A parametric derivation of the surfactant transport equation along a deforming fluid interface

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Abstract
A parametric derivation of the surfactant transport equation along a deforming fluid interface is presented in this paper. The derivation is based on the Lagrangian formulation of the interface with a parametric representation. Comparisons with some of the existing derivations are also given.

Keywords: Surfactant transport equation; Surface divergence; Interfacial flow; Parametric representation

1 Introduction
Surfactant are surface active agents that adhere to the fluid interface and affect the interface surface tension. Surfactant play an important role in many applications in the industries of food, cosmetics, oil, etc. For instance, the daily extraction of ore rely on the subtle effects introduced by the presence of surfactant [2]. In a liquid-liquid system, surfactant allow small droplets to be formed and used as an emulsion. Surfactant also play an important role in water purification and other applications where micro-sized bubbles are generated by lowing the surface tension of the liquid-gas interface. In microsystems with the presence of interfaces, it is extremely important to consider the effect of surfactant since in such case the capillary effect dominates the inertial effect of the fluids [6].

The basic equation for surfactant transport equation along a deforming interface has been derived by Scriven [4], Aris [1], and Waxman [7]. All these derivations of the surfactant equation rely heavily on differential geometry. Stone [5], on the other hand, presented a simple derivation of the

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time-dependent convective-diffusion equation for surfactant transport along a deforming interface. Stone’s derivation leads a form of surfactant mass balance equation which is used later in numerical computations [10, 9]. Wong et al. [8] derived an alternative form of the surfactant transport equation and provided an interpretation of the equation by Stone.

In this paper, we present a new derivation of the surfactant equation. Our derivation is in the same spirit as Stone’s but more detailed. For the immersed interface, we use a global Cartesian position vector and a parametric representation. As a result, the meaning of the time derivative and surface divergence in Stone’s equation become clearer. Since an explicit expression for the surface divergence is given, our formulation can be readily incorporated into a front-tracking solver or other interface tracking method for numerical computations, e.g., the immersed boundary method.

2 Surfactant transport equation

Consider a two-dimensional interfacial element \( \Sigma(t) \) that is immersed in a three-dimensional incompressible fluid domain \( \Omega \). The interface is deformable and moves with the fluid. Following Stone [5], we assume that the surfactant remains on the interfacial element and does not transport (diffuse) from or to the surrounding bulk fluids, and the total amount on the element is conserved. That is, let \( \Gamma \) denote the mass of the surfactant per unit area, we have

\[
\frac{d}{dt} \int_{\Sigma(t)} \Gamma(x, y, z, t) \, dS = 0, \tag{1}
\]

where \( dS \) is the surface area element. For simplicity, we have also neglected diffusion along the interface. We use two independent parameters \((\alpha, \beta)\) to label a fixed material point of the initial reference configuration \(\Sigma(0) := \{X_0(\alpha, \beta) | (\alpha, \beta) \in S_0\}\), \(S_0\) is a fixed domain) and the parametric form of the interfacial element at time \( t \) is given by \(\Sigma(t) := \{X(\alpha, \beta, t) | (\alpha, \beta) \in S_0\}\). In other words, we have used a Lagrangian description of the time evolution of the deformable interface and the following derivation of the surfactant transport equation is based on this parametric form of the interface.

We assume the deforming interface is smooth so that the two independent unit tangent vectors (denoted by \( \tau_1 \) and \( \tau_2 \)) and its corresponding unit normal vector (denoted by \( n \)) on the surface can be explicitly expressed by

\[
\tau_1 = \frac{\partial X}{\partial \alpha}, \quad \tau_2 = \frac{\partial X}{\partial \beta}, \quad n = \frac{\tau_1 \times \tau_2}{|\tau_1 \times \tau_2|} = \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta}. \tag{2}
\]

Since the interface is immersed in a three-dimensional incompressible fluid and moves with the local flow velocity, we have

\[
\frac{\partial X(\alpha, \beta, t)}{\partial t} = u(X(\alpha, \beta, t), t), \quad X(\alpha, \beta, 0) = X_0(\alpha, \beta), \tag{3}
\]
where the fluid velocity \( u \) is defined in the fluid domain \( \Omega \) and satisfies \( \nabla \cdot u = 0 \). Before we proceed, let us prove the following lemma.

