Conservation laws of surfactant transport equations

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Equations of the interfacial convection and convection-diffusion describing the transport of surfactants, and more general interfacial balance laws, in the context of a three-dimensional incompressible two-phase flow are considered. Here, the interface is represented implicitly by a zero level set of an appropriate function. All interfacial quantities and operators are extended from the interface to the three-dimensional domain. In both convection and convection-diffusion settings, infinite families of conservation laws that essentially involve surfactant concentration are derived, using the direct construction method. The obtained results are also applicable to the construction of the general balance laws for other excess surface physical quantities. The system of governing equations is subsequently rewritten in a fully conserved form in the three-dimensional domain. The latter is essential for simulations using modern numerical methods. © *2012 American Institute of Physics.*
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I. INTRODUCTION

The transport of mass, energy, or momentum on multiphase interfaces is a topic of increasing importance with a wide range of applications. In particular, the presence of surface active agents, also known as *surfactants*, is relevant to various manufacturing and biomedical processes and has become a focus of research within this context. To outline a few examples, silicone surfactants are used as stabilizing agents for polyetherane foam by reducing interfacial tension and, consequently, promoting the formation of a coherent interfacial film.[1] Also, surfactants are used to control the formation of small droplets in industrial emulsification processes by lowering the surface tension, and hence facilitating the droplet breakup and preventing coalescence.[2,3] The delivery of surfactants into the lung helps to regulate its surface tension with prematurely born infants with a lung surfactant deficiency.[4,5]

From the numerical point of view, simulating the transport of mass at fluidic interfaces constitutes a major challenge, since these processes are modeled by equations defined on moving and deforming submanifolds of the original domain. Commonly, one has to deal with interfacial convection-diffusion equations, involving differential operators given by tangential parts of the standard differential operators with respect to the interface. On stationary surfaces, this difficulty is usually overcome by introducing interfacial grids and determining suitable basis polynomials of the interface that yield

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an adequate basis for tangential operators.[6] Alternatively, nodes on the surface may be determined and used for a suitable discretization. As another approach, each point can be mapped to one of its closest points on the surface. In this case, the standard differential operators have only tangential components and replace the surface differential operators.[7,8]

In case of moving or deforming interfaces, however, the above approaches are less adequate since they require an adaptation in every time step and re-meshing after certain periods of time.[9–11] A better representation of the interfacial differential operators may then be given extrinsically based on the Eulerian grid, i.e., by an orthogonal projection of the standard operators onto parts tangential to the interface where an implicit representation of the interface, for instance, by means of a level set function, yields the orthogonal projection without any difficulties.[12] A weak formulation of a corresponding Eulerian convection-diffusion equation is provided in Ref. [13]. Regarding the extension approach, all computations can be performed on the fixed Eulerian grid of the three-dimensional domain. Here, to restrict computational costs and guarantee the regularity of the level set function up to a certain extent, a small neighborhood of the interface—a narrow band around the interface—is used as the new computational domain normally consisting of few grid cells in the normal direction to the interface only.[14–17] Usually, the Eulerian approach is combined with a constant extension of all quantities in normal direction off the interface.[14–17] Still, this formulation is a major obstacle for numerical methods that split up the differential terms by Gaussian product rule and thus, require equations in divergence form. As an example, Discontinuous Galerkin methods may be considered. Here, a projection of differential operators onto their tangential parts can only be implemented by incorporating aggravating source terms.

Nevertheless, conservation laws can be constructed algorithmically using the direct construction method.[18–21] The direct construction method does not require the use of Noether's theorem, and, in fact, supersedes it for equations that do not admit a variational formulation.[20,21] The method has been implemented in the symbolic software package `GeM` for `Maple`[22] and successfully used to compute conservation laws of many nonlinear models, such as the equations of magnetohydrodynamics equilibria[23] and the *G*-equation for premixed combustion.[24] Many other examples can be found in Ref. [21].

In the present paper, we provide a conserved form of both the interfacial convection and the convection-diffusion equations describing the transport of surfactants in incompressible two-phase flow based on a level set formulation of the interface. The transport of surfactants is taken only as an illustrative example of a much wider class of interfacial balance laws. A short introduction to general interfacial balance laws and, in particular, the modeling of surfactant flow is given in Sec. II. The direct construction method of conservation laws is briefly outlined in Sec. III. In Sec. IV, we use the direct construction method to derive infinite families of conservation laws for the considered interfacial surfactant transport equations, both in the convection and the convection-diffusion settings, as well as for more general interfacial balance equations. The derived families of conservation laws involve arbitrary functions. Using the obtained conservation laws for the surfactant transport equation, we rewrite the corresponding systems of partial differential equations in fully conserved forms, which is optimal for the application of appropriate numerical methods. Here, the remaining equations of the system are provided in a conserved form as they stand. In particular, the freedom of choice of an arbitrary function present in the conservation law for surfactant concentration can be used to select a form of the conservation law that has desired properties for a given numerical scheme. An outline how this new formulation might be used in numerical schemes that forgo a discretization of the interface is discussed in Sec. V. The paper is concluded with Sec. VI containing a brief summary and discussion.

II. INTERFACIAL TRANSPORT EQUATIONS

Starting with the standard postulates of continuum mechanics and the general global balance statement for an arbitrary physical quantity in a physical domain of three bulk phases including singular phase interfaces and a three-phase contact line, Wang and Oberlack[25] derived, in addition to the classical local balance equations for each bulk phase, the local balance equations on the phase interfaces and at the contact line. These additional interface and line balance laws can be specified

for excess surface and line physical quantities, e.g., excess mass, momentum, angular momentum, energy, entropy, or surfactant mass, respectively. Another extensive derivation of these interfacial transport equations may be found in Ref. 26.

The local form of the general balance law on the interface $\mathfrak{S}$ can be written in the form

$$\frac{\delta^{(\mathfrak{s})}\gamma^{(\mathfrak{s})}}{\delta t} + \nabla^{(\mathfrak{s})} \cdot \left(\gamma^{(\mathfrak{s})}\boldsymbol{u}\right) + \nabla^{(\mathfrak{s})} \cdot \boldsymbol{\phi}^{(\mathfrak{s})} - H^{(\mathfrak{s})}\left(\boldsymbol{\phi}^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})}\right) - \pi^{(\mathfrak{s})} + [\![\boldsymbol{\phi} \cdot \boldsymbol{n}^{(\mathfrak{s})}]\!] = 0 \ \text{ on } \mathfrak{S}, \quad (1)$$

where $\gamma^{(\mathfrak{s})}$ denotes the surface density of the physical quantity investigated, $\boldsymbol{u}$ is the material velocity, $H^{(\mathfrak{s})} = \nabla^{\mathfrak{s}} \cdot \boldsymbol{n}^{(\mathfrak{s})}$ is the total surface curvature, $\boldsymbol{n}^{(\mathfrak{s})}$ is the unit normal vector of the interface $\mathfrak{S}$, pointing from the domain $\mathfrak{B}^{(1)}$ into the domain $\mathfrak{B}^{(2)}$, $[\![\mathcal{G}]\!] = \mathcal{G}^{(2)} - \mathcal{G}^{(1)}$ denotes the jump of the quantity $\mathcal{G}$ over the interface $\mathfrak{S}$ between the phases $\mathfrak{B}^{(1)}$ and $\mathfrak{B}^{(2)}$, $\boldsymbol{\phi}^{(i)}$ ($i = 1, 2$) and $\boldsymbol{\phi}^{(\mathfrak{s})}$ are the respective non-convective fluxes in the bulk phases ($i = 1, 2$) and on the interface $\mathfrak{S}$, $\pi^{(\mathfrak{s})}$ is the surface production/supply rate density, and $\nabla^{(\mathfrak{s})}$ indicates the surface gradient operator, respectively. For the case of a material interface, assuming that the interfacial non-convective flux $\boldsymbol{\phi}^{(\mathfrak{s})}$ is tangential to the interface, an equivalent formulation of (1) is provided in Ref. 26. For a bulk field that is well-defined and smooth up to the surface from both sides, the surface gradient is simply the tangential component of the standard gradient, defined by

$$\nabla^{(\mathfrak{s})} = \left[\boldsymbol{I} - \boldsymbol{n}^{(\mathfrak{s})} \otimes \boldsymbol{n}^{(\mathfrak{s})}\right] \cdot \nabla \equiv \boldsymbol{I}^{(\mathfrak{s})} \cdot \nabla, \quad (2)$$

where $\boldsymbol{I}^{(\mathfrak{s})} \equiv \boldsymbol{I} - \boldsymbol{n}^{(\mathfrak{s})} \otimes \boldsymbol{n}^{(\mathfrak{s})}$ is the surface projection tensor.

