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Numerical method for coupled interfacial surfactant transport on dynamic surface meshes of general topology

Kathrin Dieter-Kissling, Holger Marschall *, Dieter Bothe

Mathematical Modeling and Analysis, Center of Smart Interfaces, Technische Universität Darmstadt, Germany

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ABSTRACT

We consider surfactant transport on moving and deforming fluid interfaces with main emphasize on the case of mixtures of several surfactants. Since the interface can be significantly covered by surfactants, the model incorporates cross-effects in terms of both cross-diffusion as well as non-idealities of the surfactant mixtures. This is accounted for by means of the interfacial Maxwell–Stefan equations with appropriate thermodynamic driving forces.

Our numerical method for detailed computation of surfactant transport is based on the collocated Finite Area Method on meshes of general topology, including automatic mesh motion and remeshing methods to allow for strongly deforming interfaces. This allows for mass conservative solution of the interfacial transport equations, which are solved in a block-coupled manner to accurately describe the cross-effects. The diffusive fluxes, which are to be inserted into the system of surfactant balances, come from an iterative inversion of the Maxwell–Stefan equations. The cross-effects lead to heterogeneous diffusivities, which in turn can cause numerical instabilities at increasing heterogeneity. Therefore, we propose an enhanced discretization procedure which is easy to implement for the finite area diffusion operator, yielding numerical conservation, robustness and boundedness. While the method can be extended to soluble surfactants in a straightforward manner, we focus here on the insoluble case.

1. Introduction

In dispersed gas–liquid or liquid–liquid systems, surfactants are commonly present on the fluid interface, either on purpose as additives or as surface active constituents of the bulk mixture or in form of impurities. In general, strongly coupled non-linear interfacial transport processes have to be considered, while the interface itself is deformable and moving.

Direct Numerical Simulation (DNS) of interfacial transport processes comprising multiple surfactants poses severe challenges to the underlying numerical method. The system is described by the two-phase Navier Stokes equations and appropriate interfacial jump conditions and the transport equations for the surfactants in the bulk and on the interface. Since surfactants accumulate at the interface, their area concentration is large such that cross-effects become relevant and the diffusive fluxes become interdependent. The system is to be described by the surface Maxwell–Stefan equations for multicomponent diffusion, resulting in a significant coupling of interfacial surfactant transport equations by the diffusive terms. Moreover, the transport of surfactants within the bulk phases and on the interface is typically coupled through sorption processes.

DNS of surfactant transport on fluid interfaces involves the numerical solution of surface PDEs, in particular advection–diffusion equations on moving/evolving surfaces. The existing methods for the DNS of two-phase flow can be categorized into Lagrangian interface tracking and Eulerian interface capturing approaches. While the first represent the interface in an explicit manner, in particular by resolving the interface with a surface mesh, the latter exhibit an implicit interface representation for which color or marker functions are introduced characterizing one of the fluid phases or the interface itself. The methods describing the numerical solution of surface PDEs are equally sub-categorized into Eulerian and Lagrangian methods. Since the majority of publications are motivated by surfactant transport processes, for the following literature review, we do not distinguish between methods for general surface PDEs and developments particularly regarding surfactants but give a general overview.

For Eulerian interface capturing approaches (e.g., Level-Set methods, Volume-of-Fluid methods, etc.) the field describing the interfacial transport quantity is extended from the interface into the adjacent volume. First developments of numerical methods for the solution of surface PDEs for Level-Set methods [1–4] are

* Corresponding author.
E-mail address: marschall@csi.tu-darmstadt.de (H. Marschall).

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based on stationary predefined Level-Set distributions [5–8]. Adalsteinson and Sethian [9,10] describe a method for solving partial differential equations on moving interfaces, considering both diffusive and advective transport on interfaces which are subject to stretching and shrinking. Xu and Zhao [11] extended the surface quantity within a narrow band around the interface, solving for advection and diffusion on a fixed Cartesian grid with a predefined velocity field. In a subsequent study ([12]), the interfacial transport method was coupled to a flow solver for incompressible Stokes flow. Also based on Level-Set methods, the surface PDEs are solved on discrete representation of the interface in form of a piecewise planar interface by Olshanski and Reusken [13]. Dziuk and Elliott [14] solve the partial differential equation on all level set surfaces by formulating an appropriate weak form of the conservation law with respect to time and space. Kallendorf et al. [15] provide a conserved formulation of the surface transport equation, building on the direct method of Anco and Bluman [16–18].

Volume-of-Fluid methods (cf. [19–21]) have been extended to cover the influence of insoluble surfactants on droplet deformation processes [22,23]. James and Lowengrub [24] show a method with exact mass conservation of the surfactant, where the evolution of the interfacial area and the surfactant mass are calculated separately. This work was combined with the Volume-of-Fluid method of Rudman [25] by Davidson and Harvie [26] and applied to rising droplets. A further enhancement of the method of James and Lowengrub [24] was published by Yang and James [27], in combination with the hybrid CLSVOF [28] method, which combines the strengths of both method. The evolution of the surfactant mass is computed applying an ALE (Arbitrary Lagrangian Eulerian) method. In [29], Alke and Bothe present a method for soluble surfactants, which is appropriate for diffusion controlled sorption processes. There, an iso-surface is constructed, on which the interfacial concentrations are explicitly evaluated from a predefined sorption isotherm and then transported on this temporal surface mesh according to the interface PDE.

