Computational study of the role of surfactants in sheared foams for foam stability

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Résumé :

Nous étudions numériquement la dynamique de mousses humides cisaillées. Pour cela, nous avons étendu un code (parallèle) 3D de la méthode level set pour des écoulements diphasiques incompressibles pour tenir compte de la dynamique de tensioactifs solubles dans le liquide, qui modifient le saut de contrainte à l'interface. En particulier, au-delà des modèles simples de tensioactifs, nous prenons en compte la rhéologie de la surface (comme la viscosité surfacique) dans l'objectif de décrire des systèmes réalistes. Nous montrons que les résultats de tests 2D et 3D sont cohérents avec la littérature. Nous présentons des résultats sur le rôle des tensioactifs et de leurs propriétés sur des événements de réarrangements de bulle (T1), et discutons leur influence sur la stabilité de la mousse.

Abstract :

The dynamics of sheared wet foams is investigated computationally in this study. For this purpose, an established 3D (parallel) implementation of a level-set method for incompressible two-phase flow has been extended to account for the presence of surfactants that are soluble in the liquid, and the associated modified stress conditions at interfaces. In particular, we account for surface rheological behavior (such as surface viscosity) beyond minimal surfactant models, to describe realistic systems. The results of 2D and 3D tests will be demonstrated to compare favourably with the literature. We shall report on the role of surfactants and their properties on T1 events, wherein adjacent bubbles are sheared past each other, with implications for foam instability.

Mots clefs : Méthode level-set, surfactants, Matériaux cellulaires, mécanique des fluides, mousse, isolation

1 Introduction

Foams are used for combining thermal or phonic insulation with low weight. On the other hand, the use of solid foams is limited due to problems with stability. To investigate this, we consider here a model of the precursor to solid foams, which are liquid foams (e.g., [1]). Liquid foams are stabilized by the introduction of surfactants : a judicious choice of surfactant can reduce the likelyhood of coalescence of large bubbles in foams that would otherwise result in collapse of a liquid foam. The problem now is that it remains unknown what properties of surfactants stabilize liquid foams best, and how. This is because it is very difficult to measure experimentally the local concentration of surfactants at gas/liquid interfaces that move and deform and are of complex shape. It is for this reason that we have embarked on a computational study of a model of liquid foams. Our long-term objective is to develop a complete description at the scale of individual bubbles in liquid foams, and to make the link with the global stability properties of foams. Moreover, understanding the precise coupling between microscopical surfactant properties and macroscopic liquid flows around bubbles is a crucial step for a complete modeling of foam rheology [3].



FIGURE 1 – Problem definition sketch. the channel height is denoted by H in the main text, and the speed of the walls by U.

2 Problem statement

We consider here a 2D model of a sheared liquid foam between two parallel moving walls, presented in Fig. 1. Periodic conditions are used on the sides of the domain, which therefore corresponds to a unit cell in a periodic arrangement of bubbles. The walls translate at equal constant speed, and the contact lines are pinned to the moving walls. The bubbles deform as they slide past each other (so-called T1 events); after a few such passages, these become normally time-periodic.

The flow is governed by the Navier-Stokes equations for incompressible flow in each fluid, coupled at interfaces through jump relations for the normal and tangential stress. Herein we shall use a one-fluid formulation, that is, a single set of momentum equations with variable density and viscosity, valid throughout the entire computational domain. As the stress tensor is discontinuous across interfaces, its divergence would introduce a singular term in the momentum equation, which is balanced upon introduction of a source term. Further details of this standard approach can be found elsewhere (e.g., [13]), although the present system does include also a jump in tangential stress, besides the common jump in normal stress due to surface tension (see also [11]).

The jump in stress at interfaces is assumed herein to be entirely through a change in the local surface

tension, with associated Marangoni stress; we adopt the Langmuir formula, $\sigma = \sigma_0(1 + \beta \ln(1 - \kappa f))$ where *f* is the local surfactant interface concentration, β the elasticity number, κ the dimensionless surfactant coverage (a convenient reference for the precise definitions of these parameters is [11], for a more physical discussion, see [6]).

We consider herein surfactants that are soluble in the liquid, but not in the gas. Therefore, apart from the convection and diffusion of surfactant interface concentration, the model accounts for adsorption of surfactants to interfaces from the bulk liquid. Hence, the transport of surfactant concentration per unit volume of liquid is also determined, subject to a flux boundary condition at moving interfaces.

The transport equations for the surfactant interface concentration and the volume concentration are, for computational convenience, written in distributive form such that they can be solved numerically thoughout the computational domain. Further details of this formulation can be found elsewhere [12, 11]. At the walls, zero diffusive fluxes of surfactant concentrations are imposed. The initial conditions used are uniform equilibrium values for the concentrations.