Moreover, in (1), $\delta^{(\mathfrak{s})}/\delta^{(\mathfrak{s})}t$ is the so-called normal time derivative, denoting the time derivative for a given point on the surface following the normal trajectory of the surface. It is related to the material time derivative d/dt and the local time derivative $\partial/\partial t$ (if well-defined) by $d\gamma^{(\mathfrak{s})}/dt = \delta^{(\mathfrak{s})}\gamma^{(\mathfrak{s})}/\delta^{(\mathfrak{s})}t + \boldsymbol{u} \cdot \nabla^{(\mathfrak{s})}\gamma^{(\mathfrak{s})} = \partial\gamma^{(\mathfrak{s})}/\partial t + \boldsymbol{u} \cdot \nabla\gamma^{(\mathfrak{s})}$. In deriving (1), it has been assumed that the phase interface is a material surface with a no-slip condition between the interface and the two adjoining phases.

In the present investigation, we restrict ourselves to the case when the non-convective flux $\boldsymbol{\phi}^{(\mathfrak{s})}$ on the interface $\mathfrak{S}$ is tangential to the surface. This applies to most excess surface physical quantities. In this case, $\boldsymbol{\phi}^{(\mathfrak{s})}$ may be expressed as a surface projection of any vector in the form $\boldsymbol{\phi}^{(\mathfrak{s})} = \boldsymbol{I}^{(\mathfrak{s})} \cdot \boldsymbol{g}$, where $\boldsymbol{g}$ is a three-dimensional spatial vector. Then, the balance law on the interface (1) can be rewritten as

$$\frac{d\gamma^{(\mathfrak{s})}}{dt} + \gamma^{(\mathfrak{s})}\nabla^{(\mathfrak{s})} \cdot \boldsymbol{u} + \nabla^{(\mathfrak{s})} \cdot \left(\boldsymbol{I}^{(\mathfrak{s})} \cdot \boldsymbol{g}\right) = S^{\gamma} \ \text{ on } \mathfrak{S}, \quad (3)$$

where $S^{\gamma} = \pi^{(\mathfrak{s})} - [\![\boldsymbol{\phi} \cdot \boldsymbol{n}^{(\mathfrak{s})}]\!]$ is the sum of the surface production/supply rate density and the flux from both the adjoining bulks to the interface.

In many applications, one is interested in the transport process of a solute whose concentration is small and whose influence on the flow field is negligible. Such a solute is considered as a passive constituent, which is convected by the fluid flow and whose relative motion to the fluid flow is modeled by a diffusive flux. The mass balance equation of the solute on the interface can be established by the general local balance Eq. (1) by means of the following identifications:

$$\gamma^{(\mathfrak{s})} = c, \quad \pi^{(\mathfrak{s})} = 0, \quad \boldsymbol{\phi}^{(\mathfrak{s})} = -\alpha\nabla^{(\mathfrak{s})}c \ \text{ on } \mathfrak{S}, \quad (4)$$

where an extended Fick's first law has been employed to relate the surface diffusive flux to the concentration field with a constant diffusion coefficient α.

Substituting (4) into (1) yields the conservation law of surfactant mass

$$\frac{dc}{dt} + c\nabla^{(\mathfrak{s})} \cdot \boldsymbol{u} - \alpha\nabla^{(\mathfrak{s})} \cdot \nabla^{(\mathfrak{s})}c = S \ \text{ on } \mathfrak{S}, \quad (5)$$

where S denotes the adsorption, or desorption, respectively, from both the adjoining bulks to the interface. Other derivations of the classical surfactant transport Eq. (5) and its simplified forms may be found in Refs. 26–33.

Depending on the problem investigated, the differential Eq. (5) must be appended by appropriate initial and boundary conditions in order to define a well-posed initial-boundary-value problem.

Regarding initial conditions, an initial concentration distribution on the interface may be specified,

$$c(\boldsymbol{x}, t = 0) = c_0(\boldsymbol{x}) \ \text{ on } \mathfrak{S}. \tag{6}$$

Boundary conditions are necessary for the interfacial boundary $\partial\mathfrak{S}$, which is usually a closed curve. Generally, there exist the following three cases. For a closed interface $\partial\mathfrak{S} = \emptyset$, no boundary condition is needed. In case $\partial\mathfrak{S} \neq \emptyset$, a value of c at the domain's boundary may be prescribed, which corresponds to Dirichlet boundary conditions. For the case when the flux rate of the surfactant at the interfacial boundary $\partial\mathfrak{S}$ is known, e.g., zero flux at the solid boundary, the Neumann boundary conditions can be employed, i.e.,

$$\nabla^{(\mathfrak{s})} c \cdot \boldsymbol{s} = b \ \text{ on } \partial\mathfrak{S}, \tag{7}$$

where $\boldsymbol{s}$ denotes the unit vector normal to the boundary curve $\partial\mathfrak{S}$ but tangent to the interface $\mathfrak{S}$, outward from the system.

For the convenience of numerical simulation, we extend the differential Eq. (5) defined on the interface $\mathfrak{S}$ to the three-dimensional space by the relation (2). As a result, the extended equation is no longer in a conserved form. Our aim is to construct it in a conserved form, first, in absence of sinks or sources, $S = 0$. Then, it is shown how the source/sink term S is considered if it is present. Furthermore, it will be demonstrated that the obtained conserved form of the surfactant transport equation may be generalized for more general interfacial balance laws (3).

Let $\mathfrak{S} \subset \mathbb{R}^3$ refer to the interface in an incompressible two-phase flow application where $\boldsymbol{u} = (u^1, u^2, u^3)$ denotes a velocity field. Let $\boldsymbol{x} = (x^1, x^2, x^3)$ be the position vector and $\Omega \subset \mathbb{R}^3$ the fluid domain considered, containing the interface $\mathfrak{S}$. Numerically, the interface is represented by an implicit approach using a level set function $\Phi : \mathbb{R}^3 \to \mathbb{R}$, i.e., $\mathfrak{S} = \{\boldsymbol{x} \in \Omega : \Phi(\boldsymbol{x}) = 0\}$. The level set function Φ is transported by the flow field $\boldsymbol{u}$ according to

$$\Phi_t + \boldsymbol{u} \cdot \nabla\Phi = 0 \ \text{ in } \Omega, \tag{8}$$

where the index t indicates the local time derivative $\partial/\partial t$. Incompressibility of the flow yields the continuity equation

$$\nabla \cdot \boldsymbol{u} = 0 \ \text{ in } \Omega \tag{9}$$

implying that the above equation can simply be given in the conserved form by

$$\Phi_t + \nabla \cdot (\boldsymbol{u}\,\Phi) = 0 \ \text{ in } \Omega \tag{10}$$

by multiplying (9) by Φ and adding Eq. (8). We focus on the surface convection-diffusion Eq. (5) of the form

$$c_t + (\boldsymbol{u} \cdot \nabla)c + c\nabla^{(\mathfrak{s})} \cdot \boldsymbol{u} - \alpha\Delta^{(\mathfrak{s})}c = 0 \ \text{ on } \mathfrak{S}, \tag{11}$$

describing the interfacial transport of surfactants at this stage without any desorption or adsorption from the adjoining bulk phases. Treating surface partial differential equations (PDEs) numerically, the most convenient approach for dealing with surface differential operators is commonly by an extrinsic representation where the standard differential operators are projected to their tangential parts. Hence, the interfacial differential Eq. (11) is extended from the interface $\mathfrak{S}$ to the three-dimensional domain Ω. Correspondingly, the interfacial concentration c must also be suitably extended to $\tilde{c}$ in the domain such that $\tilde{c}|_{\mathfrak{S}} = c$. Since the initial condition c_0 in (6) is defined only on the interface $\mathfrak{S}$, it must also be extended to the whole computational domain Ω, for example, as suggested by the authors,[15, 16, 34] requiring

$$\nabla\tilde{c}_0 \cdot \nabla\Phi = 0 \ \text{ in } \Omega \quad \text{and} \quad \tilde{c}_0 = c_0 \ \text{ on } \mathfrak{S}. \tag{12}$$

This means that we require $\tilde{c}_0$ to be constant in the direction transverse to the surface. From here on, we omit tildes, always assuming that we differentiate quantities defined not only on the surface, but in the embedding space as well.