Narrow-band methods for solving interfacial transport equations based on the diffuse interface approach (cf. [30,31]) are described in [32–36].

Lagrangian interface tracking approaches are combined with a variety of discretization procedures to allow for the numerical solution of surface PDEs. Boundary integral methods [37,38] are one representative of interface tracking methods. The interface is represented by a deforming surface mesh. It has been enhanced to account for the influence of insoluble [39–45] and soluble [46–48] surfactant on drop or bubble deformation. Dziuk and Elliott [49] propose a surface finite element method to solve the Laplace–Beltrami equation on triangulated surface meshes on stationary surfaces. In order to account for moving interfaces, the method was extended towards an evolving surface finite element method in [50] for predefined moving surfaces and has been applied to application cases [51]. The recent publication [52] proposes a second-order iso-parametric surface finite element method on moving meshes. Based on Front Tracking methods [53–56], Yamamoto et al. [57] and Zhang et al. [58] developed axisymmetric methods for fluid flow containing surfactant. Muradoglu and Tryggvason [59] and Tasoglu et al. [60] applied a finite difference method for solving the surface PDE on top of a surface mesh defined by a set of connected Lagrangian marker particles. Both insoluble and soluble surfactants are covered. Based on an Arbitrary Lagrangian Eulerian (ALE) Interface-Tracking method [61,62], Tuković and Jasak developed a Finite Area Method (FAM) on unstructured, moving and deforming surface meshes [63]. The present contribution is solely concerned with the interfacial transport of multiple surfactants. Our numerical method is based on the Finite Area Method [64,63] and is extended towards dynamic surface meshes, which are topologically changing to follow the deforming interface. Focus is on numerical aspects of the method development, such as conservativity and boundedness properties arising from the equation discretization procedure as well as robustness, i.e. stability and convergence properties, of the numerical solution procedure. The complete problem with its full complexity (including the hydrodynamics, the surface transport and the sorption processes) is out of scope here and shall be addressed in a forthcoming publication; see also [65]. The mere hydrodynamics have been presented previously [66].

The numerical evaluation of the surface diffusive fluxes from the Maxwell–Stefan equations is based on the procedure for gas mixtures. While some authors present direct methods, others apply the so-called Curtis–Hirschfelder approximation [67–69]. In the following we will apply the iterative inversion algorithm of Giovangigli [70]. After inversion, the discretization of the diffusive fluxes needs careful consideration, involving strategies for heterogeneous diffusivities. A great variety of discretization strategies for heterogeneous diffusivities exists in the literature concerning diffusivity tensors instead of scalar diffusivities. Aavatsmark et al. [71–73] propose a linear method on quadrilateral two dimensional meshes, which is flux conservative. It generalizes the principle of harmonic averaging applied with a two-point flux molecule (five-point cell molecule) for orthogonal meshes and a six point flux molecule (nine-point cell molecule) for non-orthogonal meshes. The method is extended towards triangular and polyhedral grids in [72] introducing linear multi-point flux methods (MPFM). The method is discussed together with the numerical results in [73].

Eymard et al. [74] construct a finite volume scheme based on the weak solution of the steady state anisotropic diffusion equation. The strategy is based on the construction of approximate gradients using so-called Raviart–Thomas shape functions. Since these can only be applied to triangular and quadrilateral meshes, the method was enhanced to general unstructured meshes [75], accounting for the irregularity of the mesh. The discrete gradients converge weakly to the exact gradient as proven in [76]. In [77], a hybrid finite volume (HFV) scheme has been introduced for any space dimension, which is dependent on both the cell- and the edge-based variables.

Portier [78] developed a non-linear Finite Volume Method for highly anisotropic diffusion operators on unstructured meshes. The gradients are evaluated on the vertices employing cell-centered and face-centered unknowns. A flux continuity condition is enforced and the resulting coefficient matrix is symmetric and positive definite.

The mixed finite volume scheme for anisotropic diffusion problems was introduced in [79] and is applicable to strongly anisotropic diffusion problems on any grids also based on weak solutions. Here both the fluxes and the cell-centered values are treated as unknowns. Breil and Maire [80] introduce a cell-centered diffusion scheme for two-dimensional unstructured meshes, employing cell-centered unknowns only. A local stencil is assembled and the scheme results in a sparse-banded, symmetric and positive definite diffusion matrix. The method can be applied on triangular and quadrilateral two-dimensional meshes, converging with second-order for the first and with almost second-order accuracy for the latter mesh type. However, the method is only valid for anisotropic diffusion tensors, while heterogeneities have not been covered.

Based on so-called mimetic finite difference methods (MFD), Brezzi et al. [81] introduce a family of simple discretization schemes on generalized polyhedral meshes, showing super-convergence. Another cell-centered scheme called SUCESS is introduced in [82,83] for incompressible Navier–Stokes equations. Both are very effective, since only a small stencil is necessary, while lacking accuracy compared to the hybrid schemes (HVF, MVF and MFD). The combination of SUCESS with hybrid schemes