A Finite Volume Scheme for Surfactant Driven Thin Film Flow

Günther Grün[*] — Martin Lenz[**] — Martin Rumpf[***]

** Institut für Angewandte Mathematik*
Rheinische Friedrich-Wilhelms-Universität Bonn
Beringstr. 6
53115 Bonn
Germany
gg@iam.uni-bonn.de

*** Institut für Angewandte Mathematik*
Rheinische Friedrich-Wilhelms-Universität Bonn
Wegelerstr. 6
53115 Bonn
Germany
lenz@iam.uni-bonn.de

**** Institut für Mathematik*
Gerhard-Mercator-Universität Duisburg
Lotharstr. 65
47048 Duisburg
Germany
rumpf@math.uni-duisburg.de

ABSTRACT. *The flow of a thin viscous film under the influence of a surface active agent (surfactant) is described by a system of degenerate parabolic equations. A robust and effective numerical scheme based on a finite volume discretization in space and a suitable operator splitting in time is presented. The convective part, which models the effects of Marangoni forces, is treated by an higher order explicit up-wind scheme with a limited linear reconstruction. For the fourth order parabolic part, which corresponds to the classical thin film problem, we formulate a finite volume scheme that entails the same conservation properties continuous solutions have, i. e. energy and entropy estimates. The scheme and the fundamental estimates are derived in the relevant 2D case. Numerical simulations and the convergence result are currently restricted to 1D.*

KEYWORDS: *Finite Volume Scheme, Lubrication Approximation, Surfactant, Thin Films, Operator Splitting, Fourth Order Degenerate Parabolic Equation*

1. Introduction

A surfactant (SURFace ACTive AgenNT) is a chemical agent that accumulates as a mainly mono-molecular layer at the surface of a liquid and influences its surface tension and thereby its spreading behavior. Applications of surfactant-covered thin films range from medicine (the liquid lining of the human lung) to modern coating technology (e.g. aircraft anti-icing films).

The evolution of a thin film of a viscous incompressible fluid on a plain, solid surface which bears a surfactant monolayer at the liquid–gas interface can be described by a system of convection diffusion equations. In the thin film limit, lubrication approximation (cf. [ORO 97]) reduces the problem to the investigation of the following system of higher order equations:

Surfactant driven thin film

$$\partial_t u + \tfrac{1}{3}\mathcal{S}\mathrm{div}\left(u^3\nabla\Delta u\right) - \tfrac{1}{2}\mathrm{div}\left(u^2\nabla w\right) = 0 \qquad [1]$$

$$\partial_t w + \tfrac{1}{2}\mathcal{S}\mathrm{div}\left(u^2 w\nabla\Delta u\right) - \mathrm{div}\left(uw\nabla w\right) - \mathcal{D}\Delta w = 0 \qquad [2]$$

Here, u denotes the height of the film and w represents the concentration of the surfactant at the surface of the fluid.

The evolution of film height is governed by two main effects, both related to surface tension. On the one hand there are *capillary forces* modeled by the fourth order term – $\mathcal{S}$ is a rescaled capillarity number. On the other hand the presence of the surfactant gives rise to surface tension gradients (*Marangoni forces*) which correspond to the first-order term in equation [1]. A *no-slip* boundary condition at the bottom of the thin film leads to the mobility u^3 in the fourth order term.

Simultaneously, the evolution of the surfactant concentration on the surface of the film (equation [2]) is influenced by two effects: the transport by the fluid's (vertically averaged) velocity and the surface diffusion. Here, $\mathcal{D}$ is the inverse Péclet number.

In the literature (cf. [JEN 92]), the convective term of equation [1] usually has the form $+\frac{1}{2}\mathrm{div}(u^2\nabla\sigma(w))$, where σ is the surfactant concentration dependent surface tension. In this paper we use the linearization $\sigma(w) = 1 - w$ that entails the equation given above.

2. Reduced Model for Thin Film Flow

In this section, we will restrict ourselves first to the sub-problem of thin film flow solely driven by the liquids original surface tension. Hence we assume $w = 0$ and introduce a more general mobility $\mathcal{M}$ which is in our application given by $\mathcal{M}(u) := \frac{\mathcal{S}}{3}u^3$. Furthermore, we denote by $p = -\Delta u$ the observed hydrodynamical pressure and obtain the reduced problem:

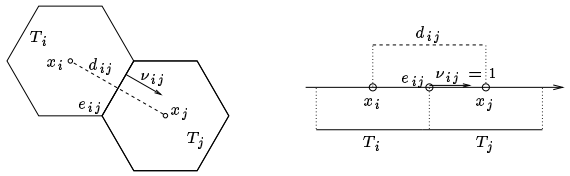

Figure 1. *Sketch of the discretization in 2D and 1D.*

Thin film equation

$$\partial_t u - \operatorname{div}(\mathcal{M}(u)\nabla p) = 0 \qquad [3]$$

$$p = -\Delta u \qquad [4]$$

In contrast to the method that was developed in [GRÜ 00] and analyzed in [GRÜ 02], we will present here a pure finite volume discretization for the complete problem. In particular, we will not need a notion of *discrete pressure* defined in an affine FE-space on the dual grid.