In particular, the above extension for the surface divergence defined on a connected surface $\mathfrak{S} \subset \mathbb{R}^3$ is given by (2), or in index notation as

$$\nabla^{(\mathfrak{s})} \cdot \boldsymbol{u} = (\delta_{ij} - n_i n_j) \frac{\partial u^i}{\partial x^j}. \tag{13}$$

The surface Laplacian, usually referred to as the Laplace-Beltrami operator, is given by

$$\Delta^{(\mathfrak{s})} c \equiv \nabla^{(\mathfrak{s})} \cdot \nabla^{(\mathfrak{s})} c = (\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} \left((\delta_{ik} - n_i n_k) \frac{\partial c}{\partial x^k} \right), \tag{14}$$

where $\boldsymbol{n} = (n_1, n_2, n_3)$ denotes the normal vector to the surface. Here, δ_{ij} is the Kronecker delta symbol: $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$. Also note that Einstein summation in repeated indexes is assumed throughout the paper. As an advantage to the level set formulation, we have that the normal vector to the interface is simply provided by

$$\boldsymbol{n} = -\frac{\nabla \Phi}{|\nabla \Phi|}.$$

In the following, we will always assume that the level set function is regular in the domain considered, in particular, Φ is sufficiently smooth, and $\nabla \Phi \neq \boldsymbol{0}$. We will get back to this issue later.

Using the incompressibility condition (9) and rewriting the the surface divergence (13) as

$$\nabla^{(\mathfrak{s})} \cdot \boldsymbol{u} = -n_i n_j \frac{\partial u^i}{\partial x^j}$$

one obtains the extended convection-diffusion surfactant transport equation

$$c_t + u^i \frac{\partial c}{\partial x^i} - c n_i n_j \frac{\partial u^i}{\partial x^j} - \alpha (\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} \left((\delta_{ik} - n_i n_k) \frac{\partial c}{\partial x^k} \right) = 0 \ \text{ in } \Omega, \tag{15}$$

or more generally, the extended general interfacial balance law (from (3) with $S^\gamma = 0$),

$$\gamma_t^{(\mathfrak{s})} + u^i \frac{\partial \gamma^{(\mathfrak{s})}}{\partial x^i} - \gamma^{(\mathfrak{s})} n_i n_j \frac{\partial u^i}{\partial x^j} + (\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} \left((\delta_{ik} - n_i n_k) g^k \right) = 0 \ \text{ in } \Omega \tag{16}$$

in the form to be investigated below.

III. CONSTRUCTION OF CONSERVATION LAWS USING THE DIRECT METHOD

For a given system of partial differential equations, it is often important to find its divergence-type conservation laws, i.e., expressions of the form

$$\frac{\partial \Theta}{\partial t} + \frac{\partial \Psi^i}{\partial x^i} = 0 \tag{17}$$

that hold on the solutions of the given system. In (17), the conservation law density Θ and the spatial fluxes Ψ^i, $i = 1, 2, 3$, can depend on independent and dependent variables of the given equations, as well as their partial derivatives, and possibly on nonlocal (integral) quantities.

Conservation laws of the form (17) provide the mathematical expression of basic conservation principles holding for a given model, such as the conservation of mass, energy, momentum, charge, etc. They are also used for multiple other purposes, such as existence, uniqueness, and global solution behavior analysis or linearisation mappings. An important application, which is in the focus of the current contribution, is the formulation of a given system of equations in a *fully conserved form*, which makes the application of many modern numerical methods straightforward, as discussed above.

An algorithmic way to seek local conservation laws (17) of a given system of PDEs is provided by the direct construction method.[18–21] Existence of conservation laws is often associated with symmetries through the famous Noether's theorem. However, this only holds for equations that follow from a variational principle, which is often not the case for equations arising in applications. Even when equations are variational, it turns out that Noether's theorem is not the optimal way

for conservation law computations. On the other hand, the direct construction method is practically efficient whether or not the given equations are variational.

We now briefly overview the direct construction method in application to a general PDE system

$$R^\sigma = 0, \quad \sigma = 1, \ldots, N \tag{18}$$

of N partial differential equations, with independent variables $\boldsymbol{z} = (z^1, \ldots, z^n)$, one of which can be time, and m dependent variables $\boldsymbol{u} = (u^1, \ldots, u^m)$. We wish to find conservation laws

$$\frac{\partial \Psi^i}{\partial z^i} = 0 \tag{19}$$

of the PDE system (18). Expressions (19) coincide with (17) when one of the independent variables is time and others are spatial variables x^i.

Consider an Euler operator with respect to each dependent variable u^j, written as

$$\mathcal{E}_{u^j} = \frac{\partial}{\partial u^j} - \mathrm{D}_i \frac{\partial}{\partial u_i^j} + \cdots + (-1)^s \mathrm{D}_{i_1} \ldots \mathrm{D}_{i_s} \frac{\partial}{\partial u_{i_1 \ldots i_s}^j} + \cdots \tag{20}$$

in terms of the total derivative operators

$$\mathrm{D}_i = \frac{\partial}{\partial z^i} + u_i^j \frac{\partial}{\partial u^j} + u_{i i_1}^j \frac{\partial}{\partial u_{i_1}^j} + u_{i i_1 i_2}^j \frac{\partial}{\partial u_{i_1 i_2}^j} + \cdots, \tag{21}$$

where $u_{i_1 \ldots i_s}^j \equiv \partial^s u^j / \partial z^{i_1} \ldots \partial z^{i_s}$ and $u_{i i_1 \ldots i_s}^j \equiv \partial^{s+1} u^j / \partial z^i \partial z^{i_1} \ldots \partial z^{i_s}$ are partial derivatives of order s and $s + 1$, respectively.

The idea of the direct construction method is based on the fact that any divergence expression is annihilated by an Euler operator with respect to each u^j:

$$\mathcal{E}_{u^j} \left(\frac{\partial \Psi^i}{\partial z^i} \right) \equiv 0, \quad j = 1, \ldots, m. \tag{22}$$

Vice versa, if an expression is annihilated by all Euler operators, then it is a divergence expression (19).

Let us seek conservation laws as linear combinations of given equations R^σ with unknown multipliers Λ^σ:

$$\Lambda^\sigma R^\sigma \equiv \frac{\partial \Psi^i}{\partial z^i} = 0. \tag{23}$$

The unknown multipliers may be chosen by a user to depend on independent and dependent variables and perhaps partial derivatives of dependent variables up to some prescribed order. Due to (22), the multipliers Λ^σ are found from the *determining equations*

$$\mathcal{E}_{u^j}(\Lambda^\sigma R^\sigma) = 0, \quad j = 1, \ldots, m. \tag{24}$$

After the linear determining equations (24) are solved and multipliers Λ^σ are found, one proceeds to finding conservation law density and fluxes by means of (23). Methods of flux computation are reviewed in Ref. 35. In particular, one of these methods requires the knowledge of point symmetries[21] of a given system of equations. For completeness, point symmetries of the Eqs. (8), (9), and (11) considered in the current paper are given in the Appendix.

The direct construction method is implemented in the symbolic software package GeM for Maple[22] which has been used for the computations in the present paper.

