Chemical Engineering Science 94 (2013) 138–149

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Science

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

Phase field modeling of Taylor flow in mini/microchannels, Part I: Bubble formation mechanisms and phase field parameters

Harish Ganapathy [a,b], Ebrahim Al-Hajri [b], Michael M. Ohadi [a,*]

[a] Smart and Small Thermal Systems Laboratory, Center for Environmental Energy Engineering, University of Maryland, College Park, MD 20742, USA
[b] Department of Mechanical Engineering, The Petroleum Institute, PO Box 2533, Abu Dhabi, UAE

HIGHLIGHTS

- Multiphase model capable of accurately predicting hydrodynamics of fluid flow.
- Finite element implementation of phase field model applied to simulate Taylor flow.
- Addresses effect of phase field parameters for mobility and interface thickness.
- Numerical Taylor bubble length compared with experimental and empirical data.
- Gas void fraction varied linearly with volumetric flow ratio at all diameters.

ARTICLE INFO

Article history:
Received 6 February 2012
Received in revised form
29 December 2012
Accepted 20 January 2013
Available online 30 January 2013

Keywords:
Hydrodynamics
Multiphase flow
Numerical analysis
Fluid mechanics
Taylor flow
Phase field

ABSTRACT

Multiphase heat and mass transfer in microscale devices is a growing field of research due to the potential of these devices for use in various engineering applications. Before the heat and mass transport phenomena in such systems can be modeled, the hydrodynamics of adiabatic multiphase flow, in the absence of specie transport across interfaces, must be accurately predicted. In the present paper, a finite element implementation of the phase field method is applied to simulate Taylor flow in mini/microchannels. Channels with characteristic dimensions ranging from 100 to 500 μm are modeled and criteria present in the literature for domain discretization are assessed. The effects of phase field parameters, namely mobility and interface thickness, on the predicted flow features are discussed. The predicted Taylor bubble lengths are compared against empirical correlations as well as available experimental data in the literature. The predicted gas void fraction data for different channel dimensions are compared with numerous experimental studies. The present results indicate a linear variation of gas void fraction with respect to volumetric flow ratio for all channel sizes.

1. Introduction

Microscale technologies are quickly penetrating new application areas due to their proven potential for process enhancement and/or equipment size/volume reduction in diverse engineering applications. When optimally designed, the inherent higher surface area to volume ratio of microscale systems substantially enhances heat and mass transfer while keeping pressure drops at moderate levels. Before the heat and mass transport phenomena in such devices can be modeled, however, the hydrodynamics of adiabatic multiphase flow in the absence of species transport across interfaces must be accurately predicted. This is because the flow features at the microscale differ from those at larger length scales and therefore accurate prediction of the flow field directly results in improved accuracy of the predicted heat/mass transport phenomena.

On the experimental front, there are many published works, starting from the early studies of Fairbrother and Stubbs (1935), Bretherton (1961) and Taylor (1961), to more recent studies that primarily focus on microscale flows. Comprehensive reviews of these works have been presented by Ghiaasiaan and Abdel-Khalik (2001), Kreutzer et al. (2005), Angeli and Gavriilidis (2008), Shao et al. (2009) and Gupta et al. (2010). In general, two-phase flow patterns can be classified into the surface tension dominated type, comprising Taylor (or slug) and bubbly flows; the transitional type, comprising churn and Taylor-annular flows; and the inertia dominated type, comprising dispersed and annular flows. Among these flow patterns, Taylor flow (Davies and Taylor, 1950) is characterized by several features that renders it an optimum choice for assessing the performance of numerical modeling

* Correspondence to: Center for Environmental Energy Engineering (CEEE), 4164C Glenn L. Martin Hall, University of Maryland, College Park, MD 20742 Tel.: +1 301 405 5263; fax: +1 301 405 2025.
E-mail address: ohadi@umd.edu (M.M. Ohadi).

0009-2509/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ces.2013.01.049

approaches. It consists of gas bubbles of length typically larger than the characteristic dimension of the channel and separated by liquid slugs. A thin film of liquid separates the gas bubble from the channel wall. Recirculating velocity components are present within the liquid slugs, as seen from the moving frame of reference. Taylor flow has also been a dominant research interest, especially for microchannel heat exchangers and reactors on account of enhanced convective mixing phenomena, as described by Salman et al. (2004). For the purposes of this paper, we will define minichannels as channels having characteristic dimensions between 200 μm and 3 mm and microchannels as those between 10 and 200 μm (Kandlikar and Grande, 2003).

The present work studies the application of the phase field method to numerical simulation of Taylor flow in mini/micro-channels. Select simulations have also been performed using an alternative volume of fluid (VOF) model for comparison purposes. The present paper is part I of a two-part study. Part I focuses on Taylor bubble formation and presents an analysis of the effects of the phase field parameters on Taylor bubble length and gas void fraction. Disagreement in the literature over linear vs. non-linear trends for gas void fraction are reviewed and compared against the present predictions to validate the numerical model. Part II of this work (Ganapathy et al., 2013) is devoted to modeling of wall adhesion and modeling of thin liquid films. The flow field, pressure distribution and the effect of channel inlet configuration are analyzed.

