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Computing Visco-Elastic Microjetting in Manufacturing, Blood Flow, and Drug Delivery Systems

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Summary: We have developed a numerical model of two-phase viscoelastic flow, which can be used to simulate a wide collection of nanoscale devices and flow phenomena.

In many physical and engineering systems, ordinary fluid phenomena have a far more complex behavior when devices are shrunk to small scales. In these environments, normal fluid flow, which is governed by Newton's Laws, can be replaced by viscoelastic behavior which exhibits subtle stresses and behaviors. Fluid injection devices, which are part of applications such as the microdispensing of bioactive fluids through high throughput injection devices, creation of cell attachment sites, scaffolds for tissue engineering, coatings and drug delivery systems for controlled drug release, and viscoelastic blood flow flow past valves, all become delicate at nanoscales.

Our goal is build numerical algorithms to accurately simulate some of the most delicate viscoelastic jetting phenomena, including ejection, fluid mixing, and the effects of walls and nozzle geometry on the tiny micromotions that determine where the fluid goes, and how it behaves.

We have successfully tested and applied these algorithms in the context of inkjet plotters. Regular dye-based inks used in desktop printers are Newtonian, which means that the relation between the stress tensor and the rate of deformation tensor at an instant is linear and not related to any other instant. The use of pigment-based inks at the end of the 1990's improved the color durability of a ink jet printout. Pigment-based inks and inks used in industrial printing applications are usually viscoelastic, i.e. the relation between the stress tensor and the rate of deformation tensor depends on the deformation history. These viscoelastic jets now form core new technology for such varied applications as printing plasma screens and automated drug design.

In our numerical simulations, we have been able to couple two state-of-the art technologies, namely high order projection methods for computing incompressible fluid flows, and level set methods for tracking intricate interface dynamics. In addition, we have extended these ideas to capturing non-Newtonian viscoelastic flow, and developed software to compute such flows in complex geometries.

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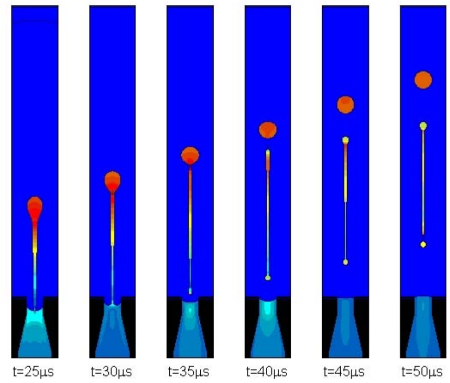
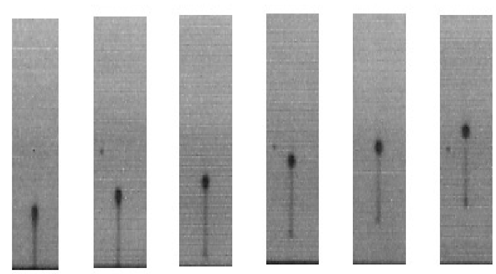
The fluid model considered in this work is the Oldroyd-B viscoelastic fluid model, in which both the dynamic viscosity and relaxation time are constant. Our purpose is to simulate two-phase immiscible incompressible flows in the presence of surface tension and density jump across the interface separating a viscoelastic fluid and from air, incorporated with a macroscopic slipping contact line model which describes the air-fluid-wall dynamics. The fluid interface between the air and the fluid is treated as an infinitely thin immiscible boundary, separating regions of different but constant densities and viscosities. The flow is axisymmetric, and solid wall boundary conditions both assume vanishing fluid velocity; this is amended by the contact model at places where the interface meets walls. Here, we wish to be able to simulate air/wall/fluid interactions and such effects as interactions between geometry and viscoelastic forces. The computational model and algorithm are general enough to handle problems in which either of the two fluids is either viscoelastic or Newtonian.

In the figure below, we model the three dimensional ejection of ink in a nozzle geometry. In the shown time sequence, an electric current is passed to an activator below the bottom of the ink path, and a droplet is expelled upwards into the air. As the three-dimensional bubble is expelled through the pinching nozzle, fluid and surface tension forces break it into multiple satellites: an experimental simulation is shown below the simulation. Controlling the fluid ejection and the size and motions of the satellites is a key part of understanding microjetting devices.

Numerical Simulation of MicroJetting



Experimental Simulation of MicroJetting



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