**Lemma.** The material time derivative of the surface element is given by

\[
\frac{d}{dt} \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| = (\nabla_s \cdot u) \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| \tag{4}
\]

where the surface divergent is defined as

\[
\nabla_s \cdot u = \left( \frac{\partial u}{\partial \tau_1} \cdot b_2 + \frac{\partial u}{\partial \tau_2} \cdot b_1 \right) \left| \frac{\partial X}{\partial \alpha} \right| \left| \frac{\partial X}{\partial \beta} \right| / \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right|. \tag{5}
\]

Here \( b_1 = n \times \tau_1 \) and \( b_2 = \tau_2 \times n \) are the tangential unit vectors normal to \( \tau_1 \) and \( \tau_2 \), respectively, as illustrated in Figure 1.

![Figure 1: Illustration of tangential and normal vectors on the surface and their relationships: \( b_1 = n \times \tau_1 \), \( b_2 = \tau_2 \times n \).](image)

**Proof.** Firstly, we review some vector identities that will be used in the following. Let us denote \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) and \( \mathbf{d} \) all time-dependent vectors in \( \mathbb{R}^3 \). The identity

\[
(\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) - (\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c}) \tag{6}
\]

can be easily checked and found in [3]. From \( n \cdot n = 1 \), we have

\[
\frac{dn}{dt} \cdot n = 0. \tag{7}
\]

\(^1\)A comparison between Eq. (5) and the surface divergence used in the literature [5] is given in Section 3.
We also note that
\[ \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} = \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| n. \]  
(8)

We start with the left-hand-side (LHS) of Eq. (4) by using Eqs. (7) and (8) to obtain
\[ \frac{d}{dt} \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| = n \cdot \frac{d}{dt} \left( \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right) = n \cdot \left( \frac{\partial^2 X}{\partial t \partial \alpha} \times \frac{\partial X}{\partial \beta} \right) + n \cdot \left( \frac{\partial X}{\partial \alpha} \times \frac{\partial^2 X}{\partial t \partial \beta} \right) = n \cdot \left( \frac{\partial u}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right) + n \cdot \left( \frac{\partial X}{\partial \alpha} \times \frac{\partial u}{\partial \beta} \right). \]

Substituting \( n = \tau_1 \times \tau_2 / |\tau_1 \times \tau_2| \) into the above expression and applying vector identity (6), we obtain
\[ \frac{d}{dt} \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| = \frac{G}{\left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right|^2} \]  
(9)

where
\[ G = \left[ \frac{\partial X}{\partial \alpha} \cdot \frac{\partial u}{\partial \alpha} \right] \left| \frac{\partial X}{\partial \beta} \right|^2 + \left[ \frac{\partial X}{\partial \beta} \cdot \frac{\partial u}{\partial \beta} \right] \left| \frac{\partial X}{\partial \alpha} \right|^2 - \frac{\partial X}{\partial \alpha} \cdot \frac{\partial X}{\partial \beta} \left( \frac{\partial X}{\partial \alpha} \cdot \frac{\partial u}{\partial \alpha} + \frac{\partial X}{\partial \beta} \cdot \frac{\partial u}{\partial \beta} \right). \]

To compute the right-hand-side (RHS) of Eq. (4), it is straightforward to verify that
\[ b_1 = \left( \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right) \times \frac{\partial X}{\partial \alpha} \left/ \left( \left| \frac{\partial X}{\partial \alpha} \right| \left| \frac{\partial X}{\partial \beta} \right| \right) \right. \]
\[ = \left[ \left| \frac{\partial X}{\partial \alpha} \right|^2 \frac{\partial X}{\partial \beta} - \left( \frac{\partial X}{\partial \alpha} \cdot \frac{\partial X}{\partial \beta} \right) \frac{\partial X}{\partial \alpha} \right] \left/ \left( \left| \frac{\partial X}{\partial \alpha} \right| \left| \frac{\partial X}{\partial \beta} \right| \right) \right. \), \]
\[ b_2 = \frac{\partial X}{\partial \beta} \times \left( \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right) \left/ \left( \left| \frac{\partial X}{\partial \alpha} \right| \left| \frac{\partial X}{\partial \beta} \right| \right) \right. \]
\[ = \left[ \left| \frac{\partial X}{\partial \beta} \right|^2 \frac{\partial X}{\partial \alpha} - \left( \frac{\partial X}{\partial \alpha} \cdot \frac{\partial X}{\partial \beta} \right) \frac{\partial X}{\partial \beta} \right] \left/ \left( \left| \frac{\partial X}{\partial \alpha} \right| \left| \frac{\partial X}{\partial \beta} \right| \right) \right. \). \]