To begin with the domain discretization (cf. figure 1), let us assume the computational domain Ω to be polygonal bounded and completely covered by non degenerate, polygonal finite volume cells $T_i \in \mathcal{T}$ for $i \in \mathcal{I}$, where I is some index set. The cells are assumed to overlap only at faces and all interior cell faces are shared by exactly two cells. For neighboring cells T_i, T_j (written $j \in \mathcal{N}(i)$), there exists a common edge which we denote by e_{ij}, furthermore $|e_{ij}|$ is its length and $\mathcal{E}$ denotes the set of all edges. Let ν_{ij} be the normal on e_{ij} oriented from T_i to T_j, and we assume that there is a family of points x_i, one for every cell, such that $\nu_{ij} = \frac{x_j - x_i}{|x_j - x_i|}$ for all faces e_{ij}. Finally let $d_{ij} := |x_j - x_i|$.

In one space dimension, e_{ij} is the common point of two neighboring intervals T_i and T_j, and we set $|e_{ij}| := 1$. The normal $\nu_{ij} = \pm 1$ so that the restriction $\nu_{ij} = \frac{x_j - x_i}{|x_j - x_i|}$ holds true for arbitrary choices of the points x_i within T_i.

Let h be the maximum diameter of the cells and τ the time step applied for the discretization of the time interval $[0;T]$. Finite volume functions that are constant on cells and time intervals are denoted by capital letters $U, P, \ldots$ By writing U_i^k, we mean the constant values of U on cell T_i in the k-th time step.

Based on these notional preliminaries we now discretize the thin film flow problem. Here, we pick up ideas for the discretization of second order degenerate diffusion problems due to Hilhorst at al. [EYM 98] and in a similar fashion used by Mikula and Ramarosy [MIK 01] and transfer them to a mixed formulation for the actual fourth order degenerate diffusion problem. It will turn out to be essential to replace the continuous mobility $\mathcal{M}$ by a discrete mobility. The special choice for M will be explained below. Finally, we obtain the following discrete problem:

Finite volume scheme

$$\frac{U_i^{k+1} - U_i^k}{\tau} = \frac{1}{|T_i|} \sum_{j \in N(i)} M(U_i^{k+1}, U_j^{k+1}) \, |e_{ij}| \, \frac{P_j^{k+1} - P_i^{k+1}}{d_{ij}} \qquad [5]$$

$$P_i^{k+1} = -\frac{1}{|T_i|} \sum_{j \in N(i)} |e_{ij}| \, \frac{U_j^{k+1} - U_i^{k+1}}{d_{ij}} \qquad [6]$$

For this scheme, we derive a number of estimates that especially will allow us to prove a convergence result. The names underline analogies to the corresponding continuous results.

Proposition 2.1 (Discrete Energy Estimate) *Let U and P be a solution of the finite volume scheme. Then the following equation holds:*

$$\sum_{e_{ij} \in \mathcal{E}} \frac{|e_{ij}|}{d_{ij}} (U_j^N - U_i^N)^2 + \sum_{k=0}^{N-1} \sum_{e_{ij} \in \mathcal{E}} \frac{|e_{ij}|}{d_{ij}} \left((U_j^{k+1} - U_i^{k+1}) - (U_j^k - U_i^k) \right)^2 +$$

$$2\tau \sum_{k=0}^{N-1} \sum_{e_{ij} \in \mathcal{E}} M(U_i^{k+1}, U_j^{k+1}) \frac{|e_{ij}|}{d_{ij}} (P_j^{k+1} - P_i^{k+1})^2 = \sum_{e_{ij} \in \mathcal{E}} \frac{|e_{ij}|}{d_{ij}} (U_j^0 - U_i^0)^2 \qquad [7]$$

The proof of this lemma is rather straightforward following the advice in [GRÜ 00] and [EYM 98] and thus left to the reader.