2. Brief review of relevant literature

Various models have been developed for multiphase systems and have been applied towards two-phase flow in both minichannels and microchannels. The VOF method (Hirt and Nichols, 1981), which has proven to be the most popular, and the level set method (Osher and Sethian, 1988; Sussman et al., 1994), belong to the class of diffuse-interface modeling approaches. They are primarily based on the approximation of surface tension forces in the interfacial region as a body force, using the continuum surface force (CSF) formulation of Brackbill et al. (1992). These approaches have been implemented in numerous studies including Taha and Cui (2004), Qian and Lawal (2006), Liu and Wang (2008), Kumar et al. (2007), Carlson et al. (2008), Fang et al. (2008), Lakhehal et al. (2008), Chen et al. (2009), Gupta et al. (2009), Krishnan et al. (2010), Santos and Kawaji (2010), Asadolahi et al. (2011, 2012). Likewise, the front tracking model by Unverdi and Tryggvason (1992) is also a diffuse-interface formulation, wherein the center of the interface is marked by following the advection of control points (Jacqmin, 1999). The surface tension forces are estimated from the positions of the control points and fluid properties across the interface varies over multiple cells.

The phase-field method also belongs to the class of diffuse interface techniques but governs the interface based on the fluid free energy. The free energy density is comprised of the gradient energy and the bulk energy density (van der Waals, 1893). Cahn and Hilliard (1959) defined the phase-field variable, ϕ, which is considered as a measure of phase. It assumes two distinct values in either phase and undergoes a rapid smooth change across the interface. In the interfacial region, the two phases are considered to be mixed and are thereby associated with a mixing energy. An implementation of the phase field method was presented by Jacqmin (1999), following which several others have presented their modifications to deal with different types of systems. Among these, the work of Yue et al. (2004) is suitable for the present work and is therefore reviewed here.

Based on van der Waals' theory, the expression for mixing energy density is given by Eq. (1). By considering a double-well potential for $f_0(\phi)$, as given by Eq. (2), the Ginzburg–Landau form of mixing energy density is obtained (Eq. (3)). This mixing energy adds to the total free energy density of the system. The first and second terms on the right side in Eq. (3) represent the gradient energy and bulk free energy density, respectively. λ is the magnitude of mixing energy and ξ scales with the thickness of the interface.

$$f_{\mathrm{mix}}(\phi,\nabla\phi)=\lambda\left[\frac{1}{2}|\vec{\nabla}\phi|^2+f_0(\phi)\right] \tag{1}$$

$$f_0(\phi)=\frac{1}{4\xi^2}(\phi^2-1)^2 \tag{2}$$

$$f_{\mathrm{mix}}(\phi,\nabla\phi)=\frac{1}{2}\lambda|\vec{\nabla}\phi|^2+\frac{\lambda}{4\xi^2}(\phi^2-1)^2 \tag{3}$$

The rate of change of free energy with respect to the phase field variable, ϕ, yields the chemical potential of the system, G, given by Eq. (4). The chemical potential is zero at an interface at equilibrium.

$$G=\frac{\partial f_{\mathrm{mix}}}{\partial\phi}=\lambda\left[-\vec{\nabla}^2\phi+\frac{\phi(\phi^2-1)}{\xi^2}\right] \tag{4}$$

By integrating Eq. (4) once, and in conjunction with the conditions specified by Eq. (5), we obtain Eq. (6). The solution of Eq. (6) gives the equilibrium profile for $\phi(x)$, which is reported by Eq. (7).

$$f_0(\pm\infty)=0;\quad \left.\frac{d\phi}{dx}\right|_{x=\pm\infty}=0 \tag{5}$$

$$f_0(\phi)=\frac{1}{2}\left(\frac{d\phi}{dx}\right)^2 \tag{6}$$

$$\phi(x)=\tanh\left(\frac{x}{\sqrt{2}\xi}\right) \tag{7}$$

The diffuse mixing energy in the interfacial region must be equal to the traditional surface energy (Eq. (8)). Eqs. (7) and (8) together, result in the final expression for interfacial tension, given by Eq. (9), which corresponds to the sharp interface formulation while the limit of ξ tending to zero.

$$\sigma=\lambda\int_{-\infty}^{\infty}\left[\frac{1}{2}|\vec{\nabla}\phi|^2+f_0(\phi)\right]dx \tag{8}$$

$$\sigma=\frac{2\sqrt{2}\lambda}{3\xi} \tag{9}$$

Based on the above formulation, Yue et al. (2004) derived the following governing equations for the phase field approach to model multiphase flows.

$$\frac{\partial\phi}{\partial t}+\mathbf{U}\times\nabla\phi=\nabla\times\frac{\gamma\lambda}{\xi^2}\nabla\psi \tag{10}$$

$$\psi=-\nabla\times\xi^2\nabla\phi+\left(\phi^2-1\right)\phi+\left(\frac{\xi^2}{\lambda}\right)\frac{\partial f_{\mathrm{ext}}}{\partial\phi} \tag{11}$$

As noted by Jacqmin (1999), the phase field governing equations are a function of the time scale of Cahn–Hilliard diffusion, γ.

$$\gamma=\chi\xi^2 \tag{12}$$

As per the definition in Eq. (12), the functional dependence of γ on two user-defined parameters: mobility, χ, and interface thickness, ξ, posed difficulties on account of the absence of definitive guidelines on their selection which are to be taken into consideration while determining the element size, h. Subsequently, a criterion, $h\leq\xi$, was proposed by Yue et al. (2006), and further, the h/ξ ratio was varied from 0.5 to 1 in order to ensure that the region occupied by the interface would be sufficiently resolved