Conservation Laws of Surfactant Transport Equations

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Outline

1 Surfactants
   - Brief Overview
   - Applications
   - Surfactant Transport Equations

2 Conservation Laws
   - Definition and Examples
   - Applications

3 Direct Construction Method for Conservation Laws
   - The Idea
   - Completeness

4 Conservation Laws of Examples of Surfactant Dynamics Equations
   - The Convection Case
   - The Convection-Diffusion Case

5 Conclusions
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Surfactants - Brief Overview

"Surfactant" = "Surface active agent".

Act as detergents, wetting agents, emulsifiers, foaming agents, and dispersants.

Consist of a hydrophobic group (tail) and a hydrophilic group (head).
Surfactants - Brief Overview

**Surfactants**

- "Surfactant" = "Surface active agent".
- Act as detergents, wetting agents, emulsifiers, foaming agents, and dispersants.
- Consist of a hydrophobic group (tail) and a hydrophilic group (head).

- Sodium lauryl sulfate:

\[
\text{H}_3\text{C} - \text{C} - \text{C} - \text{C} - \text{C} - \text{C} - \text{C} - \text{C} - \text{O}^- \text{SO}_3^- \text{Na}^+ 
\]

- Saponification: e.g., triglyceride (fat) + base \(\rightarrow\) sodium stearate (soap)

\[
\begin{align*}
\text{R} - \text{O} - \text{C} - \text{O} - \text{R} \\
\text{R} - \text{O} - \text{C} - \text{O} - \text{R} \\
\text{R} - \text{O} - \text{C} - \text{O} - \text{R} \\
\end{align*}
\]

\[3 \text{NaOH} / \text{H}_2\text{O} \xrightarrow{\text{heat}} 3 \text{R} - \text{O} - \text{C} - \text{ONa} + \text{H}_2\text{O} - \text{OH} \]
Surfactants - Brief Overview

**Surfactants**

- "Surfactant" = "Surface active agent".
- Act as detergents, wetting agents, emulsifiers, foaming agents, and dispersants.
- Consist of a hydrophobic group (*tail*) and a hydrophilic group (*head*).

- Hydrophilic groups (heads) can have various properties:

![Surfactant Diagram]
Surfactants - Applications

- Surfactant molecules adsorb at phase separation interfaces.
  - Stabilization of growth of bubbles / droplets.
  - Creation of emulsions of insoluble substances.
  - Multiple industrial and medical applications.
- Can form micelles, double layers, etc.
Soap bubbles...
Surfactant Transport Equations

Derivation:

Can be derived as a special case of multiphase flows with moving interfaces and contact lines:

[Y. Wang, M. Oberlack, 2011]

Illustration:

- Illustration:
Surfactant Transport Equations (ctd.)

Parameters

- Surfactant concentration $c = c(x, t)$.
- Flow velocity $u(x, t)$.
- Two-phase interface: phase separation surface $\Phi(x, t) = 0$.
- Unit normal: $n = -\frac{\nabla \Phi}{|\nabla \Phi|}$.
Surfactant Transport Equations (ctd.)

Surface gradient

- Surface projection tensor: \( p_{ij} = \delta_{ij} - n_i n_j \).
- Surface gradient operator: \( \nabla^s = p \cdot \nabla = (\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} \).
- Surface Laplacian:

\[
\Delta^s F = (\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} \left( (\delta_{ik} - n_i n_k) \frac{\partial F}{\partial x^k} \right).
\]
Surfactant Transport Equations (ctd.)

Governing equations

- Incompressibility condition: \( \nabla \cdot \mathbf{u} = 0 \).
- Fluid dynamics equations: Euler or Navier-Stokes.
- Interface transport by the flow: \( \Phi_t + \mathbf{u} \cdot \nabla \Phi = 0 \).
- Surfactant transport equation:

\[
ct + u^i \frac{\partial c}{\partial x^i} - cn_i n_j \frac{\partial u^i}{\partial x^j} - \alpha(\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} \left( (\delta_{ik} - n_i n_k) \frac{\partial c}{\partial x^k} \right) = 0.
\]
Surfactant Transport Equations (ctd.)

\[ \Phi = 0 \]

\[ n \cdot u = 0 \]

Fully conserved form

- Specific numerical methods (e.g., discontinuous Galerkin) require the system to be written in a **fully conserved form**.
- Straightforward for continuity, momentum, and interface transport equations.
- Can the surfactant transport equation be written in the conserved form?

\[ c_t + u^i \frac{\partial c}{\partial x^i} - cn_i n_j \frac{\partial u^i}{\partial x^j} - \alpha (\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} \left( (\delta_{ik} - n_i n_k) \frac{\partial c}{\partial x^k} \right) = 0. \]
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Conservation Laws: Some Definitions