The following dimensionless groups will be used in the presentation of the results. With reference to Fig. 1, we define **Péclet numbers** $Pe_F = HU/D_F$ and $Pe_f = HU/D_f$ for the surfactant concentration in the liquid and at interfaces, respectively, where D_F and D_f are the diffusivity of surfactants in the liquid and at interfaces, respectively. A **Biot number** $Bi = r_d H/U$ involves the desorption coefficient r_d , which is an inverse timescale for the desorption from the liquid to interfaces. Reference will also be made to a **capillary number**, $Ca_{eq} = \mu U/\sigma_{eq}$ and a **Reynolds number** $Re = \rho HU/\mu$ where σ_{eq} is the equilibrium surface tension, μ the liquid shear viscosity and ρ the liquid density.

3 Numerical method

We have implemented and tested solvers for the surfactant interface and liquid concentrations in a preexisting level-set method for two-phase flows, that has been used and tested in prior work on the route towards atomization of droplets from a sheared liquid film without surfactants [8]. A cartesian MAC grid of square cells is used, and the Navier-Stokes equations are solved using a projection method. To improve mass conservation of each of the fluids, the level-set method used in that prior work has been replaced by a more advanced method [10] after extensive comparative study of level-set methods [9]. The computational methods used for the surfactant concentration equations is a counterpart for level-set methods of the approach developed in [11] for diffuse-interface methods. Results of tests obtained with our method can be found elsewhere [12], including 3D tests for a sheared droplet.

4 Results

A sample instantaneous view is presented in Fig. 2. It is seen that the surfactants are swept to the rear of bubbles, resulting there in a lower surface tension; this only arises at sufficiently large values of the interfacial Péclet number, Pe_f . Our results show that although the minimum gap between opposite bubbles is increased by surfactants, the gap between adjacent bubbles is reduced, at some distance from the contact lines. The largest variation in surfactant interface concentration, where Marangoni stress is the most significant, is near the gap between opposite bubbles.

These results have been quantified in detail in a parametric study of the system behaviour on the scale of bubbles. The numerical simulations allow extracting the surfactant concentration, along with other



FIGURE 2 – Sample instantaneous view of a numerical simulation result. The colour and greyscales represent the surfactant concentration in the liquid, respectively (red/light : high, blue/dark : low). the interfaces have been thickened for clarity of presentation. $Ca_{eq} = 0.2$, Bi = 0.1, $Pe_F = Pe_f = 10$.

quantities, to be plotted versus the arc length along a bubble surface, as well as the minimal thickness of the liquid film between bubbles that slide past each other.



FIGURE 3 – Sample time signals of forces whereby work is done by moving the walls : (A), capillary force; (B), integrated gas swall stress; (C), integrated liquid wall stress. $Ca_{eq} = 0.2$, Bi = 10, $Pe_F = Pe_f = 1$.

Here we focus on derived quantities to characterise the liquid foam - in particular, towards characterisation of the rheology of liquid foams. As a measure of dissipation in the foam, we study the work done by moving the walls. In these simulations, the shear rate is imposed, and the work done by moving the walls can be determined from the results.

In Fig. 3 we show example time signals for three contributions into which we have decomposed the total force exerted by the walls : the integrated wall shear stress in the gas an liquid, and the capillary contribution at the contact lines. Of these, the capillary contribution is generally dominant in our results.

Naturally, these forces are time-periodic, after an initial transient, the period corresponding to the duration of a T1 event. We focus herein on the time-average (taken after the initial transient) of the principal, capillary contribution to the total force. In Fig. 4, this average force is plotted versus capillary number for different parameter values.



FIGURE 4 – Averaged capillary force vs capillary number for various Biot and Péclet number values.

Interestingly, each set of results exhibits a power-law dependency on the capillary number. Fitted exponents for the results in Fig. 4 with surfactants are close to 0.6, whereas that for the results for the corresponding surfactant-free foam is approximately 0.8. Such power-law dependencies are reminiscent of friction laws that have been measured or predicted for bubbles slipping against a solid wall [2, 5, 7], as well as for bubble-bubble friction [4].

The coefficient of proportionality between the force and the power of the capillary number is seen to increase with increasing Péclet numbers and lower Biot numbers, that is, for less homogeneous surface concentrations. Further work will be focussed on the origin of this enhanced friction, which can be attributed either to the impact of Marangoni stresses on flow features (mobile or rigid-like surfaces [2]) or to surface dissipation [5].

5 Conclusion

A two-dimensional model of sheared wet foams has been studied computationally. Some first observations at the scale of individual bubbles include an elucidation of the non-uniform surfactant distribution at moderately large advection compared to surfactant surface diffusion. At elevated Péclet number, the liquid film between sheared bubbles is thickened, whereas that between adjacent bubbles is thinned. Further analysis is required of the extended results, including on the dependency of the minimal film thickness during T1 events on system parameters.

The overall rheological behaviour has been studied by the work done when shearing the wet foam. The results show an interesting power-law dependency on a capillary number that will have to be analyzed further.

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