In Sec. IV below, the direct construction method is used to discover infinite families of conservation laws of the system of Eqs. (9), (10), and (15) and in particular, to write all those equations in the conserved form. This is done for the cases of both zero and nonzero diffusion coefficient α.

It is important to note that the majority of PDE systems arising in applications can be written in a *solved form* with respect to some leading derivatives. It has been proven that for such systems, *all of their local conservation laws* follow from some multipliers through linear combinations (23) see, e.g., Ref. 21. The equations considered below, in both convection and convection-diffusion settings, can be written in a solved form.

In seeking conservation laws, one naturally avoids *trivial* conservation laws like div curl$(\cdot) \equiv 0$, or those whose fluxes and density vanish on solutions of the given system. For details, see Ref. 21.

IV. CONSERVED FORM OF THE EQUATIONS

In this section, we assume that sets of initial values and boundary conditions are provided where necessary; they will not be stated explicitly. These conditions will neither influence, nor be influenced by the construction of the conserved form of the considered differential equations.

A. The convection case

In the case of no surface diffusion ($\alpha = 0$), the governing Eqs. (9), (10) and (15) in the index notation can be written as

$$R^1 = \frac{\partial u^i}{\partial x^i} = 0 \ \text{ in } \Omega, \tag{25a}$$

$$R^2 = \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0 \ \text{ in } \Omega, \tag{25b}$$

$$R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - c n_i n_j \frac{\partial u^i}{\partial x^j} = 0 \ \text{ in } \Omega. \tag{25c}$$

Equations (25a) and (25b) are in the conserved form as they stand. We now seek multipliers Λ^1, Λ^2, Λ^3 of conservation laws for the Eqs. (25) such that the linear combination

$$\Lambda^i R^i = \frac{\partial \Theta}{\partial t} + \frac{\partial \Psi^i}{\partial x^i} = 0 \tag{26}$$

yields a conservation law and the conserved density Θ involves the surfactant concentration c. Consequently, one must take $\Lambda^3 \neq 0$.

The first step is to choose the dependence of the multipliers Λ^i for the direct construction method.

It can be shown that choosing multipliers independent of second-order derivatives does not yield any solution of the equations determining the multipliers (24). Hence, to construct any conservation form (26) with $\Lambda^3 \neq 0$, a dependence of the multipliers on the second-order spatial derivatives of physical quantities is necessary.[21]

One is successful when using the multiplier ansatz

$$\Lambda^i = \Lambda^i(t, \mathbf{x}, \Phi, c, \mathbf{u}, \partial\Phi, \partial c, \partial\mathbf{u}, \partial^2\Phi, \partial^2 c, \partial^2\mathbf{u}), \tag{27}$$

where

$$\partial\Phi \equiv \left\{ \frac{\partial\Phi}{\partial x^k}, \ k = 1, 2, 3 \right\}, \quad \partial^2\Phi \equiv \left\{ \frac{\partial^2\Phi}{\partial x^j \partial x^k}, \ j, k = 1, 2, 3 \right\}$$

are sets of first-order and second-order derivatives of Φ, or c and components of $\mathbf{u}$, respectively. In (27), one may additionally include time derivatives of components of $\mathbf{u}$ but does not need to include time derivatives of Φ and c, since the latter are defined by spatial derivatives through the Eqs. (25b) and (25c).

Requiring that the conservation law (26) holds and solving the multiplier determining Eqs. (22), one obtains an infinite set of admitted conservation law multipliers Λ^1, Λ^2, Λ^3. Importantly, the multiplier Λ^3 can be nonzero. It has a general form

$$\Lambda^3 = |\nabla\Phi| \ \mathcal{K}(\Phi, \ c|\nabla\Phi|), \tag{28}$$

where $\mathcal{K}$ is an arbitrary sufficiently smooth function of its arguments. The form of the multipliers Λ^1, Λ^2 is highly complicated; however, a rather simple explicit form of an equivalent conservation law can be found. The following statement holds.

Principal Result 1:

(a)   *The system of surfactant transport equations in the absence of surface diffusion* (25a)–(25c) *admits an infinite family of conservation laws given by*

$$\frac{\partial}{\partial t}\mathcal{G}(\Phi, c|\nabla\Phi|) + \frac{\partial}{\partial x^i}\left(u^i\mathcal{G}(\Phi, c|\nabla\Phi|)\right) = 0 \ \ in\ \Omega, \tag{29}$$

   where $\mathcal{G}$ is an arbitrary sufficiently smooth function of its arguments.

(b)   *Each of the conservation laws* (29) *with $\mathcal{G} \neq 0$ is a conserved form of the dynamic equation* (25c) *for the surfactant concentration.*

(c)   *The conservation laws* (29) *can be written in the material form as*

$$\frac{d}{dt}\mathcal{G}(\Phi, c|\nabla\Phi|) = 0, \tag{30}$$

   where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \boldsymbol{u} \cdot \nabla$$

   denotes the material derivative. This means that the quantity $\mathcal{G}$ is invariant to a fixed particle.

(d)   *The arbitrary functions $\mathcal{K}$ and $\mathcal{G}$ are related by*

$$\mathcal{K}(\Phi, \ c|\nabla\Phi|) = \frac{\partial\mathcal{G}}{\partial\xi}(\Phi, \xi)|_{\xi=c|\nabla\Phi|}. \tag{31}$$

Remark 1: To preserve the number of independent equations in the rewritten system, as compared to the equation system (25), $\mathcal{G}$ has to be chosen as an invertible function in its second argument. With this restriction, the surfactant transport equation without diffusion, (25c), can be replaced by the conserved form (29).

Statement (b) follows from the observation that, since Λ^3 given by (28) is generally nonzero, the linear combination (26) essentially involves the surfactant transport Eq. (25c). Statement (c) is a direct consequence of the incompressibility condition (9). This indicates that in the pure convection case, $\mathcal{G}(\Phi, c|\nabla\Phi|)$ is a material conservation quantity.

The statement (a) follows from the direct construction method. A straightforward way to verify that (29) holds on solutions of (25) is as follows. Denote the differential consequences of equation $R^2 = 0$ (25b) with respect to spatial coordinates x^j by

$$R_j^2 = \frac{\partial}{\partial x^j}\Phi_t + \frac{\partial}{\partial x^j}\left(u^i\frac{\partial\Phi}{\partial x^i}\right) = 0, \quad j = 1, 2, 3, \tag{32}$$

and denote $\mathcal{G}(\Phi, c|\nabla\Phi|) = \widetilde{\mathcal{G}}(\Phi, c^2|\nabla\Phi|^2) = \widetilde{\mathcal{G}}$ for the simplicity of notation. Then a direct computation yields

$$\frac{\partial}{\partial t}\left(\mathcal{G}(\Phi, c|\nabla\Phi|)\right) + \frac{\partial}{\partial x^i}\left(u^i\mathcal{G}(\Phi, c|\nabla\Phi|)\right) \equiv \frac{\partial}{\partial t}\widetilde{\mathcal{G}} + \frac{\partial}{\partial x^i}\left(u^i\widetilde{\mathcal{G}}\right)$$

$$= \{\widetilde{\mathcal{G}} - \Phi D_1\widetilde{\mathcal{G}} - 2c^2|\nabla\Phi|^2 D_2\widetilde{\mathcal{G}}\} \ R^1 + \{D_1\widetilde{\mathcal{G}}\} \ R^2 + \{2c|\nabla\Phi|^2 D_2\widetilde{\mathcal{G}}\} \ R^3 + \left\{2c^2 D_2\widetilde{\mathcal{G}}\frac{\partial\Phi}{\partial x^j}\right\} \ R_j^2,$$

where $D_1\widetilde{\mathcal{G}}, D_2\widetilde{\mathcal{G}}$ denote the partial derivatives of $\widetilde{\mathcal{G}}$ by its first and second argument, respectively. Consequently, the divergence expression (29) is indeed a linear combination of the equations $R^1 = 0$, $R^2 = 0$, $R^3 = 0$ (25) and the differential consequences $R_j^2 = 0$ (32) with multipliers given in the curly brackets, and the Principal Result 1 is fully established.