Conservation law:

**Given:** some model.

**Independent variables:** \( x = (t, x, y, ...) \); **dependent variables:** \( u = (u, v, ...) \).

**A conservation law:** a divergence expression equal to zero

\[
D_t \Theta(x, u, ...) + D_x \Psi^1(x, u, ...) + D_y \Psi^2(x, u, ...) + \cdots = 0.
\]

Time-independent:

\[
D_i \Psi^i \equiv \text{div}_{x, y, \ldots} \Psi = 0.
\]

Time-dependent:

\[
D_t \Theta + \text{div}_{x, y, \ldots} \Psi = 0.
\]

**A conserved quantity:**

\[
D_t \int_V \Theta \, dV = 0.
\]

Example: small string oscillations, 1D wave equation

Independent variables: \( x, t \); dependent: \( u(x, t) \).

\[ u_{tt} = c^2 u_{xx}, \quad c^2 = T/\rho. \]

Conservation of momentum:

- **Divergence expression:** \( D_t(\rho u_t) - D_x(Tu_x) = 0. \)

- **Arises from a multiplier:**

\[ D_t(\rho u_t) - D_x(Tu_x) = \Lambda(u_{tt} - c^2 u_{xx}) = \rho(u_{tt} - c^2 u_{xx}) = 0; \]

- **Conserved quantity:** total momentum \( M = \int \rho u_t \, dx = \text{const.} \)
Example: small string oscillations, 1D wave equation

Independent variables: \( x, t \); dependent: \( u(x, t) \).

\[
  u_{tt} = c^2 u_{xx}, \quad c^2 = \frac{T}{\rho}.
\]

Conservation of Energy:

- **Divergence expression:** \( D_t \left( \frac{\rho u_t^2}{2} + \frac{T u_x^2}{2} \right) - D_x( T u_t u_x ) = 0 \).

- **Arises from a multiplier:**
  \[
  D_t \left( \frac{\rho u_t^2}{2} + \frac{T u_x^2}{2} \right) - D_x( T u_t u_x ) = \rho u_t (u_{tt} - c^2 u_{xx}) = 0;
  \]

- **Conserved quantity:** total energy \( E = \int \left( \frac{\rho u_t^2}{2} + \frac{T u_x^2}{2} \right) dx = \text{const.} \)
Applications of Conservation Laws

**ODEs**
- Constants of motion.
- Integration.

**PDEs**
- Direct physical meaning.
- Constants of motion.
- Differential constraints (\( \text{div} \mathbf{B} = 0 \), etc.).
- Analysis: existence, uniqueness, stability.
- Nonlocally related PDE systems, exact solutions. Potentials, stream functions, etc.:
  \[
  \mathbf{V} = (u, v), \quad \text{div} \mathbf{V} = u_x + v_y = 0,
  \begin{cases}
    u = \Phi_y, \\
    v = -\Phi_x.
  \end{cases}
  \]
- An infinite number of conservation laws can indicate integrability / linearization.
- Numerical simulation.
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The Idea of the Direct Construction Method

**Definition**

The *Euler operator* with respect to $U^j$:

$$E_{U^j} = \frac{\partial}{\partial U^j} - D_i \frac{\partial}{\partial U^i_j} + \cdots + (-1)^s D_{i_1} \cdots D_{i_s} \frac{\partial}{\partial U^i_{j_{1\ldots s}}} + \cdots, \quad j = 1, \ldots, m.$$  

Consider a general DE system $R^\sigma[u] = R^\sigma(x, u, \partial u, \ldots, \partial^k u) = 0, \quad \sigma = 1, \ldots, N$ with variables $x = (x^1, \ldots, x^n), \quad u = u(x) = (u^1, \ldots, u^m)$.

**Theorem**

*The equations*

$$E_{U^j} F(x, U, \partial U, \ldots, \partial^s U) \equiv 0, \quad j = 1, \ldots, m$$

hold for arbitrary $U(x)$ if and only if

$$F(x, U, \partial U, \ldots, \partial^s U) \equiv D_i \Psi^i$$

for some functions $\Psi^i(x, U, \ldots)$.  

Consider a general DE system \( R^\sigma [u] = R^\sigma (x, u, \partial u, \ldots, \partial^k u) = 0, \quad \sigma = 1, \ldots, N \) with variables \( x = (x^1, \ldots, x^n) \), \( u = u(x) = (u^1, \ldots, u^m) \).

### Direct Construction Method [Anco, Bluman (1997, 2002)]

- Specify dependence of multipliers: \( \Lambda^\sigma = \Lambda^\sigma (x, U, \ldots) \), \( \sigma = 1, \ldots, N \).

