Theoretical & numerical simulation on the formation of coated microbubbles

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1. Introduction

Microfluidic devices have emerged as a powerful tool for the formation of encapsulated drops and microbubbles, which are used in medicine for imaging via ultrasound and as drug delivery vectors [1]. Among other techniques, microfluidics are more preferable, because of the high production rates and the monodispersity in size of the microbubbles [2].
Unlike T-juction shape microfluidics, recent developments in flow focusing geometries demonstrate the formation of stable coated microbubbles with size less than 10 μm, which is crucial for biomedical applications. In the former case, capillary and viscous forces destabilize the gas-liquid interface leading to absolute instability with small wave numbers or relative big microbubbles (~100 μm) [3]. Capillary forces are less important in flow focusing devices, while the pressure drop in gas phase and the volumetric flow rate of the liquid are expected to affect the stability of the interface and create smaller microbubbles [4].
In fact, the orifice of a flow focusing device accelerates the flow, while the presence of surfactants reduces the surface tension on the gas-liquid interface; hence, Marangoni stresses are developed [5,6]. Both phenomena are responsible for destabilization of the interface, which leads to bubble formation. In addition, understanding and controlling the surfactant transfer on microbubbles surface is also important, because the amount of the attached material will greatly affect the mechanical properties; hence, the microbubbles behavior in vascular bed. The above phenomena and the mechanisms that lead to the instability of the pinching process are not extensively discussed in the literature. The present work investigates these processes with a coupled mass-hydrodynamic model; see also figure 1.

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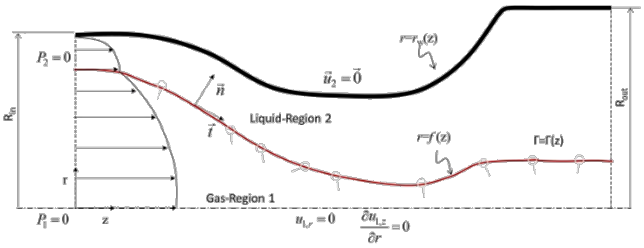

Figure 1: Schematic representation of two phase flow in a convergent-divergent tube

2. Methods

2.1 Mathematical Formulation-FEM

We consider the axisymmetric steady-state flow of two immiscible fluids in a horizontal tube with a varied cross section. The Navier-Stokes and the continuity equations are employed for each phase, coupled with the appropriate kinematic and dynamic conditions at the interface:

$$\vec{\nabla}\cdot\vec{u}_i=0 \tag{2-1}$$

$$\mathrm{Re}_i\left(\vec{u}\cdot\vec{\nabla}\right)\vec{u}=-\vec{\nabla}P+\vec{\nabla}\cdot\underline{\underline{\tau}} \tag{2-2}$$

where $\underline{\underline{\tau}}$ is the newtonian viscous stress tensor and $\mathrm{Re}_i=\rho_i U R_0/\mu_i$ is the Reynolds number of each phase (i=1→gas, i=2→liquid).

$$\vec{u}\cdot\vec{n}=0 \tag{2-3}$$

$$\left(P_1-\lambda P_2\right)\underline{\underline{I}}\cdot\vec{n}+\left(\lambda\underline{\underline{\tau}}_2-\underline{\underline{\tau}}_1\right)\cdot\vec{n}=\frac{2k_m}{Ca}\sigma\vec{n}-\frac{\vec{\nabla}_s\sigma}{Ca} \tag{2-4}$$

with $\lambda=\mu_2/\mu_1$ is the ratio of viscosities, $Ca=\mu_1 U/\sigma_0$ is the capillary number, $\vec{n}$ is the normal vector on the interface pointing towards the liquid phase and $\vec{\nabla}_s=\left(\underline{\underline{I}}-\vec{n}\vec{n}\right)\cdot\vec{\nabla}$ is the surface gradient operator. The second term in (2-4) denotes the Marangoni stresses developed due to surface tension gradients, where we assume the following constitutive relation:

$$\frac{\sigma}{\sigma_0}=1-\beta\left(\Gamma-1\right) \tag{2-5}$$

σ_0 is the initial uniform surface tension. Parameter β denotes the so-called elastic number and it is interpreted as a measure of the surfactant strength.
Assuming insoluble surfactant, a mass balance is written on the interface in terms of its surface concentration [7-8]:

$$u_z\frac{\partial\Gamma}{\partial z}+\Gamma\vec{\nabla}_s\cdot\vec{u}=\frac{1}{Pe}\vec{\nabla}_s^2\Gamma+J_B \tag{2-6}$$

