Viscoelastic jet formation with impulsive boundary motion using Basilisk


Emre Turkoz, Luc Deike, Craig B. Arnold
with Jens Eggers
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**Motivation**

Need of Printing Viscoelastic Materials

- **Flexible electronics**

- **Sensors**

- **3D printing**

- **Tissue engineering**
Motivation

Printing Techniques

- Nozzle should be designed for the ink and application
- Clogging
- Drop diameters $\geq 10 \mu m$

- Nozzle → no clogging
- Droplets with smaller diameters

Inkjet printing

Laser-induced forward transfer

- Ink
- Nozzle
- Droplet
- Piezoelectric transducer
- Substrate
- Substrate Motion

- Mirror
- Objective
- Laser
- Glass
- Transfer Material
- Receiver Substrate
- Translation Stage
Description of our technique

**Blister-Actuated Laser-Induced Forward Transfer (BA-LIFT)**


Microfluid. Nanofluid. 11.2, 199-207 (2011)

Mechanical impulse and subsequent jet formation

Droplet pinch-off through Rayleigh-Plateau instability

Material transfer onto acceptor surface
BA-LIFT has many parameters

**Parameter Space**

- $E_b$: Laser beam energy
- $R_b$: Laser spot size
- $H_p$: PI layer thickness
- $H$: Film thickness
- $\mu$: Viscosity
- $\rho$: Density
- $\gamma$: Surface tension
- $\lambda$: Viscoelasticity

Blister profile

Jet formation

Ink properties

This parameter space determines the outcome of the process

NMP - newtonian solvent

0.1 wt.% xanthan gum in water - A viscoelastic solution
Develop a fully adaptive Basilisk model to simulate BA-LIFT with Newtonian fluids

Determine the dimensionless parameters

Solid boundary deformation

Grid convergence with static and adaptive meshing

Validation with experiments

Validate the viscoelastic models in Basilisk with the literature

Modify the BA-LIFT model slightly by introducing an extra dimensionless parameter
Problem Setup

How the computation domain should look like

Three phases
- Polymer
- Ink
- Air

Solid boundary deformation: From empirical measurements [1]

Flow is axially symmetric

Impulsive Boundary Deformation during BA-LIFT is already formulated [1].

\[ \delta(r, E, t) = X(r, E) \cdot T(t) \]

\[ X(r, E) = H_0(E) \left( 1 - \left( \frac{r}{R_0(E)} \right)^2 \right)^C \]

\[ T(t) = \frac{2}{\pi} \arctan(t/\tau_b) \]

Non-dimensionalization of the Problem

**Dimensionless parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_a$</td>
<td>Air viscosity</td>
</tr>
<tr>
<td>$\mu_l$</td>
<td>Liquid viscosity</td>
</tr>
<tr>
<td>$\rho_a$</td>
<td>Air density</td>
</tr>
<tr>
<td>$\rho_l$</td>
<td>Liquid density</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Surface tension</td>
</tr>
<tr>
<td>$\tau_b$</td>
<td>Blister expansion time</td>
</tr>
<tr>
<td>$R_b$</td>
<td>Blister radius</td>
</tr>
</tbody>
</table>

**Dimensionless numbers**

\[
\tau_c = \sqrt{\frac{\rho R_b^3}{\gamma}}
\]

$\mu_a / \mu_l$

$\rho_a / \rho_l$

$\tau_b / \tau_c$

$Oh = \mu_l / \sqrt{\rho \gamma R_b}$

Blister expansion time / capillary time scale

$H_b = f(R_b)$
Modeling the solid layer [1,2,3] & Algorithm

- **Solid layer is represented with a tracer (f12)**
- **Reinitialized every time step**
- **Velocity values throughout the solid are assigned at each time step**

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**Advance the solid boundary**

**Reinitialize the velocity everywhere in the solid**

**Calculate material properties**

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Every timestep!