- Solve the set of determining equations

\[
E_{Uj}(\Lambda^\sigma R^\sigma) \equiv 0, \quad j = 1, \ldots, m,
\]

for arbitrary \( U(x) \) (off of solution set!) to find all such sets of multipliers.

- Find the corresponding fluxes \( \Phi^i(x, U, \ldots) \) satisfying the identity

\[
\Lambda^\sigma R^\sigma \equiv D_i \Phi^i.
\]

- Each set of fluxes and multipliers yields a local conservation law

\[
D_i \Phi^i(x, u, \ldots) = 0,
\]

holding for all solutions \( u(x) \) of the given PDE system.
Completeness of the Direct Construction Method

For the majority of physical DE systems (in particular, all systems in solved form), all conservation laws follow from linear combinations of equations!

\[ \Lambda_\sigma R^\sigma \equiv \partial_i \Phi^i. \]
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Governing equations ($\alpha = 0$)

\[ R^1 = \frac{\partial u^i}{\partial x^i} = 0, \]

\[ R^2 = \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0, \]

\[ R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - cn_i n_j \frac{\partial u^i}{\partial x^j} = 0. \]
Governing equations \((\alpha = 0)\)

\[
R^1 = \frac{\partial u^i}{\partial x^i} = 0, \\
R^2 = \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0, \\
R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - c n_i n_j \frac{\partial u^i}{\partial x^j} = 0.
\]

Multiplier ansatz

\[
\Lambda^i = \Lambda^i(t, x, \Phi, c, u, \partial \Phi, \partial c, \partial u, \partial^2 \Phi, \partial^2 c, \partial^2 u).
\]
CLs of the Surfactant Dynamics Equations: The Convection Case

**Governing equations \( \alpha = 0 \)**

\[
R^1 = \frac{\partial u^i}{\partial x^i} = 0,
\]
\[
R^2 = \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0,
\]
\[
R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - cn_i n_j \frac{\partial u^j}{\partial x^i} = 0.
\]

**Multiplier ansatz**

\[
\Lambda^i = \Lambda^i(t, x, \Phi, c, u, \partial \Phi, \partial c, \partial u, \partial^2 \Phi, \partial^2 c, \partial^2 u).
\]

**Conservation Law Determining Equations**

\[
\mathcal{E}_{uj}(\Lambda^\sigma R^\sigma) = 0, \quad j = 1, \ldots, 3; \quad \mathcal{E}_\Phi(\Lambda^\sigma R^\sigma) = 0; \quad \mathcal{E}_c(\Lambda^\sigma R^\sigma) = 0.
\]
CLs of the Surfactant Dynamics Equations: The Convection Case (ctd.)

Governing equations \((\alpha = 0)\)

\[
R^1 = \frac{\partial u^i}{\partial x^i} = 0,
\]

\[
R^2 = \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0,
\]

\[
R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - cn_i n_j \frac{\partial u^i}{\partial x^j} = 0.
\]

Principal Result 1 (multipliers)

- There exist an **infinite family** of multiplier sets with \(\Lambda^3 \neq 0\), i.e., essentially involving \(c\).
- Family of conservation laws with

\[
\Lambda^3 = |\nabla \Phi| \mathcal{K}(\Phi, c|\nabla \Phi|).
\]
Governing equations ($\alpha = 0$)

\[ R^1 = \frac{\partial u^i}{\partial x^i} = 0, \]
\[ R^2 = \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0, \]
\[ R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - c n_i n_j \frac{\partial u^i}{\partial x^j} = 0. \]

Principal Result 1 (divergence expressions)

- Usual form:
  \[ \frac{\partial}{\partial t} G(\Phi, c|\nabla \Phi|) + \frac{\partial}{\partial x^i} \left( u^i G(\Phi, c|\nabla \Phi|) \right) = 0. \]
- Material form:
  \[ \frac{d}{dt} G(\Phi, c|\nabla \Phi|) = 0. \]
Governing equations (\(\alpha = 0\))

\[ R^1 = \frac{\partial u^i}{\partial x^i} = 0, \]
\[ R^2 = \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0, \]
\[ R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - cn_i n_j \frac{\partial u^i}{\partial x^j} = 0. \]

Simplest conservation law with \(c\)-dependence

- Can take \(G(\Phi, c|\nabla \Phi|) = c|\nabla \Phi|\).

\[ \frac{\partial}{\partial t} (c|\nabla \Phi|) + \frac{\partial}{\partial x^i} \left( u^i c|\nabla \Phi| \right) = 0. \]
The Convection-Diffusion Case

