

# A Numerical Method for Soluble Surfactants on Moving Interfaces

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We present a numerical method modeling soluble surfactants on deforming interfaces. The method uses an explicit Eulerian discretization of the interface allowing the use of standard finite difference schemes to solve coupled time-dependent differential equations for the concentration of surfactant on the interface and for the concentration of surfactant in the bulk.

*Keywords:* Soluble surfactants, Interfaces, Segment projection method

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## 1 Introduction

In many practical multiphase flow problems, surfactants are present. Surfactants, or surface reacting agents, modify the strength of surface tension. The work here can be applied to problems dealing with gas emboli [6], microfluidic applications, and electrical components, in which the surface tension plays a significant role.

The concentration of surfactant on the interface is modeled with a time-dependent differential equation defined on the time-dependent and deforming interface. For soluble surfactants, this is also coupled to a PDE for the concentration of surfactant in the bulk. We model the adsorption and desorption of surfactant to the interface from the bulk fluid using Langmuir kinetics [1], which assumes that the surfactant is absorbed as a monomolecular layer [4].

We present a second order method based on an explicit but yet Eulerian discretization of the interface. We use standard finite difference schemes on the discretization of the interface to solve the PDE for the surface concentration of surfactant. The PDE for the concentration in the bulk is, in the spirit of interface tracking methods, solved on a fixed uniform grid. The interface arbitrarily cuts through the uniform grid so the boundary flux condition for the bulk surfactant needs a special treatment. We discuss some details of this implementation and show results in two dimensions.

## 2 Equations

We assume the fluid is incompressible and viscous. The governing equations are the Navier-Stokes equations, including the force from the interface,  $[T\hat{n}]_{\Gamma} = \vec{f} = \sigma\kappa\hat{n} - \nabla_s\sigma$ , where  $T$  is the stress tensor,  $\kappa$  is curvature,  $\hat{n}$  is the unit normal vector,  $\sigma(s, t)$  is the surface tension coefficient, and  $\nabla_s$  is the surface gradient operator. The surface tension coefficient depends on the concentration of surfactant on the interface,  $\sigma(s, t) = F(\rho(s, t))$ , where  $F$  is given by different possible constitutive laws. For the results shown here, we do not solve the Navier-Stokes equations for the velocity,  $\vec{u}$ , but rather assume a given divergence free velocity field, which allows us to focus on the numerical methods for surfactant treatment.

We use the segment projection method (SPM) [5] to represent the interface,  $\Gamma$ . The SPM gives an explicit and Eulerian description of the interface. The interface is divided into multiple overlapping segments, so that each segment can be considered as a function (of one variable in two dimensions and of two variables in three dimensions). The results shown here will consider interfaces with just one segment in two dimensional flow. The points on the interface are given by  $\Gamma(t) = (x, f(x, t))$  and then the interface is updated using,  $f_t + uf_x = v$ , where  $\vec{u} = (u, v)$  is the interfacial velocity.

We solve for the interface surfactant concentration,  $\rho$ , and the bulk surfactant concentration,  $C$ , using advection diffusion PDEs and using a model for the mass flux of surfactant from the interface to the bulk,  $j_n$ . For the interface surfactant concentration, following [3], we have,  $\rho_t + \rho(\nabla_s \cdot \vec{u}) = D_{\Gamma}\nabla_s^2\rho + j_n$ . When using the SPM to represent the interface, this equation becomes a PDE for  $\rho(x, t)$  where the interface  $\Gamma$  is represented by  $(x, f(x, t))$ ,

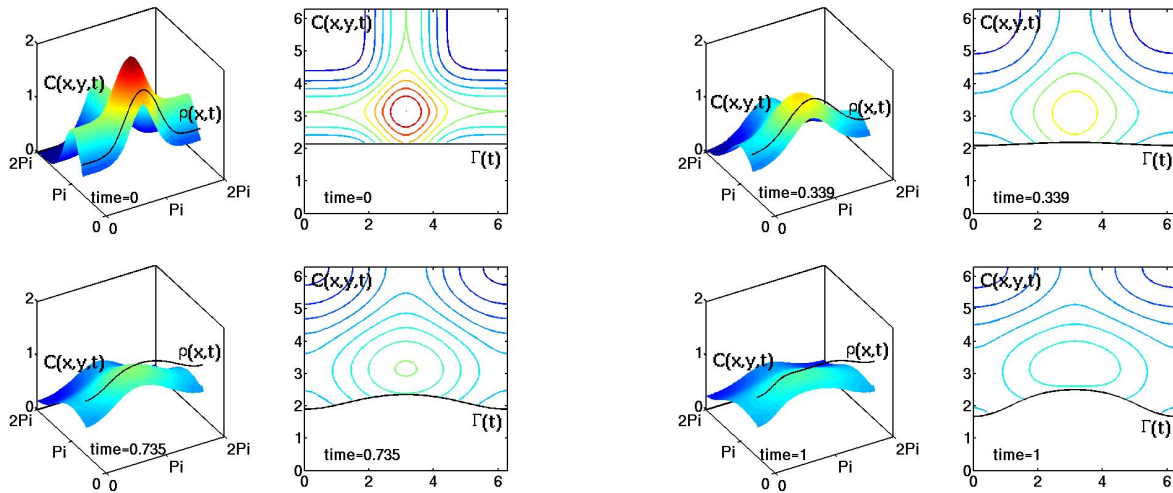
$$\frac{\partial\rho}{\partial t} + u\frac{\partial\rho}{\partial x} + \rho\frac{u_x + v_x f_x}{1 + f_x^2} = D_{\Gamma}\nabla_s^2\rho + j_n, \quad (1)$$