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Adaptive grid for parallelization

Results
Comparison of different parallelization schemes

Grid Convergence

Transferred volume at 5.14 μJ (10^{-15} m^3)

Level | Cells/μm
--- | ---
7 | 1.34
8 | 2.67
9 | 5.34
10 | 10.68
11 | 21.37

Mesh size (cells/μm)

Jet length (μm)

- OpenMP static
- MPI adaptive (XSEDE)
- OpenMP adaptive (Tiger)
Validation with Experiments

Comparison with experiments

![Graph showing comparison between experiment data, Basilisk simulations, and Brown (2012) with CFD-ACE+ results. The graph plots transferred volume of ink (10^-15 m^3) against energy (μm).]
Now: Viscoelastic Models

Develop a fully adaptive Basilisk model to simulate BA-LIFT with Newtonian fluids

- Determine the dimensionless parameters
- Solid boundary deformation
- Grid convergence with static and adaptive meshing
- Validation with experiments

Verify the viscoelastic models in Basilisk with the literature

Modify the BA-LIFT model by introducing an extra dimensionless parameter to model viscoelasticity

Transfer model
A Sidetack from BA-LIFT: Viscoelastic Simulations in Basilisk

Possible thanks to the model [1] implemented by Jose M. Lopez-Herrera Sanchez [2]

Log-conformation technique to overcome “the high-Weissenberg number problem”

\[ \nabla \cdot \mathbf{u} = 0, \]

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \mathbf{\tau} \]

\[ \frac{\partial \mathbf{c}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{c} - (\nabla \mathbf{u} \cdot \mathbf{c} + \mathbf{c} \cdot \nabla \mathbf{u}^T) = f_s(\mathbf{c}) \]

\[ \mathbf{\tau} = \mathbf{\tau}_S + \mathbf{\tau}_P \]

\[ \mathbf{\tau}_S = 2\eta_S \mathbf{D} \quad \mathbf{D} = (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)/2 \]

\[ \mathbf{\tau}_P = G_0 f_s(\mathbf{c}) \quad G_0 = \frac{\lambda_p}{\eta_p} \]

Conformation tensor!

\[ \text{De} = \frac{\lambda_p}{\sqrt{\rho h^3 / \gamma}} \quad \beta = \frac{\mu_s}{\mu_0} \]

Oldroyd-B

\[ f_s(\mathbf{c}) = \mathbf{c} - \mathbf{I} \]

FENE-P

\[ f_s(\mathbf{c}) = \frac{\mathbf{c}}{1 - \text{tr}(\mathbf{c})/L^2} - \mathbf{I} \]


Verifying the Oldroyd-B model: Comparison with Clasen

Clasen [1]

- 1D along the axial direction
- Finite-difference
- Slender jet equations

Basilisk

- 2D axially symmetric
- Log-conformation technique

Minimum Filament Radius vs. Time

$min_h$

Time

$H = 0.252e^{-0.00362t}$
The model cannot capture the experimental trends

**Oldroyd-B with Basilisk: Accuracy**

\[ h(t) = h_0 \exp(-1/3De) \]

\[ \sigma_{zz}(t) = \sigma_0 \exp(1/3De) \]
The model cannot capture the experimental trends. The slope for the axial stress should be improved!

Oldroyd-B with Basilisk: Accuracy

\[ h(t) = h_0 \exp\left(-\frac{1}{3De}\right) \]
\[ \sigma_{zz}(t) = \sigma_0 \exp\left(\frac{1}{3De}\right) \]

A different strategy to solve Oldroyd-B equations?
A note on Oldroyd-B: Comparison with Experiments

The model can not capture the experimental trends

Experimental thinning is faster at early times

The last step: BA-LIFT simulations with the current models

Simulating BA-LIFT with Oldroyd-B and FENE-P

Develop a fully adaptive Basilisk model to simulate BA-LIFT with Newtonian fluids

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Verify the viscoelastic models in Basilisk with the literature

Modify the BA-LIFT model by introducing an extra dimensionless parameter to model viscoelasticity
Unique Jet Features during BA-LIFT with Viscoelastic Inks

Jetting without breakup

Multiple-drop formation

Shoulder formation

Hanging drop formation and delayed breakup
Viscoelastic BA-LIFT simulations

0.1 wt.% PEO in 60-40 wt.% WG

22 us  42 us  62 us  292 us  342 us  >1s

Droplet shape!
Strategy: Try to observe these features with a parameter sweep and compare with experimental parameters!