**Governing equations ($\alpha \neq 0$)**

\[ R^1 = \frac{\partial u^i}{\partial x^i} = 0, \]
\[ R^2 = \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0, \]
\[ R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - cn_i n_j \frac{\partial u^j}{\partial x^j} - \alpha (\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} \left( (\delta_{ik} - n_i n_k) \frac{\partial c}{\partial x^k} \right) = 0. \]

**Conservation Law Determining Equations**

\[ \mathcal{E}_{u^j}(\Lambda^\sigma R^\sigma) = 0, \quad j = 1, \ldots, 3; \quad \mathcal{E}_\Phi(\Lambda^\sigma R^\sigma) = 0; \quad \mathcal{E}_c(\Lambda^\sigma R^\sigma) = 0. \]
The Convection-Diffusion Case (ctd.)

Governing equations ($\alpha = 0$)

\begin{align*}
R^1 &= \frac{\partial u_i}{\partial x^i} = 0, \\
R^2 &= \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0, \\
R^3 &= c_t + u^i \frac{\partial c}{\partial x^i} - cn_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.
\end{align*}

Principal Result 2 (multipliers)

\begin{align*}
\Lambda^1 &= \Phi F(\Phi) |\nabla \Phi|^{-1} \left( \frac{\partial}{\partial x^j} \left( c \frac{\partial \Phi}{\partial x^j} \right) - cn_i n_j \frac{\partial^2 \Phi}{\partial x^i \partial x^j} \right), \\
\Lambda^2 &= -F(\Phi) |\nabla \Phi|^{-1} \left( \frac{\partial}{\partial x^j} \left( c \frac{\partial \Phi}{\partial x^j} \right) - cn_i n_j \frac{\partial^2 \Phi}{\partial x^i \partial x^j} \right), \\
\Lambda^3 &= F(\Phi) |\nabla \Phi|,
\end{align*}
The Convection-Diffusion Case (ctd.)

**Governing equations (\(\alpha = 0\))**

\[
R^1 = \frac{\partial u^i}{\partial x^i} = 0,
\]

\[
R^2 = \Phi_t + \frac{\partial (u^i \Phi)}{\partial x^i} = 0,
\]

\[
R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - c n_i n_j \frac{\partial u^i}{\partial x^j} - \alpha (\delta_{ij} - n_i n_j) \frac{\partial}{\partial x^j} (\delta_{ik} - n_i n_k) \frac{\partial c}{\partial x^k} = 0.
\]

**Principal Result 2 (divergence expressions)**

- An infinite family of conservation laws:

\[
\frac{\partial}{\partial t} (c \mathcal{F}(\Phi) |\nabla \Phi|) + \frac{\partial}{\partial x^i} \left( A^i \mathcal{F}(\Phi) |\nabla \Phi| \right) = 0,
\]

where

\[
A^i = c u^i - \alpha \left( (\delta_{ik} - n_i n_k) \frac{\partial c}{\partial x^k} \right), \quad i = 1, 2, 3,
\]

and \(\mathcal{F}\) is an arbitrary sufficiently smooth function.
The Convection-Diffusion Case (ctd.)

Governing equations \((\alpha = 0)\)

\[
R^1 = \frac{\partial u^i}{\partial x^i} = 0,
\]

\[
R^2 = \Phi_t + \frac{\partial (u^i\Phi)}{\partial x^i} = 0,
\]

\[
R^3 = c_t + u^i \frac{\partial c}{\partial x^i} - cn_i n_j \frac{\partial u^i}{\partial x^j} - \alpha (\delta_{ij} - n_in_j) \frac{\partial}{\partial x^j} \left( (\delta_{ik} - n_in_k) \frac{\partial c}{\partial x^k} \right) = 0.
\]

Simplest conservation law with \(c\)-dependence

- Can take \(\mathcal{F}(\Phi) = 1\):

\[
\frac{\partial}{\partial t} (c |\nabla \Phi|) + \frac{\partial}{\partial x^i} \left( A^i |\nabla \Phi| \right) = 0.
\]
Some conclusions

- Conservation laws can be obtained systematically through the **Direct Construction Method**, which employs multipliers and Euler operators.
- The method is implemented in a symbolic package **GeM** for **Maple**.
- Surfactant dynamics equations can be written in a fully conserved form.
- Infinite families of $c$-dependent conservation laws for cases with and without diffusion.
Conclusions

Some conclusions

- Conservation laws can be obtained systematically through the Direct Construction Method, which employs multipliers and Euler operators.
- The method is implemented in a symbolic package GeM for Maple.
- Surfactant dynamics equations can be written in a fully conserved form.
- Infinite families of $c$-dependent conservation laws for cases with and without diffusion.

Open problems

- Higher order conservation laws?
- Can we get more by including fluid dynamics equations?