where  $D_{\Gamma}$  is the diffusion coefficient along the interface. For the bulk concentration of surfactant we solve,

$$C_t + \vec{u} \cdot \nabla C = D\nabla^2 C \text{ in } \Omega \in \mathbb{R}^2 \text{ with } D\frac{\partial C}{\partial n} = j_n \text{ at } \Gamma, \quad (2)$$

where  $\Omega$  is the bulk fluid on one side of the interface and  $D$  is the diffusion coefficient in the bulk. The mass flux is modeled following [1],  $j_n = k_a C_{\Gamma}(\rho_{\infty} - \rho) - k_d \rho$ , where  $k_a$  and  $k_d$  are the adsorption and desorption coefficients,  $\rho_{\infty}$  is the maximum

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**Fig. 1** In this test case, the given velocity field is  $\vec{u}(x, y, t) = (t \sin x \cos y, -t \sin y \cos x)$ , the initial conditions are  $f(x, 0) = \pi - 1$ ,  $\rho(x, 0) = (3e^{-(x-\pi)^2} + 2e^{-1}) / (1 + e^{-1} + e^{-(x-\pi)^2})$ , and  $C(x, y, 0) = e^{-(x-\pi)^2} + e^{-(y-\pi)^2}$ , and the parameter values are set to  $D = 1$ ,  $\rho_\infty = 3$ ,  $k_a = 1$ ,  $k_d = 1$ , and  $D_\Gamma = 1$ . We show results at times 0, 0.339, 0.735, and 1.

surfactant concentration on the interface, and  $C_\Gamma$  is the bulk surfactant concentration at the interface. When  $j_n$  is substituted into equation (2), we get a mixed Neumann-Dirichlet boundary condition for  $C$  at the interface,  $D \frac{\partial C}{\partial n} = k_a C(\rho_\infty - \rho) - k_d \rho$ .

### 3 Discretization

As described in Section 2, we here consider the simplified case where  $\Gamma(t) = (x, f(x, t))$ . We discretize the shape function,  $f(x, t)$ , and the associated interface surfactant concentration,  $\rho(x, t)$  on the same uniform one dimensional grid. For the bulk concentration,  $C(x, y, t)$ , we use a uniform two dimensional grid. Since we are using uniform grids, we can use standard finite difference schemes with Strang splitting to solve for the different variables. (In the results here we use Lax-Wendroff for the advection terms and Crank-Nicholson for the diffusion terms.) The difficulty arises since the boundary condition for  $C(x, y, t)$  is applied at the interface which cuts arbitrarily through the two dimensional grid we use for  $C$ . We use the Kreiss-Petersson-Yström Embedded Boundary method [2] to handle the boundary condition. The idea behind this method is to extrapolate  $C$  to ghost points using the boundary condition at the interface and values of  $C$  in  $\Omega$ .

### 4 Results and Conclusion

For numerous test cases with one segment and a given velocity, we get second order convergence for  $f$ ,  $\rho$  and  $C$ , and also for the conservation of total surfactant. In figure 1, we show one test case with time dependent velocities. The height in the three dimensional figures gives the concentration of surfactant and the black line shows the location of the interface and the amount of surfactant on the interface. The bulk surfactant only exists on one side of the interface in these cases.

Here, we have shown that we have developed a new computational method for the solution of PDEs on dynamics interfaces, using the SPM, with an explicit and Eulerian representation of the interface. We have handled soluble surfactants by solving differential equations using standard numerical methods and having a special treatment of the mixed Neumann-Dirichlet boundary condition for  $C$ . We are currently further developing the numerical method to allow for interfaces represented by multiple segments. This will be coupled to the Navier-Stokes equations to enable the study of surfactants in multiphase flows.

**Acknowledgements** The authors acknowledge the support from an Alfred P. Sloan Research Fellowship and DOE Grant DE-FG02-88ER25053. The work presented here was mostly done at KTH and we would like to thank them for their hospitality.

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