Remark 2: In the case $\mathcal{G}(\Phi, c|\nabla\Phi|) = 1$, formula (29) reduces to the incompressibility condition (25a). Simplest concentration-dependent conservation laws in the family (29) can be obtained, for

example, by setting $\mathcal{G}(\Phi, c|\nabla\Phi|) = (c|\nabla\Phi|)^p$, $p \in \mathbb{N}$, and are given by

$$\frac{\partial}{\partial t}[(c|\nabla\Phi|)^p] + \frac{\partial}{\partial x^i}[u^i(c|\nabla\Phi|)^p] = 0. \tag{33}$$

In particular, when p is an even number, the density and the fluxes in (33) do not involve square roots, which are due to $|\nabla\Phi|$.

Another possible case of interest for applications is the separated form $\mathcal{G}(\Phi, c|\nabla\Phi|) = F_1(\Phi)F_2(c|\nabla\Phi|)$, where F_1 and F_2 are suitable arbitrary functions.

B. The convection-diffusion case

In the presence of diffusion, the extended surfactant dynamic equations take the form

$$\tilde{R}^1 = \frac{\partial u^i}{\partial x^i} = 0 \ \text{ in } \Omega, \tag{34a}$$

$$\tilde{R}^2 = \Phi_t + \frac{\partial(u^i\Phi)}{\partial x^i} = 0 \ \text{ in } \Omega, \tag{34b}$$

$$\tilde{R}^3 = c_t + u^i\frac{\partial c}{\partial x^i} - cn_in_j\frac{\partial u^i}{\partial x^j} - \alpha(\delta_{ij} - n_in_j)\frac{\partial}{\partial x^j}\left((\delta_{ik} - n_in_k)\frac{\partial c}{\partial x^k}\right) = 0 \ \text{ in } \Omega. \tag{34c}$$

Similar to the purely convective case, for the system (34), there exist no conservation laws where the multipliers depend only on independent and dependent variables as well as first order derivatives of the dependent variables. Hence, no c-dependent conservation law can be constructed.[22]

If the multiplier dependence is further generalized to include second order derivatives of Φ, then one finds an infinite family of sets of local conservation law multipliers corresponding to c-dependent conservation laws. Such multipliers are given by

$$\begin{aligned}
\Lambda^1 &= \Phi\mathcal{F}(\Phi)|\nabla\Phi|^{-1}\left(\frac{\partial}{\partial x^j}\left(c\frac{\partial\Phi}{\partial x^j}\right) - cn_in_j\frac{\partial^2\Phi}{\partial x^i\partial x^j}\right), \\
\Lambda^2 &= -\mathcal{F}(\Phi)|\nabla\Phi|^{-1}\left(\frac{\partial}{\partial x^j}\left(c\frac{\partial\Phi}{\partial x^j}\right) - cn_in_j\frac{\partial^2\Phi}{\partial x^i\partial x^j}\right), \\
\Lambda^3 &= \mathcal{F}(\Phi)|\nabla\Phi|,
\end{aligned} \tag{35}$$

where $\mathcal{F}$ is an arbitrary sufficiently smooth function. The conservation law density Θ and the fluxes Ψ^i are again found directly using the flux determining Eq. (26). The following result holds.

Principal Result 2:

(a)   *The system of surfactant transport Eqs. (34a)–(34c) in the case of a nonzero surface diffusion ($\alpha \neq 0$) admits an infinite family of conservation laws given by*

$$\frac{\partial}{\partial t}\left(c\,\mathcal{F}(\Phi)\,|\nabla\Phi|\right) + \frac{\partial}{\partial x^i}\left(A^i\,\mathcal{F}(\Phi)\,|\nabla\Phi|\right) = 0 \ \text{ in } \Omega, \tag{36}$$

where

$$A^i = cu^i - \alpha\left((\delta_{ik} - n_in_k)\frac{\partial c}{\partial x^k}\right), \quad i = 1, 2, 3, \tag{37}$$

and $\mathcal{F}$ is an arbitrary sufficiently smooth function of its argument, cf. (35).

(b)   *Each of the conservation laws (36) with $\mathcal{F} \neq 0$ is a conserved form of the dynamic Eq. (34c) for the surfactant concentration. In this case, (34c) can be replaced by (36).*

The simplest concentration-dependent conservation law of the family (36) is obtained by setting $\mathcal{F}(\Phi) = 1$, and has the form

$$\frac{\partial}{\partial t} \left(c \, |\nabla \Phi| \right) + \frac{\partial}{\partial x^i} \left(u^i \, c \, |\nabla \Phi| \right) = \alpha \frac{\partial}{\partial x^i} \left(|\nabla \Phi| \, (\delta_{ik} - n_i n_k) \frac{\partial c}{\partial x^k} \right) \quad \text{in } \Omega. \qquad (38)$$

Remark 3: As it is expected, one can observe that when $\alpha = 0$, formulas (36) collapse to a subfamily of conservation laws (29) for the no-diffusion case, with $\mathcal{G}(\Phi, c|\nabla\Phi|) = c\mathcal{F}(\Phi)|\nabla\Phi|$.

Remark 4: Conservation laws (36), as well as conservation laws (29) for the no-diffusion case, are dimensionally consistent for any choice of dimension units for the arbitrary functions $\mathcal{F}$ and $\mathcal{G}$.

C. Conservation forms for general interfacial balance laws

Conserved forms of the surfactant transport Eq. (15) in the convection-diffusion setting were constructed in Sec. IV A above. The Eq. (15) follows from a surface extension of the Fick's law, i.e., the third identity in (4). However, it is easy to see that neither the obtained multipliers (35), nor the conservation laws (36) themselves depend on the choice of the surface diffusion law. This allows for the following generalization.

Let $\gamma^{(\mathfrak{s})}$ be some excess surface physical quantity on the surface $\mathfrak{S}$ whose non-convective flux can be expressed as the surface projection of an arbitrary vector in the form $\boldsymbol{\phi}^{(\mathfrak{s})} = \boldsymbol{I}^{\mathfrak{s}} \cdot \boldsymbol{g}$. The balance law for $\gamma^{(\mathfrak{s})}$ in the absence of the source term is given by (16), which is almost identical to the surfactant transport Eqs. (15) and (34c). It follows that the analysis of Sec. IV B can be carried over to a system of Eqs. (16), (34a) and (34b), to obtain an infinite family of conservation laws

$$\frac{\partial}{\partial t} \left(\gamma^{(\mathfrak{s})} \, \mathcal{F}^\gamma(\Phi) \, |\nabla \Phi| \right) + \frac{\partial}{\partial x^i} \left(A^{i,\gamma} \, \mathcal{F}^\gamma(\Phi) \, |\nabla \Phi| \right) = 0, \qquad (39)$$

where

$$A^{i,\gamma} = \gamma^{(\mathfrak{s})} u^i + \phi_i^{(\mathfrak{s})} = \gamma^{(\mathfrak{s})} u^i + \left(\delta_{ij} - n_i n_j \right) g^j, \quad i = 1, 2, 3, \qquad (40)$$

for any excess surface physical quantity $\gamma^{(\mathfrak{s})}$. In (39), $\mathcal{F}^\gamma$ is an arbitrary sufficiently smooth function.

D. Interfacial transport equations in the presence of source terms

So far, we have only considered surfactant transport equations and balance laws that do not involve source terms. In many cases, the source terms may occur, e.g., for the surfactant transport equation when adsorption or desorption from both the adjoining bulk phases to the interface or chemical production on the interface take place.