Using the definition of the surface divergence of Eq. (5), we find that
\[ \nabla_s \cdot u = G \left/ \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right|^2 \right. \]  
(10)

Combining (9) and (10) completes the proof.
To derive the governing equation for the surfactant concentration $\Gamma$, we begin by applying the law of mass conservation, which yields

\[
0 = \frac{d}{dt} \int_{\Sigma(t)} \Gamma(x, y, z, t) \, dS
= \frac{d}{dt} \int_{\Sigma(0)} \Gamma(X(\alpha, \beta, t), t) \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| \, d\alpha \, d\beta
= \int_{\Sigma(0)} \frac{d}{dt} \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| \, d\alpha \, d\beta + \int_{\Sigma(0)} \Gamma \frac{d}{dt} \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| \, d\alpha \, d\beta,
\]

where the material derivative is defined as usual $\frac{d}{dt} \big|_{X} = \frac{\partial}{\partial t} |X + u \cdot \nabla \Gamma$, and the subscript $X$ denotes that the derivative is taken with respect to time while $X$ is fixed. In order to simplify the notation, we drop the subscript in the rest of the paper. Using the previous lemma and combining these two integrands, we have

\[
0 = \int_{\Sigma(0)} \left( \frac{\partial \Gamma}{\partial t} + u \cdot \nabla \Gamma + \Gamma(\nabla_s \cdot u) \right) \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| \, d\alpha \, d\beta,
\]

which leads to the same surfactant transport equation as in [5]. Thus we have established that the time derivative in Stone’s derivation is identical to the one used here, i.e., with $X$ fixed.
In [8], Wong et. al. argued that in Stone’s derivation, the time derivative has the meaning that the derivative follows the fixed point which moves normal to the interface rather than the usual meaning of the partial derivative which keeps the surface coordinates \((\alpha, \beta)\) fixed. Therefore, they derived another surfactant transport equation in which the time derivative is taken by fixing the surface coordinates. The difference between those two derivations can be easily seen by defining \(\Gamma(X(\alpha, \beta, t), t) = \hat{\Gamma}(\alpha, \beta, t)\). Going back to the material derivative, we immediately obtain that

\[
\frac{D\Gamma}{Dt} + \Gamma \nabla_s \cdot u = \frac{\partial \hat{\Gamma}}{\partial t} + \hat{\Gamma} \nabla_s \cdot u = 0.
\] (14)

It is important to note that the second equation above is exactly the one derived by Wong et.al. in [8] without the diffusion term.

The above surfactant equation can also be derived under the present formulation as follows. By assuming the surfactant concentration \(\hat{\Gamma}(\alpha, \beta, t)\) is a function of initial parameters \(\alpha, \beta\) and the time \(t\), the conservation of mass becomes

\[
0 = \frac{d}{dt} \int_{\Sigma(0)} \hat{\Gamma}(\alpha, \beta, t) \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| d\alpha d\beta
\]

\[
= \int_{\Sigma(0)} \frac{\partial \hat{\Gamma}}{\partial t} \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| d\alpha d\beta + \int_{\Sigma(0)} \frac{d}{dt} \hat{\Gamma} \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| d\alpha d\beta,
\]

\[
= \int_{\Sigma(0)} \left( \frac{\partial \hat{\Gamma}}{\partial t} + \hat{\Gamma} \nabla_s \cdot u \right) \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right| d\alpha d\beta.
\]

Since the material element \(\Sigma(0)\) is arbitrary, we immediately obtain the second equation of (14). The time derivative here is taken by fixing \(\alpha\) and \(\beta\), which is simply the material derivative.

