Fiber spinning is an industrial process that can be applied to solutions of carbon nanotubes (CNTs) to create fibers which exhibit the unique mechanical and electrical properties of CNTs on the macro-scale. This process involves the extrusion of a CNT-superacid solution through a die and subsequent coagulation of the extruded solution in water or air to produce a pure CNT fiber. However, morphological irregularities that appear in the viscous outer layer of the fiber before it has fully solidified may lead to degradation of fiber strength and elasticity. In this viscous outer layer, we suspect that radial buckling too is related to the degradation of properties. In order to describe these irregularities, we have modeled the flow as an isothermal solution and chosen a physical model to take into account the viscoelasticity of the material and examine changes in the stress and radial position profile for various conditions on viscosity ($\mu$) and relaxation time. For example, we may force a $\mu$-profile in space and time to simulate coagulation, where the range of possible values was informed by rheological data of uncoagulated CNTs. Though a 2D model may be necessary to fully capture radial buckling, we first develop a 1D model which will allow us to investigate the effects of axially varying $\mu$ on surface profile and stresses within the solution in one dimension along the axis of flow.
**Numerical Analysis of Free Surface Flows in Fiber Spinning of Carbon Nanotubes**

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### Background

- Fibers can be produced from solutions of carbon nanotubes (CNTs) dissolved in sulfuric acid\(^1\).  
- These exhibit CNTs’ unique mechanical and electrical properties on the macroscale.  
- Irregular morphologies in some of these fibers may lead to degradation of material properties.  
- Morphological features are typically difficult to measure experimentally.

### Governing Equations

**Key assumptions:**  
1) 1D  
2) Isothermal  
3) Relatively inviscid medium

An upper-convected Maxwell (UCM) constitutive equation was chosen to model stress:

\[
\tau + \frac{\partial \tau}{\partial t} = \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)
\]

(1)

UCM takes into account stress relaxation, and thus is suitable for modeling a viscoelastic fluid where \(\delta\) is Oldroyd’s convected derivative.

**CNT fiber spinning shares characteristics with polymer melts spinning:**  
1) Primarily extensional flow  
2) Non-Newtonian  
3) Viscoelastic behavior

Assuming velocity only varies along z and neglecting gravity, the constitutive equation in x and z reduces to

\[
\tau_{xx} + \frac{\partial \tau_{zx}}{\partial z} + \tau_{zx} + \frac{\partial \tau_{zz}}{\partial x} = 2\mu \left( \frac{\partial u_z}{\partial z} - \frac{\partial u_x}{\partial x} \right)
\]

(2)

\[
\tau_{xx} + \frac{\partial \tau_{zx}}{\partial z} = 2\mu \left( \frac{\partial u_z}{\partial z} - \frac{\partial u_x}{\partial x} \right)
\]

(3)

The reduced momentum balance in z is

\[
\rho \frac{\partial v_z}{\partial t} + \frac{\partial p}{\partial z} = \frac{\partial \tau_{zz}}{\partial x}
\]

(4)

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### Boundary Conditions

**Assuming constant volumetric flow rate,**

\[
\mathbf{u}_v(t,z) = \frac{Q}{2\pi r(\zeta)^3}
\]

(5)

**If we assume the fiber is fully solidified at the chill roll,**

\[
\mathbf{u}_v(t,z) = \mathbf{u}_f
\]

(6)

**If we know the velocity at some point on the boundary, all velocities there may be determined by applying (9) and assuming an initial radial profile, (r, t) (2)**

**Start-up transients are not treated here, but we assume that prior to observing the flow, stress gradients near the endpoint have become negligible, allowing us to introduce two more boundary conditions,**

\[
\tau_{xx} = 2\mu \frac{\partial u_z}{\partial z}
\]

(7)

\[
\tau_{xx} = \frac{2\mu}{(\zeta)^2}
\]

(8)

**We use a solution from the literature for a high Deborah number polymer at steady state as an initial condition for T and \(\mathbf{p}\).**

### Discussion

**A solution was obtained by a forward Euler method for velocity and first and third normal stresses, but the method’s limited stability prevents examining the system over long run times.**

- **Implicit methods could be implemented to better understand the time evolution of features such as a forced viscous or radial profile, based either on the above boundary conditions or w/ steady solutions as ICs.**

### References


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