Generally, when a transport equation contains a source term, it may not be written in a fully conserved form, except for some special cases. However, using the previously derived conserved forms for the no-source case, one can rewrite a transport equation with sources in a more compact form. As an example, consider a surfactant transport equation with sources. It can be written in the form

$$R^{3*} = \tilde{R}^3 - S(c, \boldsymbol{x}, t),$$

$$= c_t + u^i \frac{\partial c}{\partial x^i} - c n_i n_j \frac{\partial u^i}{\partial x^j} - \alpha (\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} \left((\delta_{ik} - n_i n_k) \frac{\partial c}{\partial x^k} \right)$$

$$- S(c, \boldsymbol{x}, t) = 0 \quad \text{in } \Omega. \qquad (41)$$

A linear combination of (34a) and (34b) and the above Eq. (41) by the multipliers (35) yields

$$\Lambda^1 \tilde{R}^1 + \Lambda^2 \tilde{R}^2 + \Lambda^3 R^{3*}$$

$$= \Lambda^1 \tilde{R}^1 + \Lambda^2 \tilde{R}^2 + \Lambda^3 \tilde{R}^3 - \Lambda^3 S(c, \boldsymbol{x}, t),$$

$$= \frac{\partial}{\partial t} \left(c \, \mathcal{F}(\Phi) \, |\nabla \Phi| \right) + \frac{\partial}{\partial x^i} \left(A^i \, \mathcal{F}(\Phi) \, |\nabla \Phi| \right) - \Lambda^3 S(c, \boldsymbol{x}, t) = 0. \qquad (42)$$

Consequently, the interfacial convection-diffusion equation with sources can be rewritten as

$$\frac{\partial}{\partial t}\left(c\,\mathcal{F}(\Phi)\,|\nabla\Phi|\right) + \frac{\partial}{\partial x^i}\left(A^i\,\mathcal{F}(\Phi)\,|\nabla\Phi|\right) = \mathcal{F}(\Phi)|\nabla\Phi|S(c,\boldsymbol{x},t)\ \text{in}\ \Omega. \tag{43}$$

Similarly, the purely convective surfactant dynamics equation can be rewritten as

$$\frac{\partial}{\partial t}\mathcal{G}(\Phi,c|\nabla\Phi|) + \frac{\partial}{\partial x^i}\left(u^i\mathcal{G}(\Phi,c|\nabla\Phi|)\right) = |\nabla\Phi|\,\frac{\partial\mathcal{G}}{\partial\xi}(\Phi,\xi)|_{\xi=c|\nabla\Phi|}(\Phi,\,c|\nabla\Phi|)S(c,\boldsymbol{x},t)\ \text{in}\ \Omega. \tag{44}$$

V. PERSPECTIVES FOR NUMERICAL TREATMENT

Evolving interfacial physical quantities, such as surfactant concentration, along a moving deformable surface is a highly challenging task, and depending on the method applied, tracking or capturing an interface also requires great expertise. In most research works, a Lagrangian grid is used to track the phase interface and employed to discretize interfacial equations implying that these equations are only solved on the interface, see e.g., Refs. [36–42].

Up to now, considerably fewer works on numerical simulations of interfacial equations are based on an Eulerian approach. Several limited examples may be found in Refs. [13–17] for various interfacial differential equations, but not for surfactant transport. Xu *et al.*[34] presented a level-set/immersed interface method for two dimensional interfacial flows with insoluble surfactant. The evolution of the surfactant concentration was performed by solving a convection-diffusion equation using an Eulerian approach, first presented in Ref. [43].

In the Eulerian approach considered in the current work, the surface differential operators are expressed in terms of global derivatives, and the interfacial physical quantities, such as the surfactant concentration, which are supposed to be only defined along the interface, are extended off the interface into a higher dimensional domain. To reduce the amount of computational cost caused by the additional dimension, computations are typically restricted to a tube around the interface consisting of few grid cells only. The extended physical quantities are then evolved in this narrow band. The interface is captured by the level set method. By suitably choosing this narrow band, the sufficient regularity of the level set function ($\nabla\Phi\neq\boldsymbol{0}$) is assured. Thus, the evolution of the physical quantity investigated, for instance of the surfactant concentration, along the interface (zero level-set contour) is embedded in the evolution of the extended quantity in the narrow band. An advantage of this method is that the evolution of the extended physical quantity can be easily performed using standard numerical methods on the same Eulerian grid as used for the representation of the flow field, avoiding an explicit discretization of the interface. A disadvantage is that the possible conserved form of the interfacial balance law may be destroyed by the extension of the interfacial differential equation to the three-dimensional domain, as shown before for the surfactant transport equation. From the viewpoint of numerical accuracy, the conserved form of a differential equation is always favorable to reduce numerical errors and preserve the quantity numerically. The conserved form of Eqs. (25) and (34) offers new perspectives to the numerical treatment of interfacial convection-diffusion equations that attempt to forgo the discretization of fluidic interfaces and maintain the high-order numerical accuracy.

Numerical computing in this domain requires choosing conditions at the boundary of the narrow band. The correct boundary conditions remain unclear, or to some extent they can be chosen arbitrarily, since for the interfacial differential equation, any transport process occurs only along the interface. This implies that no information is shared between level sets and any analytic solution on the interface is unaffected by these additional boundary conditions. However, in numerical simulation, the computational domain is discretized, and the numerical solution will depend on the choice of the boundary conditions, though this dependence should decrease as spatial and temporal resolutions increase. Previous works have used either homogeneous Neumann, or Dirichlet boundary conditions at the boundary of the computational domain.[13–17,34,43,44]

As we have pointed out in Sec. II, in order to solve the interfacial differential equation in a neighborhood of the surface, initial data must be extended from the surface into the larger Eulerian

domain. Many authors suggested to extend the surface data by requiring the initial condition to be constant normal to the surface, thus minimizing variations in the solution off the interface and hopefully limiting numerical errors due to discretization. On this account, a natural condition at the boundary of the narrow band may be

$$\frac{\partial c}{\partial x^i} \frac{\partial \Phi}{\partial x^i} = 0, \tag{45}$$

which is automatically satisfied if the solution normal to the surface is constant. Unfortunately, the numerical solution of the extended differential equation does not retain this property at later times. As a result, long-time calculations may often require intermittent re-extension of data off the surface[16,43] and the above boundary condition may be a suitable limitation to reduce numerical errors. Furthermore, taking into account that the domain boundaries may not correspond to isocontours of the level set function, a slightly modified convenient boundary condition may be used in the form
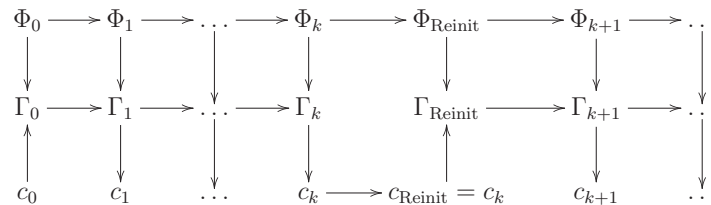
$$\frac{\partial c}{\partial x^i} n_i^b = 0, \tag{46}$$

where $\boldsymbol{n}^b$ represents the outer normal of the narrow band. The suitability of a boundary condition must be examined numerically. A further way to reduce the influence of the conditions at the boundary of the narrow band on the numerical solution of the interface is to take the advantage of arbitrary functions $\mathcal{G}$ in (29) and $\mathcal{F}$ in (36) by requiring them to decay exponentially with the distance to the interface, e.g., in the form $\sim\exp(-\lambda\,\Phi^2)$ with $\lambda > 0$. As a result, the differential equation and its corresponding solution are restricted to a very narrow region around the interface.