### 3 Surface divergence

In this section, we show that our definition of surface divergence is consistent to the one used in the literature [5]

\[
\nabla_s \cdot u = (I - n \otimes n) \nabla \cdot u = \nabla \cdot u - n \cdot \nabla u \cdot n.
\] (15)

In order to simplify the notation, we use \(z^k\) as the parameters for the surface with \(z^1 = \alpha\) and \(z^2 = \beta\). The third parameter \(z^3\) is used for the parameter along the normal direction. We use \(x^i\) as the Cartesian coordinates and \(e^i\) as the corresponding unit vectors for \(i = 1, 2, 3\). Therefore, the position and velocity vectors can be expressed as

\[
X = x^i e^i, \quad u = u^i e^i
\]
where the repeated indices indicate the summation. To deal with non-Cartesian coordinates one often uses the co-variant and contra-variant basis vectors as follows

\[ g_k = \frac{\partial x^i}{\partial z^k} e^i, \quad g^k = \frac{\partial z^k}{\partial x^i} e^i, \quad k = 1, 2, 3 \]  

(16)

with the orthogonal property

\[ g^i \cdot g^j = \delta^i_j \]  

(17)

where \( \delta^i_j \) is the Kronecker delta symbol. Comparing with our earlier notation, we have

\[ \tau_1 = \frac{g_1}{|g_1|}, \quad \tau_2 = \frac{g_2}{|g_2|}, \quad b_1 = \frac{g_2}{|g_2|}, \quad b_2 = \frac{g_1}{|g_1|}, \quad n = \frac{g_3}{|g_3|} = \frac{g^3}{|g^3|}. \]

Using Eq. (16) and the fact that \( e^i \) are constant unit vectors, we have

\[ \nabla \cdot u = \frac{\partial (e^i \cdot u)}{\partial x^i} = \frac{\partial (e^i \cdot u)}{\partial z^k} \frac{\partial z^k}{\partial x^i} = e^i \cdot \frac{\partial u}{\partial z^k} \frac{\partial z^k}{\partial x^i} = g^k \cdot \frac{\partial u}{\partial z^k}. \]

Similarly, we have

\[ \nabla u = \frac{\partial u}{\partial x^i} e^i = \frac{\partial u}{\partial z^k} g^k \]

and

\[ n \cdot \nabla u \cdot n = n \cdot \frac{\partial u}{\partial z^k} g^k \cdot n = n \cdot \frac{\partial u}{\partial z^k} |g^3| = g^3 \cdot \frac{\partial u}{\partial z^3}. \]

Therefore,

\[ \nabla \cdot u - n \cdot \nabla u \cdot n = g^1 \cdot \frac{\partial u}{\partial z^1} + g^2 \cdot \frac{\partial u}{\partial z^2} \]

\[ = \left| g^1 \right| \left| g_1 \right| b_2 \cdot \frac{\partial u}{\partial \tau_1} + \left| g^2 \right| \left| g_2 \right| b_1 \cdot \frac{\partial u}{\partial \tau_2}. \]  

(18)

From Eq. (17), we have

\[ \left| g^1 \right| \left| g_1 \right| \tau_1 \cdot b_2 = \left| g^2 \right| \left| g_2 \right| \tau_2 \cdot b_1 = 1. \]

Using

\[ \tau_1 \cdot b_2 = \tau_1 \cdot (\tau_2 \times n) = n \cdot (\tau_1 \times \tau_2) = |\tau_1 \times \tau_2| \]

and

\[ \tau_2 \cdot b_1 = \tau_2 \cdot (n \times \tau_1) = n \cdot (\tau_1 \times \tau_2) = |\tau_1 \times \tau_2|, \]

we obtain

\[ \left| g^1 \right| \left| g_1 \right| = \left| g^2 \right| \left| g_2 \right| = 1/|\tau_1 \times \tau_2| = \left| \frac{\partial X}{\partial \alpha} \right| \left| \frac{\partial X}{\partial \beta} \right| / \left| \frac{\partial X}{\partial \alpha} \times \frac{\partial X}{\partial \beta} \right|. \]  

(19)

Combining Eq. (19) and Eq. (18) shows that the surface divergence given by Eq. (15) is consistent with our definition (5).
Acknowledgment

M.-C. Lai is supported in part by National Science Council of Taiwan under research grant NSC-95-2115-M-009-010-MY2 and H. Huang is supported by grants from the Natural Science and Engineering Research Council (NSERC) of Canada and the Mathematics of Information Technology and Complex Systems (MITACS) of Canada.

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