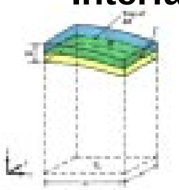
MODELING OF MULTI-COMPONENT VISCOELASTIC FLOWS

W. W. Miles and V. J. Ervin
DEPARTMENT OF MATHEMATICAL SCIENCES
L. L. Thompson and D. A. Zumbrunnen
DEPARTMENT OF MECHANICAL ENGINEERING

Objectives

- Formulate and implement computationally efficient model equations of interfacial forces, including variable interfacial tension, that govern the in situ formation of multi-layer films and fibers within multi-component polymer melts.
- Develop and implement accurate methodologies to track the interfacial regions between multi-component melts, including non-Newtonian flow.
- Make available methods and algorithms for interfacial modeling for future generalizations to multi-component melts of Thrust I fiber/film extrusion models which currently consider one polymer component.

Interfacial Tension Effects



- To derive the interface condition between two fluids, the momentum balance of a volume element which contains the interface is examined.

$$\frac{d}{dt}\int_{\Omega} \rho \vec{u}\, dV = \int_{\Omega} \rho \vec{b}\, dV + \int_{\partial\Omega} \vec{t}\, dS$$

- The interface force is derived from the surface integral for stress.

$$\int_{\partial\Omega} \vec{t}\, dS = \int_{\Omega} \nabla \bullet \underline{\underline{T}}\, dV + \int_{I} \Delta \underline{\underline{T}} \bullet \vec{n}\, dS$$

Above, *T* is the total stress tensor, *t* is the traction vector, *n* is the outward unit normal, and $\Delta T = T^1 - T^2$. Below, N is the unit vector which is tangent to the interfacial surface and normal to the interfacial boundary, C.

$$\int_{I} \Delta \underline{\underline{T}} \bullet \vec{n}\, dS = \int_{C} \sigma \vec{N}\, dS$$

Boundary Condition/ Continuum Surface Force Model

Converting the right-hand integral into a surface integral leads to the point-wise boundary condition:

$$\Delta \underline{\underline{T}} \cdot \vec{n} + \sigma\kappa\vec{n} + \nabla_s \sigma = 0$$

The interfacial condition is imposed by a Continuum Surface Force (CSF) Model. We express the interfacial tension forces as local volume forces, thereby allowing the boundary condition to be imposed conveniently within the balance of momentum equation. This "spreading" of the interface is accomplished by the use of the delta distribution.

Continuum Model

The modified balance of momentum equation including *spatially varying interfacial tension effects*, together with the incompressibility condition, may be expressed as:

$$\begin{aligned} &\rho\frac{\partial \vec{u}}{\partial t} + \rho\vec{u}\bullet\nabla\vec{u} - \nabla\bullet\underline{\underline{T}} = -(\sigma\kappa\vec{n} + \nabla_s\sigma)\delta(\vec{n}(x_s)\bullet(x - x_s)) && \text{in } \Omega \\ &\nabla\bullet\vec{u} = 0 \quad \text{in } \Omega && (A) \\ &\vec{u} = 0 \quad \text{on } \partial\Omega && \end{aligned}$$

Non-Newtonian behavior is modeled through the constitutive equation. Using an Oldroyd *constitutive* model, we have proved mathematically that an approximating solution exists and is unique for both the steady-state and time-dependent problems.

Existence Theorem

The existence theorem establishes the confidence and reliability in numerical simulations for complex solution behavior and is of significance within the mathematics community.

Theorem: Given problem (A) has a solution (with some regularity constraints). Then the corresponding weak form of (A) has a solution in the approximating space.

Outline of the proof of the theorem:

- Define an iterative map such that if two consecutive iterates are the same, then the iterate is a solution to the desired problem.
- We show the map is well-defined and bounded on bounded sets.
- We show the map is continuous and is a contraction.
- Finally, we employ fixed point theory to show a solution exists.

Continuum Surface Force Model

In the continuum, the interface may be thought of as a surface of discontinuity (Figure A). Our CSF model allows a smooth transition of "color" (and hence, other fluid properties) from fluid 1 to fluid 2 through an interfacial region (Figure B).

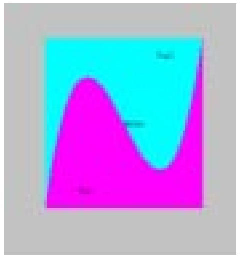


Figure A

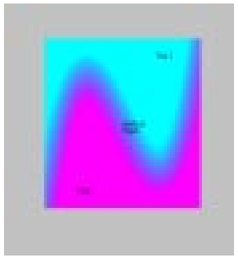
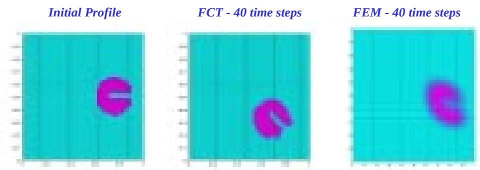


Figure B

Interface Tracking

Two new methods of interface tracking have been studied: Flux-Corrected Transport (FCT) and the Defect Correction Finite Element Method (DCFEM). Both techniques use convection to track the interface. Our results show that FCT outperforms the DCFEM in both speed and accuracy.



$$\frac{\partial C}{\partial t} + \nabla\cdot(\vec{v}C) = 0$$

*__The Advection Equation:__ C(**x**) is a "color" function which is defined to be 0 in phase A, 1 in phase B, and some fraction between 0 and 1 in the interfacial region.*

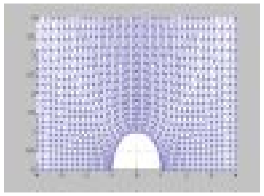
Flux Corrected Transport

1. Compute the flux at each boundary using both a low order and higher order, stable scheme. Denote these fluxes as $F^{L}_{i+\frac{1}{2}}$ and $F^{H}_{i+\frac{1}{2}}$ respectively.
2. Define the anti-diffusive flux, $A^{R}_{i+\frac{1}{2}} = F^{H}_{i+\frac{1}{2}} - F^{L}_{i+\frac{1}{2}}$
3. Advect the color function using the low order fluxes. $C_i^{temp} = C_i^{n} - \left(\frac{F^{L}_{i+\frac{1}{2}} - F^{L}_{i-\frac{1}{2}}}{\Delta x}\right)$
4. Limit $A_{i+\frac{1}{2}}$ so that applying it to the approximation will not introduce any new extrema. That is, determine constants $f_{i+\frac{1}{2}}$ such that $A^{R}_{i+\frac{1}{2}} = f_{i+\frac{1}{2}} A_{i+\frac{1}{2}} \;;\; 0 \le f_{i+\frac{1}{2}} \le 1$
5. Compute the new "corrected" approximation: $C_i^{n+1} = C_i^{temp} - \left(\frac{A^{R}_{i+\frac{1}{2}} - A^{R}_{i-\frac{1}{2}}}{\Delta x}\right)$

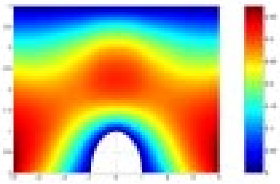
Ongoing Work

Code has been written which solves for velocity, pressure and stress within a single-component flow. The finite element method is used in coordination with the theta method. The Oldroyd *constitutive* model is employed. This solver will be modified to allow for multi-component flows by incorporating the Continuum Surface Force Model and imposing an advection of the color function in each iteration.

Computational Grid



First Component of Velocity



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