We do not require the level set function to maintain the signed distance property throughout the entire computation. Our test computations have also shown that with sufficiently high-order numerical methods, e.g., the Discontinuous Galerkin (DG) method, a re-initialization of the level set function may be often not necessary. However, in some cases in order to assure the numerical convergence, a re-initialization may be unavoidable. Indeed, the conserved form of the surfactant transport equation obtained before, e.g., (36), or its modified form

$$\frac{\partial \Gamma}{\partial t} + \frac{\partial}{\partial x^i}\left(u^i \Gamma\right) = \alpha\,\frac{\partial}{\partial x^i}\left(\mathcal{F}(\Phi)|\nabla\Phi|\,(\delta_{ik} - n_i n_k)\,\frac{\partial}{\partial x^k}\left(\frac{\Gamma}{\mathcal{F}(\Phi)|\nabla\Phi|}\right)\right) \tag{47}$$

rewritten for the new conserved quantity $\Gamma = c\,\mathcal{F}(\Phi)\,|\nabla\Phi|$, is based on the convection equation of the level set function (34b) without the re-initialization. When the obtained conserved form (47) is employed to simulate the evolution of the conserved quantity Γ (or the concentration c), the possible necessity of re-initialization forces the respective time stepping scheme to be interrupted, and re-started with the new level set function after re-initialization and the previous value of the surfactant concentration both of which yield a new initial value for Γ, as displayed in the diagram below:

$$
\begin{array}{ccccccccc}
\Phi_0 & \longrightarrow & \Phi_1 & \longrightarrow & \cdots & \longrightarrow & \Phi_k & \longrightarrow & \Phi_{\text{Reinit}} & \longrightarrow & \Phi_{k+1} & \longrightarrow & \cdots \\
\downarrow & & \downarrow & & \vdots & & \downarrow & & \downarrow & & \downarrow & & \\
\Gamma_0 & \longrightarrow & \Gamma_1 & \longrightarrow & \cdots & \longrightarrow & \Gamma_k & & \Gamma_{\text{Reinit}} & \longrightarrow & \Gamma_{k+1} & \longrightarrow & \cdots \\
\uparrow & & \downarrow & & \vdots & & \downarrow & & \uparrow & & \downarrow & & \\
c_0 & & c_1 & & \cdots & & c_k & \longrightarrow & c_{\text{Reinit}} = c_k & & c_{k+1} & & \cdots
\end{array}
$$

Certainly, this constitutes additional computational cost and a loss in efficiency. However, choice of a suitable method can make a frequent re-initialization redundant, as that indicated by numerical experiments in case of Discontinuous Galerkin methods.[45]

VI. SUMMARY AND CONCLUSIONS

In the present paper, the interfacial convection equations (25) and convection-diffusion equations (34) describing the transport of surfactants on a two-phase interface in a three-dimensional incompressible flow were studied. The formulation considered is based on an implicit representation

of the interface by a level set function and an extrinsic formulation of differential operators acting on the interface.

Infinite sets of conservation laws essentially involving the surfactant concentration c have been discovered for both convection and convection-diffusion formulations using the direct construction method involving local conservation law multipliers. The results obtained can be generalized further to interfacial balance laws where the non-convective flux is tangential to the surface.

For the purely convective case, conserved densities and fluxes of the new conservation laws (29) generally depend on the level set function Φ, the norm of its gradient $|\nabla\Phi|$, the flow velocity $\mathbf{u}$, and the surfactant concentration c itself. Conservation laws depend on an arbitrary function $\mathcal{G}(\Phi, c|\nabla\Phi|)$, and hold for all sufficiently smooth globally or locally defined level set functions $\Phi = \Phi(t, x, y, z)$. For the convection-diffusion setting, the fluxes (36) additionally involve the diffusion coefficient α as well as the surface gradient of c as compared to the fluxes (29). In fact, the set of conservation laws is larger in the case of zero diffusion.

The obtained families of conservation laws yield a fully conserved form of each respective system of equations, in cases with and without diffusion. In particular, each equation becomes a divergence-type conservation law.

The conserved forms obtained for surfactant transport dynamics equations were further generalized in Sec. IV C to provide conserved forms of the source-free transport equation (16) of any excess surface physical quantity, satisfying an arbitrary appropriate surface diffusion law.

From a numerical point of view, the fully conserved form is desirable for any solver that is based on Riemann solvers and offers much better perspectives than, for example, treating the extrinsic operator formulation by the product rule or the introduction of artificial variables. Derivatives present in the fluxes require numerical treatment. Hence, the fully conserved form obtained in the present paper seems to be particularly suitable for Discontinuous Galerkin methods.

As an important aspect, arbitrary functions that appear in the new conservation laws admit a lot of freedom regarding the dependence of density and fluxes on the level set function itself. On one hand, one should, of course, be careful to avoid degenerate formulations of the problem, keeping in mind that by definition Φ vanishes exactly on the interface. On the other hand, the functions $\mathcal{G}$ in (29) and $\mathcal{F}$ in (36) provide means to approximate the equation in a variety of ways, for example, to localize it to a narrow region around the interface.

APPENDIX: POINT SYMMETRIES OF THE SURFACTANT TRANSPORT EQUATIONS

In the current section, standard notation is used to denote symmetries. For details, see Ref. 21 or any text on symmetries of differential equations.

1. The case of no diffusion, $\alpha = 0$.

In this case, the surfactant transport equations (25) have an infinite set of point symmetries spanned by the following families of infinitesimal generators.

- Translations in space and time:

$$\mathrm{X}_j = \frac{\partial}{\partial x^j}, \, j = 1, 2, 3; \qquad \mathrm{X}_4 = \frac{\partial}{\partial t}.$$

- Dilations

$$\mathrm{X}_5 = t\frac{\partial}{\partial t} + x^i\frac{\partial}{\partial x^i}.$$

- Generalized scalings

$$X_6 = h_1(\Phi)\frac{\partial}{\partial \Phi}, \quad X_7 = h_2(\Phi)c\frac{\partial}{\partial c}, \quad X_8 = f(t)\frac{\partial}{\partial t} - f'(t)u^i\frac{\partial}{\partial u^i}.$$

- The Galilean group

$$X_9 = g_1(t)\frac{\partial}{\partial x^1} + g_1'(t)\frac{\partial}{\partial u^1}, \quad X_{10} = g_2(t)\frac{\partial}{\partial x^2} + g_2'(t)\frac{\partial}{\partial u^2}, \quad X_{11} = g_3(t)\frac{\partial}{\partial x^3} + g_3'(t)\frac{\partial}{\partial u^3}.$$

- The generalized rotation around the x^3 axis, given by

$$X_{12} = k_1(t)\left(x^2\frac{\partial}{\partial x^1} - x^1\frac{\partial}{\partial x^2} + u^2\frac{\partial}{\partial u^1} - u^1\frac{\partial}{\partial u^2}\right) + k_1'(t)\left(x^2\frac{\partial}{\partial u^1} - x^1\frac{\partial}{\partial u^2}\right),$$

  and the corresponding generalized rotations around the axes of x^1, x^2 given by X_{13}, X_{14} involving arbitrary functions $k_2(t)$, $k_3(t)$ and cyclic index permutations $1 \to 2 \to 3 \to 1$. [The generalized rotations X_{12}, X_{13}, X_{14} include usual rotations when the corresponding $k_i(t) = 1$, $i = 1, 2, 3$.]

  In the above generators, $f(t)$, $g_i(t)$, $h_i(t)$, $k_i(t)$ are arbitrary functions.

2. The case of nonzero diffusion, $\alpha \neq 0$.

In the case when the surface diffusion is present, $\alpha \neq 0$, the surfactant transport equations (34) also have an infinite set of point symmetries, spanned by the following infinitesimal generators:

$$X_1, X_2, X_3, X_4, X_6, X_7, X_9, X_{10}, X_{11}, X_{12}, X_{13}, X_{14}$$

from above, and an additional scaling symmetry

$$X_{15} = 2t\frac{\partial}{\partial t} + x^i\frac{\partial}{\partial x^i} - u^i\frac{\partial}{\partial u^i}.$$

[Note that symmetries X_5 and X_8 hold when $\alpha = 0$ but do not hold when $\alpha \neq 0$.]

[1] S. A. Snow, U. C. Pernisz, and R. J. Braun, "'Tying up loose ends'—Silicone surfactants as stabilizing agents for flexible polyurethane foam," Silicon Chem. **3**, 1–10 (2006).

[2] J. J. M. Janssen, A. Boon, and W. G. M. Agterof, "Influence of dynamic interfacial properties on droplet breakup in simple shear flow," AIChE J. **40**, 1929–1932 (1994).

[3] C. D. Eggleton, T.-M. Tsai, and K. J. Stebe, "Tip streaming from a drop in the presence of surfactants," Phys. Rev. Lett. **87**(4), 048302 (2001).

[4] J. B. Grotberg, "Pulmonary flow and transport phenomena," Annu. Rev. Fluid Mech. **26**, 529–571 (1994).

[5] J. B. Grotberg, D. Halpern, and O. E. Jensen, "Interaction of exogenous and endogeneous surfactant: Spreading-rate effects," J. Appl. Physiol. **78**, 750–757 (1995).