- Oldroyd-B model
- Infinitely stretchable polymer chains
- Can resolve with uniform mesh level 11
- Could not get adaptive meshing + MPI work with viscoelastic model yet!

De = 160 Oldroyd-B model
Future Work

Maybe the answer lies in a new model!

Later stages: Beads-on-a-string formation

Implement refinement with filament radius
Make it work with adaptive and MPI

A model proposed in [1] to explain this sinusoidal instability!

Acknowledgements

- Members of the Arnold group
- Jose M. Lopez-Herrera Sanchez for numerous e-mail exchanges
- Prof. Jens Eggers
- Antonio Perazzo and Prof. Howard A. Stone
Future Work: We need to implement a better model! [1]

\[
\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \nabla \cdot \mathbf{\sigma}_p + \eta_s \Delta \mathbf{v}
\]

\[
\frac{D\mathbf{\sigma}_p}{Dt} = (\nabla \mathbf{v})^T \cdot \mathbf{\sigma}_p + \mathbf{\sigma}_p \cdot (\nabla \mathbf{v}) - \frac{\mathbf{\sigma}_p}{\lambda} + nk_B T \left((\nabla \mathbf{v})^T + (\nabla \mathbf{v})\right) - k_B T \frac{Dn}{Dt} \delta + D \Delta \mathbf{\sigma}_p
\]

\[
\frac{Dn}{Dt} = -\frac{D}{k_B T} \nabla \nabla : \mathbf{\sigma}_p + D \Delta n
\]

Perturbation analysis yields a novel mechanism for an instability which grows sinusoidally and might explain the formation of beads-on-a-string structure.

Experimental observation: Polymer concentration is very high along the thread.

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Algorithm for Log-conformation Technique (as in log_conform_1.h by Lopez)

1. Initialize parameters $S, \psi$ (tensor type)
2. Evaluate the RHS of (2)
3. Calculate (1)
4. Evaluate B, M and $\Omega$
5. Integrate (2)
6. Diagonalize A and evaluate $\psi$
7. Evaluate $A$ from $S$ as $A = \frac{\lambda}{\mu} S + I$
8. Recover the conformation tensor $A = e^\psi$
9. Integrate (3) analytically
10. Evaluate the stress tensor S for the next time step

\[
\frac{\partial \psi}{\partial t} + \nabla \cdot (\psi \mathbf{u}) = 0
\]

\[
\frac{\partial \psi}{\partial t} = 2B + (\Omega \cdot \psi - \psi \cdot \Omega)
\]

\[
\frac{\partial A}{\partial t} = \frac{1}{\lambda} (I - A)
\]
Minimum Filament Radius vs. Time

\[ h(t) = h_0 \exp(-1/3De^*) \]

<table>
<thead>
<tr>
<th>De</th>
<th>( h_0 )</th>
<th>( h_0' )</th>
<th>De*</th>
</tr>
</thead>
<tbody>
<tr>
<td>94.9</td>
<td>0.2520</td>
<td>96.57</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>0.3045</td>
<td>56.84</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>0.3343</td>
<td>48.34</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>0.3835</td>
<td>38.46</td>
<td></td>
</tr>
</tbody>
</table>
Effect of elasticity on BA-LIFT jets
Still localized pinch-off & beads-on-a-string not

De = 0.2
Oh = 0.2
b=1000

De = 0.4
Oh = 0.2
b=1000

De = 0.6
Oh = 0.2
b=1000
Maximum Axial Stress along the Filament vs. Time

\[ \sigma_{zz}(t) = \sigma_0 \exp\left(\frac{1}{3De^*}\right) \]

\[ \sigma_0 = \frac{2}{h_0} \]

<table>
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<th>(h_0)</th>
<th>(h_0^*)</th>
<th>De*</th>
</tr>
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<tbody>
<tr>
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<td>0.2374</td>
<td>7.564</td>
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<tr>
<td>50</td>
<td>0.3343</td>
<td>4.616</td>
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<tr>
<td>40</td>
<td>0.3835</td>
<td>3.918</td>
<td>35.43</td>
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