$J_B=k_a C_S\Gamma_\infty-k_d\Gamma$ is the adsorption/desorption flux and $Pe=UR_0/D_s$ is the Peclet number.
The problem is completed with typical non-slip boundary condition (bc) at the solid wall and symmetry bc on the axis of symmetry. We impose a known velocity profile at the tube inlet and open (or free) bc at the tube exit.

The system of equations is discretized with the finite element method using Lagrangian polynomials to interpolate each unknown. The computational mesh is generated by a mapping of the physical domain with the necessary spine transformations of coordinates [9]. The final algebraic system is solved via Newton iterations for the unknown vector $\vec{x} = \left(u_z, u_r, P, f, \Gamma\right)^{T}$.

The super-imposed velocity profile at the entrance is pre-described by the volumetric flow rate of each phase (Q_1,Q_2). We seek numerical solutions in the parameter space defined by Q_1, Q_2.

3. Results and discussion

Employing the model presented above, we perform simulations in order to obtain the steady state of two co-flowing fluids in a tube with radius R_0 and length $10R_0$. In this simulation we assume that the gas phase is perfluorobutane C_4F_{10} with physical properties ρ_1=11.2 kg/m^3 & μ_1=1.22·10^{-5} Pa·s. The liquid is taken to be water (ρ_2=10^3 kg/m^3, μ_2=10^{-3} Pa·s). The other physical properties are σ_0=0.04 N/m, D_s=10^{-9} m^2/s, Γ_{∞} =10^{-6} mol/m^2 and β=0.015. We also assume that Q_1=Q_2=12 μL/min and R_0=11 μm. These properties have been chosen as indicative values from similar experimental studies [2].

Preliminary results of our study recover the analytical solution in terms of the fully developed axial velocity profile in a tube of constant cross section. In this case, the shape of the interface exhibits entrance effects and at the exit reaches the height that theory predicts, figure 2(a). Then, we consider a convergent-divergent tube having a sinusoidal shape, figure 2(b). As can be seen, the shape of the interface is now more disturbed. Clearly, such geometry alters the flow regime and the distribution of the surfactant concentration.

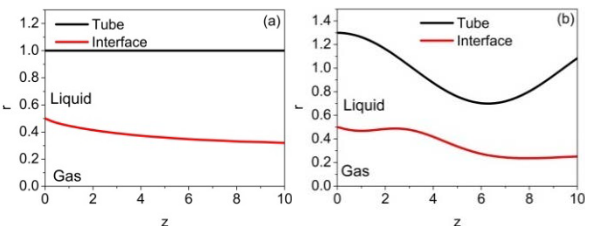

Figure 2: (a) Shape of the interface in a typical tube and (b) a convergent-divergent tube.

4. Conclusions

In this work we investigate the pinch-off process during the formation of coated microbubbles in a flow focusing geometry.

Currently, our model can predict the steady state analytical solution for two co-flowing fluids. In addition, the ongoing effort concentrates in mesh refinement tests and simulations in convergent-divergent geometry.

We anticipate that the concentration of the surfactant will gradually increase due to relative big values of the interfacial Peclet number leading to a reduction of surface tension. Therefore, Marangoni stresses and inertia forces will destabilize the interface.

Further calculations are under way to investigate the mechanisms that determine the evolution of the interface and perform parametric analysis to obtain the flow arrangement that will serve as base flow for a subsequent stability analysis that will provide the size selection mechanism.

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6. References

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