To formulate an entropy estimate, we need the following definition:

Definition 2.2 (Admissible Entropy-Mobility Pair) *Assume that m is a (continuous, non negative) approximation of $\mathcal{M}$ and $s_0 \in \mathbb{R}^+$. Then functions $G : \mathbb{R} \to \mathbb{R}_0^+$ and $M : \mathbb{R}^2 \to \mathbb{R}_0^+$ are called an admissible entropy-mobility pair iff:*

- *M is continuous and symmetric with respect to its two arguments*
- *$M(U, U) = m(U)$*
- *$M(U_i, U_j)(G'(U_j) - G'(U_i)) = U_j - U_i$,*

where $g(s) = \int_{s_0}^{s} \frac{1}{m(r)}$ and $G(s) = \int_{s_0}^{s} g(r)$

These assumptions are especially satisfied if we choose M as the harmonic integral mean of the continuous mobility $\mathcal{M}$ on the interval spanned by the corresponding height values U_i and U_j:

$$M(U_i, U_j) = \begin{cases} \left(\int_{U_i}^{U_j} \frac{1}{m(r)} \right)^{-1} & \text{if} \quad U_i \neq U_j \\ m(U_i) & \text{if} \quad U_i = U_j \end{cases} \qquad [8]$$

Proposition 2.3 (Discrete Entropy Estimate) *Let (G, M) be an admissible entropy-mobility pair. Then the following inequality holds:*

$$\sum_{i\in\mathcal{I}} |T_i|\, G(U^N) + \tau \sum_{k=1}^{N} \sum_{i\in\mathcal{I}} |T_i| \left(P_i^k\right)^2 \leq \sum_{i\in\mathcal{I}} |T_i|\, G(U^0) \qquad [9]$$

Since this is the part most unique to our problem and the proposed finite volume scheme (as compared to [GRÜ 00]), we will demonstrate the proof of this lemma.

Proof We start with equation [5] of our finite volume scheme and test with $G'(U^{k+1})$, i.e. we multiply by $G'(U_i^{k+1})$ and sum over i for all cells:

$$\sum_{i\in\mathcal{I}} |T_i|\,(U_i^{k+1} - U_i^k) G'(U_i^{k+1}) =$$

$$\tau \sum_{i\in\mathcal{I}} \sum_{j\in N(i)} M(U_i^{k+1}, U_j^{k+1}) \frac{|e_{ij}|}{d_{ij}} (P_j^{k+1} - P_i^{k+1}) G'(U_i^{k+1}) \qquad [10]$$

Let us emphasize that each face e_{ij} appears twice on the right side. With the convention that $\mathcal{E}$ contains each side only once, we can write

$$\sum_{k=0}^{N-1} \sum_{i\in\mathcal{I}} |T_i|\,(U_i^{k+1} - U_i^k) G'(U_i^{k+1}) =$$

$$= \tau \sum_{k=0}^{N-1} \sum_{e_{ij}\in\mathcal{E}} M(U_i^{k+1}, U_j^{k+1}) \frac{|e_{ij}|}{d_{ij}} (P_j^{k+1} - P_i^{k+1})(G'(U_i^{k+1}) - G'(U_j^{k+1}))\,. \quad [11]$$

Applying the convexity of G (on the left side) and the entropy-mobility property (on the right side) we obtain

$$\sum_{k=0}^{N-1} \sum_{i\in\mathcal{I}} |T_i|\,(G(U_i^{k+1}) - G(U_i^k)) \leq \tau \sum_{k=0}^{N-1} \sum_{e_{ij}\in\mathcal{E}} \frac{|e_{ij}|}{d_{ij}} (P_j^{k+1} - P_i^{k+1})(U_i^{k+1} - U_j^{k+1})\,. \qquad [12]$$

The left hand side simplifies further by telescopic summation, while we transform the summation on the right hand side to a summation over cells:

$$\sum_{i\in\mathcal{I}} |T_i|\, G(U_i^N) - \sum_{i\in\mathcal{I}} |T_i|\, G(U_i^0) \leq -\tau \sum_{k=0}^{N-1} \sum_{i\in\mathcal{I}} \sum_{j\in N(i)} \frac{|e_{ij}|}{d_{ij}} P_i^{k+1} (U_i^{k+1} - U_j^{k+1}) \qquad [13]$$

Plugging equation [6] into the right-hand side the statement of the proposition is established. □

Finally, we have the following result of compactness in time, whose proof is again quite analogous to the proof for the finite element discretization given in [GRÜ 02] and thus is skipped here.

Proposition 2.4 (Time Compactness) *Let (U, P) be a solution of our finite volume scheme for a time step width τ and space discretization width h and let s be such that $0 < s < T = N\tau$ and $\max\{\mathcal{M}(U_i^k, U_j^k) | e_{ij} \in \mathcal{E}, 0 \leq k \leq N\} \leq \hat{M}$. If we write $U_i(t)$ for the value of U on the cell i at the time t, then:*

$$\int_0^{T-s} \sum_i |T_i| \left(U_i(t+s) - U_i(t)\right)^2 dt \leq \hat{C}\hat{M}s \qquad [14]$$

These estimates allow us to continue as in [GRÜ 00]: The entropy estimate 2.3 allows us to construct numerical mobilities m that entail a weak non negativity result. Estimates 2.1, 2.3 and 2.4 allow to prove a compactness argument for U in time and space that leads to a convergence result in 1D.

