dimensionalized, using a characteristic length scale L, the pressure scale $P = \gamma_{\text{ref}}/L$ and the velocity scale $U = \gamma_{\text{ref}}/\mu_c$, which are build using the continuous fluids viscosity μ_c and surface tension γ_{ref}.

Low Reynolds number flows are described by the 3*D* Stokes and continuity equation, where non-dimensional operators and variables in 3*D* are denoted with a tilde.

$$\lambda_\phi \tilde{\Delta}\tilde{\mathbf{u}} - \nabla\tilde{p} = 0 \quad \text{and} \quad \tilde{\nabla}\cdot\tilde{\mathbf{u}} = 0. \tag{1}$$

The non-dimensional parameter λ_ϕ compares the viscosity of the considered fluid phase ϕ against the viscosity of the carrier fluid, $\lambda_\phi = \mu_\phi/\mu_c$. For the dispersed phase $\phi = d,\ \lambda_d = \lambda = \mu_d/\mu_c$, and for the continuous phase $\phi = c,\ \lambda_c = 1$. Because of the small size and the horizontal alignment gravitational effects are neglected.

2.1. Brinkman model for depth-averaged flow

The non-dimensional height is $h = H/L$ and is considered to be small, $h \ll 1$. As the flow is confined between two plates at a distance h, one considers only fluid motion in the x–y plane and neglects the vertical velocity component, which is equivalent to the assumption of constant pressure in the z-direction.

Under this assumption the flow field writes $\tilde{\mathbf{u}}(x,y,z) = (u_x(x,y)f(z), u_y(x,y)f(z), 0)^T$. The two-dimensional velocity vector $\mathbf{u}(x,y) = \begin{pmatrix} u_x(x,y) \\ u_y(x,y) \end{pmatrix}$ represents mean velocities, which demands $\int_0^h f(z)dz = h$. With these assumptions Eq. (1) can be written in terms of two-dimensional variables and operators:

$$\lambda_\phi\left(\Delta\mathbf{u} + \mathbf{u}\frac{\partial^2 f(z)}{\partial z^2}\right) - \nabla p = 0 \quad \text{and} \quad \nabla\cdot\mathbf{u} = 0. \tag{2}$$

When $h \ll 1$ the profile $f(z)$ becomes a parabolic Poiseuille profile and its second derivative in Eq. (2) is known. Using the parabolic profile $f(z) = 6\frac{z}{h}(1-\frac{z}{h})$ in Eq. (2) and depth-averaging over z we get the amalgam equation of Darcy equation and 2*D* Stokes equation given in Eq. (3), which is called Brinkman equation and was first applied in granular media flows [9],

$$\lambda_\phi\left(\Delta\mathbf{u} - k^2\mathbf{u}\right) - \nabla p = 0, \quad \nabla\cdot\mathbf{u} = 0, \quad k = \frac{\sqrt{12}}{h}. \tag{3}$$

We shall briefly illustrate the advantage of the Brinkman equation through a comparison of its solution for a flow in a rectangular duct of width w with the 3*D* Stokes solution. The exact solution can be found by separation of variables and is given for instance in Langlois and Deville [10]. Depth-averaging the solution of the 3*D* Stokes equation gives the mean velocity across the channel.

$$\langle\tilde{u}\rangle = -\frac{\partial p}{\partial x}\frac{h^2}{12}\left(1 - \frac{96}{\pi^4}\sum\frac{\cos h((1+2n)\pi y/h)}{(1+2n)^4\cos h((1+2n)\pi w/(2h))}\right). \tag{4}$$

In comparison, the mean velocity using of the depth-averaged Brinkman equation is:

$$u = -\frac{\partial p}{\partial x}\frac{h^2}{12}\left(1 - \frac{\cos h\left(\sqrt{12}y/h\right)}{\cos h\left(\sqrt{12}w/(2h)\right)}\right). \tag{5}$$

Both solutions show at leading order a hyperbolic cosine with similar prefactors, $96/\pi^4 \approx 0.986$ for the Stokes equation instead of 1 for the Brinkman equation and in the hyperbolic cosine a factor $\pi \approx 3.14$ instead of $\sqrt{12} \approx 3.46$. The depth-averaged velocity profiles are plotted in Fig. 1 for different aspect ratios. One observes that the solution from the Brinkman equation tends the solution of the 3*D* Stokes equation as the aspect ratio increases. Already for square channels, $w/h = 1$, the solutions are not too far from each other. Whereas a comparison with the Darcy equation, which is constant in y, gives $\overline{u}_{Darcy} = -\frac{\partial p}{\partial x}\frac{h^2}{12}$. Far away from the walls the Darcy equation gives correct results for high aspect ratios but fails near walls and for a moderate confinement.

In a more detailed analysis Gallaire et al. [11] showed that even in the complex thermo-capillary flow around a droplet the averaged model agrees almost perfectly with 3*D* Stokes. Including the in-plane Laplacian yields two important improvements in comparison to Darcy's law: (1) tangential velocities and stress can be imposed on boundaries and (2) there appears a boundary layer near walls and interfaces that scales like h, the non-dimensional height of the channel.

2.2. In-flow and out-flow boundary conditions

Boundary conditions of the single-phase problem prescribe either the stress or the velocity. The typical no-slip boundary condition on channel walls is $\mathbf{u} = \mathbf{0}$. In contrast to Darcy flow, the Brinkman model imposes normal and tangential velocities. The normal and tangent are given by a vector that contains their projections on the x and y axis, e.g. $\mathbf{n} = (n_x, n_y)^T$.

As typical inflow boundary condition the solution of the Brinkman equation in a straight channel flow is used. For a straight inflow boundary of length w parameterized by s, whose origin is in the middle of the boundary:

$$u_{in}(s) = Ca\frac{\cos h(kw/2) - \cos h(ks)}{\cos h(kw/2) - 1}. \tag{6}$$

It is worth observing that the dimensionless inflow velocity is represented by the capillary number Ca because the velocity is