

# Stable finite element approximations of two-phase flow with soluble surfactant



John W. Barrett<sup>a</sup>, Harald Garcke<sup>b</sup>, Robert Nürnberg<sup>a,\*</sup>

<sup>a</sup> Department of Mathematics, Imperial College London, London, SW7 2AZ, UK

<sup>b</sup> Fakultät für Mathematik, Universität Regensburg, 93040 Regensburg, Germany

## ARTICLE INFO

### Article history:

Received 4 August 2014

Received in revised form 19 February 2015

Accepted 22 May 2015

Available online 27 May 2015

### Keywords:

Incompressible two-phase flow

Soluble surfactants

Finite elements

Front tracking

ALE-ESFEM

## ABSTRACT

A parametric finite element approximation of incompressible two-phase flow with soluble surfactants is presented. The Navier–Stokes equations are coupled to bulk and surface PDEs for the surfactant concentrations. At the interface adsorption, desorption and stress balances involving curvature effects and Marangoni forces have to be considered. A parametric finite element approximation for the advection of the interface, which maintains good mesh properties, is coupled to the evolving surface finite element method, which is used to discretize the surface PDE for the interface surfactant concentration. The resulting system is solved together with standard finite element approximations of the Navier–Stokes equations and of the bulk parabolic PDE for the surfactant concentration. Semidiscrete and fully discrete approximations are analyzed with respect to stability, conservation and existence/uniqueness issues. The approach is validated for simple test cases and for complex scenarios, including colliding drops in a shear flow, which are computed in two and three space dimensions.

© 2015 Elsevier Inc. All rights reserved.

## 1. Introduction

Surface active agents, also called surfactants, are among the most widely used molecules in industry. They may act as detergents, wetting agents, emulsifiers, foaming agents and dispersants. The reason for these many applications is that soluble surfactants can have a pronounced effect on the interface and, hence also, on the evolution in a two-phase flow. In particular, surfactants influence the surface tension at the interface, and local inhomogeneities lead to Marangoni effects. In situations where the surfactant is soluble in one or in both of the two bulk phases, the adsorption and desorption of surfactants at the interface has to be taken into account. This means surfactant molecules can attach to and detach from the interface, and the corresponding mass balances on the interface and in the bulk have to be taken into account. The fundamental transport mechanisms for surfactants are diffusion in the bulk phases and on the interface, and advection with the underlying fluid velocity.

Adsorption of surfactants to the interface decreases the surface tension, which makes it easier for the interface to deform. It also can be observed, see e.g. the numerical experiments in Section 6, that an interface moves towards regions with a high bulk surfactant concentration. The presence of surfactants typically decreases the rise velocity of bubbles. The reason for this is that Marangoni stresses at the interface imply that the shear free condition at the interface no longer holds, and

\* Corresponding author. Tel.: +44 207594857.

E-mail addresses: j.barrett@imperial.ac.uk (J.W. Barrett), harald.garcke@mathematik.uni-regensburg.de (H. Garcke), robert.nurnberg@imperial.ac.uk (R. Nürnberg).

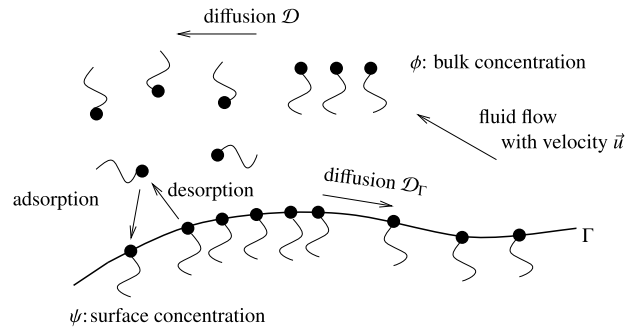


Fig. 1. The different quantities and transport phenomena in the bulk and at the interface are schematically illustrated.

hence the drag force on the bubble increases. In particular, the rise velocity of a bubble is reduced, and this effect can be used to maximize the contact time between different fluid phases, which can be important to influence the transfer of chemical components. These phenomena demonstrate that the interplay between the fluid velocity and the bulk and surface surfactant concentrations is multifaceted. Due to this versatile interaction it is often difficult to identify the sources for the different phenomena from experiments alone. It is hence important to have reliable numerical methods for this complex problem at hand in order to obtain a better understanding of the interdependence of fluid flow, adsorption, advection, Marangoni effects and diffusion, see Fig. 1 for a schematic description of the different quantities and transport processes.

In order to mathematically describe the complex physics illustrated in Fig. 1, one has to solve the following equations.

- The incompressible Navier–Stokes equations in both phases, see (2.3a)–(2.3c).
- An advection–diffusion equation for the bulk surfactant concentration in either one or in both phases, see (2.8a).
- A parabolic partial differential equation on the evolving interface describing the conservation of bulk surfactant. Here a source term stemming from adsorption and desorption of surfactants has to be taken into account, see (2.8b) and Fig. 1.
- An equilibrium of force equation on the interface, which includes curvature and Marangoni effects, see (2.5)(a).
- An additional interface equation taking the surface thermodynamics into account. Depending on whether the interface kinetics are slow or fast, this either results in a condition relating the bulk fluxes to differences of chemical potentials, or it leads to the chemical potentials having to be equal, see (2.13) and (2.15). The latter condition contains Henry's law (2.17) as a special case.

In addition,

- the interface has to be advected with a normal velocity which equals the normal part of the fluid velocity, see (2.5)(b).

Although the overall problem has many applications, not many analytical results exist for this problem. An energy inequality for the insoluble case, which we are also going to use, has been derived in [27]. In [13] energy methods and semigroup theory were used to study the stability of equilibria in the soluble case. In [26] a diffuse interface model was introduced to describe two-phase flow with soluble surfactants for which an energy inequality can be shown. Moreover, by using matched asymptotic expansions the authors of [26] could show that a novel sharp interface model can be recovered, which also satisfies an energy law. We refer to Section 2 for the precise details of this sharp interface model, which has already been outlined above.

In contrast, over the years many papers presenting numerical methods and computations for interfacial flows with soluble surfactants have appeared. Let us briefly mention the methods that have been used by different groups. In [1,39] the volume of fluid (VOF) method was used, which approximates the characteristic function of one of the phases. The level set method, which describes the interface as the level set of a function, was considered in [43]. Numerical computations based on diffuse interface models have been presented in [24,26,35,42]. The immersed boundary method has been used in [15,34]. A front tracking method for soluble surfactants has been introduced in [36,41]. In addition we mention the arbitrary Lagrangian–Eulerian approach in [25], the segment projection method in [33] and the hybrid methods studied in [12,43]. For more references and an introduction to numerical methods for two-phase flow we refer to the book [30].

In this paper we adapt the approach from [9,10] to numerically solve the governing equations for soluble surfactants at fluid interfaces. In particular, we consider the system with the novel free boundary condition in [26] that allows for a stability bound. For a particular instance of this model, where the bulk surfactant concentration is assumed to be continuous across the interface, we are able to prove a stability bound for our semidiscrete finite element approximation. To our knowledge, this is the first stability result for a numerical approximation of two-phase flow with soluble surfactant in the literature. In our finite element approximation the interface, and the surface quantities defined on it, are approximated with the help of parametric finite elements. The method is an example for an unfitted front-tracking method, in that the mesh points used to describe the interface are totally independent from the underlying bulk finite element mesh. In addition, the

Download English Version:

<https://daneshyari.com/en/article/6931319>

Download Persian Version:

<https://daneshyari.com/article/6931319>

[Daneshyari.com](https://daneshyari.com)