[6] G. Dziuk and M. C. Elliott, "Surface finite elements for parabolic equations," J. Comput. Math. **25**, 385–407 (2007).

[7] S. J. Ruuth and B. Merriman, "A simple embedding method for solving partial differential equations on surfaces," J. Comput. Phys. **227**, 1943–1961 (2008).

[8] C. B. Macdonald and S. J. Ruuth, "Level set equations on surfaces via the closest point method," J. Sci. Comput. **35**(2–3), 219–240 (2008).

[9] G. Dziuk and M. C. Elliott, "Finite elements on evolving surfaces," IMA J. Numer. Anal. **27**, 262–292 (2007).

[10] M. C. Elliott and C. Eilks, "Numerical simulation of dealloying by surface dissolution via the evolving surface finite element method," J. Comput. Phys. **227**, 9727–9741 (2008).

[11] M. Lenz, S. F. Nemadjieu, and M. Rumpf, "Finite volume method on moving surfaces," in *Finite Volumes for Complex Applications V*, edited by R. Eymard and J.-M. Hérald (Wiley, London/Hoboken, NJ, 2008), pp. 561–576.

[12] G. Dziuk and M. C. Elliott, "Eulerian finite element method for parabolic PDEs on implicit surfaces," IMA J. Numer. Anal. **10**, 119–138 (2008).

[13] G. Dziuk and C. M. Elliott, "An Eulerian approach to transport and diffusion on evolving implicit surfaces," Comput. Visualization Sci. **13**, 17–28 (2010).

[14] M. Bertalmio, S. Osher, G. Sapiro, and L.-T. Cheng, "Variational problems and partial differential equations on implicit surfaces," J. Comput. Phys. **174**, 759–780 (2001).

[15] J. B. Greer, "An improvement of a recent Eulerian method for solving PDEs on general geometries," J. Sci. Comput. **29.3**, 321–352 (2006).

[16] J. B. Greer, A. L. Bertozzi, and G. Sapiro, "Fourth order partial differential equations on general geometries," J. Comput. Phys. **216**(1), 216–246 (2006).

[17] M. Burger, "Finite element approximation of elliptic partial differential equations on implicit surfaces," Comput. Visualization Sci. **12**, 87–100 (2009).

[18] S. C. Anco and G. W. Bluman, "Direct construction method for conservation laws of partial differential equations. Part I: Examples of conservation law classifications," Eur. J. Appl. Math. **13**, 545–566 (2002).

[19] S. C. Anco and G. W. Bluman, "Direct construction method for conservation laws of partial differential equations. Part II: General treatment," Eur. J. Appl. Math. **13**, 567–585 (2002).

[20] G. W. Bluman, A. F. Cheviakov, and S. C. Anco, "Construction of conservation laws: How the direct method generalizes Noether's theorem," in *Proceedings of the Fourth International Workshop "Group Analysis of Differential Equations and Integrable Systems," Nicosia, 26–30 October 2008* (University of Cyprus, Department of Mathematics and Statistics, Protaras, Cyprus, 2009), pp. 13–35.

[21] G. W. Bluman, A. F. Cheviakov, and S. C. Anco, *Applications of Symmetry Methods to Partial Differential Equations*, Applied Mathematical Sciences Vol. 168 (Springer, New York/Dodrecht/Heidelberg/London, 2010).

[22] A. F. Cheviakov, "GeM software package for computation of symmetries and conservation laws of differential equations," Comp. Phys. Comm. **176**(1), 48–61 (2007).

[23] A. F. Cheviakov and S. C. Anco, "Analytical properties and exact solutions of static plasma equilibrium systems in three dimensions," Phys. Lett. A **372**, 1363–1373 (2008).

[24] M. Oberlack and A. F. Cheviakov, "Higher-order symmetries and conservation laws of the G-equation for premixed combustion and resulting numerical schemes," J. Eng. Math. **66**, 121–140 (2010).

[25] Y. Wang and M. Oberlack, "A thermodynamic model of multiphase flows with moving interfaces and contact line," Continuum Mech. Thermodyn. **23**, 409–433 (2011).

[26] J. C. Slattery, L. Sagis, and E. S. Oh, *Interfacial Transport Phenomena*, 2nd ed. (Springer, New York, 2007).

[27] G. M. Mavrovouniotis, H. Brenner, D. A. Edwards, and L. Ting, "A micromechanical investigation of interfacial transport processes II. Interfacial constitutive equations," Philos. Trans. R. Soc. London, Ser. A **345**, 209–228 (1993).

[28] S. Gross and A. Reusken, *Numerical Methods for Two-phase Incompressible Flows* (Springer, Berlin/Heidelberg, 2011), Vol. 1.

[29] H. A. Stone, "A simple derivation of the time-dependent convective-diffusion equation for surfactant transport along a deforming interface," Phys. Fluids A **2**(1), 111–112 (1990).

[30] D. Bothe, J. Prüss, and G. Simonett, "Well-posedness of a two-phase flow with soluble surfactant," in *Progress in Nonlinear Differential Equations and Their Applications* (Birkhäuser Verlag, Basel, 2005), Vol. 64, pp. 37–61.

[31] H. Wong, D. Rumschitzki, and C. Maldarelli, "On the surfactant mass balance at a deforming fluid interface," Phys. Fluids **8**, 3203–3204 (1996).

[32] M. G. Blyth and C. Pozrikidis, "Evolution equations for the surface concentration of an insoluble surfactant; applications to the stability of an elongating thread and a stretched interface," Theor. Comput. Fluid Dyn. **17**, 147–164 (2004).

[33] D. Halpern and A. L. Frenkel, "Destabilization of a creeping flow by interfacial surfactant: Linear theory extended to all wavenumbers," J. Fluid Mech. **485**, 191–220 (2003).

[34] J. J. Xu, Z. Li, J. Lowengrub, and H. Zhao, "A level-set method for interfacial flows with surfactant," J. Comp. Phys. **212**, 590 (2006).

[35] A. F. Cheviakov, "Computation of fluxes of conservation laws," J. Eng. Math. **66**, 153–173 (2010).

[36] H. D. Ceniceros, "The effects of surfactants on the formation and evolution of capillary waves," Phys. Fluids **15**, 245–256 (2003).

[37] A. J. James and J. S. Lowengrub, "A surfactant-conserving volume-of-fluid method for interfacial flows with insoluble surfactant," J. Comp. Phys. **201**, 685–722 (2004).

[38] Y. W. Kruijt-Stegeman, F. N. van de Vosse, and H. E. H. Meijer, "Droplet behavior in the presence of insoluble surfactants," Phys. Fluids **16**, 2785–2796 (2004).

[39] M. C. Lai, Y. H. Tseng, and H. Huang, "An immersed boundary method for interfacial flows with insoluble surfactant," J. Comp. Phys. **227**, 7279–7293 (2008).

[40] J. Lee and C. Pozrikidis, "Effect of surfactants on the deformation of drops and bubbles in Navier-Stokes flow," Comput. Fluids **35**, 43–60 (2006).

[41] M. Muradoglu and G. Tryggvason, "A front-tracking method for computations of interfacial flows with soluble surfactants," J. Comp. Phys. **227**, 2238–2262 (2008).

[42] J. Zhang, D. M. Eckmann, and P. S. Ayyaswamy, "A front tracking method for a deformable intravascular bubble in a tube with soluble surfactant transport," J. Comp. Phys. **214**, 366 (2006).

[43] J. J. Xu and H. Zhao, "An Eulerian formulation for solving partial differential equations along a moving interface," J. Sci. Comput. **19**(1–3), 573–594 (2003).

[44] D. Adalsteinsson and J. A. Sethian, "Transport and diffusion of material quantities on propagating interfaces via level set methods," J. Comp. Phys. **185**(1), 271–288 (2003).

[45] E. Marchandise, J.-F Remacle, and N. Chevaugeon, "A quadrature-free discontinuous Galerkin method for the level set equation," J. Comput. Phys. **212**, 338–357 (2006).