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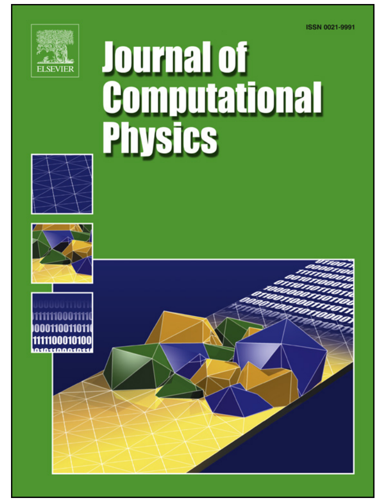

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Liquid-vapor transformations with surfactants. Phase-field model and Isogeometric Analysis

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Abstract

Surfactants are compounds that find energetically favorable to be located at the boundaries between fluids. They are able to modify the properties of those interfaces, for example, reducing surface tension. Here, we propose a new model for liquid-vapor flows with surfactants which captures the dynamics of the surfactant and accounts for phase transformations in the fluid. The aforementioned model is derived from a free energy functional by using a Coleman-Noll approach. The proposed theory emanates from the isothermal Navier-Stokes-Korteweg equations, which describe single-component two-phase flow and naturally allow for phase transformations. We believe that our model has significant potential to study the influence of surfactants in vaporization and condensation processes. From a numerical point of view, the proposed model poses significant challenges to existing discretization methods, including stiffness in space and time, internal and boundary layers as well as higher-order partial differential operators. To overcome these challenges we propose algorithms based on Isogeometric Analysis, which permit an accurate and efficient discretization. Finally, we illustrate the viability of the theoretical framework and the effectiveness of our algorithms by solving several numerical problems in two and three dimensions.

Keywords: Surfactants, Surface tension, Navier-Stokes-Korteweg (NSK), Complex fluids, Phase-field model, Isogeometric Analysis (IGA).

1. Introduction

Surfactants are very useful products in the chemical industry. They can be found in detergents, cosmetics, or the dye of our clothes. However, the chemical industry is not the only beneficiary of these extraordinary compounds. In recent decades, surfactants have also been used in other fields such as biotechnology [1, 2], electronic printing [3], microelectronics [4] or medical research [5, 6]. They also play an essential role in our organism, increasing the pulmonary compliance and preventing atelectasis [7, 8], that is, the complete or the partial collapse of the lungs.

The word surfactant is an abbreviation of *surface active agent* and is used to name different types of compounds that find energetically favorable to be located at the interfaces of a system. The consequence is that surfactants are absorbed by the interface, that is, they get trapped at the boundary between different phases. Even if they are usually very thin, interfaces play a crucial role in the system dynamics. The composition in the interfacial region can differ dramatically from that of the bulk phases. Indeed, across interfaces there are rapid property changes that lead to an excess of free energy, related to the amount of work required to create the interface. The presence of surfactants at the interface can significantly reduce the work required to generate interfaces, altering completely the behavior of the system [9–13]. For a more detailed discussion on surfactant properties the reader is referred to [14–16]

In the literature, one can find a number of computational methods that describe surfactant absorption phenomena. For this purpose, different techniques have been employed, such as phase-field models [17–21], front tracking methods [19, 22] or volume of fluid schemes [23, 24]. However, most of these models only deal with soluble or insoluble

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