3. An Operator Splitting Scheme for the Surfactant Problem

We will now discuss a finite volume scheme for the original problem of the surfactant driven motion of a thin viscous film. I.e. we consider equations [1], [2]. Let us especially focus on the time discretization. Here we apply a natural operator splitting: We isolate the vertically averaged velocity v (known from lubrication theory) from the second equation, and split each of the remaining equations as follows – indices $i + 0.5$ indicate in the usual way an intermediate time step of the splitting scheme:

Operator splitting

$$(u_{i+0.5} - u_i)/\tau_i = \frac{1}{2}\mathrm{div}(u_i^2 \nabla w_i) \qquad [15]$$

$$(u_{i+1} - u_{i+0.5})/\tau_i = -\frac{1}{3}\mathcal{S}\mathrm{div}(u_{i+1}^3 \nabla \Delta u_{i+1}) \qquad [16]$$

$$v_{i+1} = \frac{1}{2}\mathcal{S}u_{i+1}^2 \nabla \Delta u_{i+1} - u_{i+1}\nabla w_i \qquad [17]$$

$$(w_{i+0.5} - w_i)/\tau_i = -\mathrm{div}(v_{i+1} w_i) \qquad [18]$$

$$(w_{i+1} - w_{i+0.5})/\tau_i = \mathcal{D}\Delta w_{i+1} \qquad [19]$$

The terms involving higher order derivatives are all computed with an implicit method, while the first-order terms can be treated explicitly. Let us now inspect more closely the separate steps of the proposed splitting scheme and their physical meaning:

[**15**] **Marangoni Flow:** The flow of the film that is induced by surface tension gradients.

Our method is best for convection dominated problems, i.e. where $\mathcal{S}$ and $\mathcal{D}$ are very small. In order to reduce the numerical damping, which might even artificially superpose the effects of the parabolic parts, it turn out to be indispensable to use a higher order scheme where possible.

We consider the Engquist–Osher up-winding method from [ENQ 81]. The values on cell faces from both sides (that are required for evaluation of the numerical flux) are extrapolated linearly from the given (constant) values in the usual neighborhood. To avoid oscillations, a min-mod limiter function (cf. [KRÖ 97]) is applied.

[**16**] **Thin Film Flow:** The thin film flow (induced by surface tensions absolute values) is treated as described in section 2 above, except we take into account explicit terms on the right hand side of the equation.

[**17**] **Velocity:** The vertically averaged velocity is computed explicitly from values known so far.

[**18**] **Surfactant Transport:** The surfactant is transported linearly with the velocity computed in the previous step. This term is treated with the same up-winding scheme used in step [15].

[**19**] **Surface Diffusion:** The surfactant diffusion step is computed by a plain finite volume scheme. For the discretization of the Laplacian, cf. the treatment of the pressure equation in section 2.

4. Numerical Results

The scheme described above has been implemented so far for problems in one space dimension.

Figure 2 depicts two characteristic simulations that have been computed with the described scheme. On the left side, we see the evolution of a film of initially constant thickness after a drop of surfactant has been applied. The large surface tension gradients at the boundary of the surfactant droplet give rise to Marangoni forces which initiate the motion of the liquid and the spreading of the surfactant monolayer. To ensure a better visibility we apply a non physical scaling of the film height and especially of the surfactant concentration graph drawn on top of the thin film graph. On the right side, we consider an initial configuration with a surfactant on top of a compactly supported thin film. Note how, after the Marangoni flow has reached the boundary of the film, it causes the film's support to spread, which is remarkable because the film is expected not to spread in the absence of a surfactant. Furthermore the method has been tested on the similarity solution given in [JEN 92] for $\mathcal{S} = \mathcal{D} = 0$.

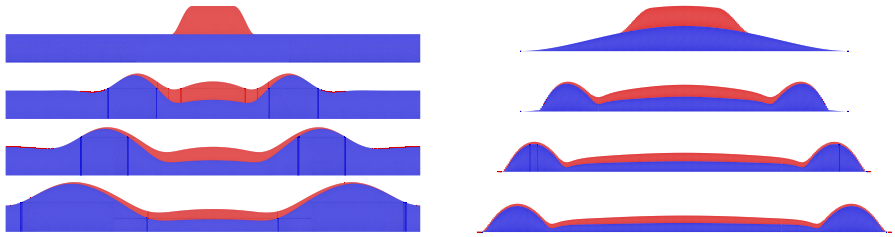

Figure 2. *Numerical results in one space dimension.*

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