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Numerical Simulation of Filling Processes with Newtonian and Shear-thinning Fluids

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Extrusion of a fluid into a container is used in many different applications, including injection molding, mold filling, encapsulation and bottle filling. Computational fluids dynamics (CFD) can be a useful approach to troubleshoot these processes by predicting defects and flow instabilities that can lead to incomplete filling and void formation. CFD can also be useful for optimizing filling processes with respect to processing parameters (e.g. flow rate, temperature, and rheology) and mold design (e.g. gate and vent location). In this paper, we investigate the physics of the filling process with numerical simulations. Here, the finite element method is used to understand the interaction of the extrusion jet with the geometry and the fluid pool. Filling dynamics are moving boundary problems, where the location of the fluid-gas interface is unknown a priori and must be solved as part of the numerical method. Here we use an Eulerian technique, where the mesh is stationary and the interface is captured using a level set method. Results are presented for several geometries including injection molding from a curtain die, mold filling into a container with obstacles, and filling of a Carreau-Yasuda fluid into a simple mold. Numerical results are validated with experimental data when possible.

Introduction

Extrusion of a fluid into a container is used in many different applications, including injection molding, mold filling, encapsulation and bottle filling. For instance, injection loading of a ceramic paste is a high rate process used to create green ceramic parts that are then run through a binder burnout and sintering process to produce the final ceramic part. Figure 1 shows short shots (or incomplete filling of a mold) for an injection loading process, illustrating some of the defects that can occur when a fluid with complex shear and temperature dependent rheology interacts with a high rate process.

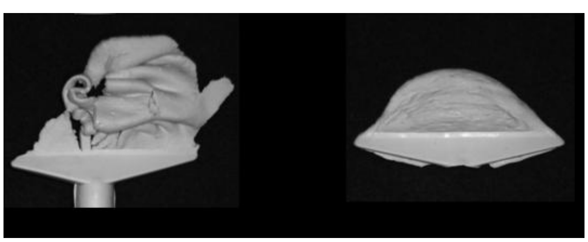

Fig. 1. Short shots of injection loading of a ceramic paste in a mold [Rao et al, 2006]. The photo on the left is injection loading using a slow injection speed, while the photo on the right uses a higher injection speed.

At low filling speed, the paste acts like a solid material. Even at high filling rates, when the paste begins to act as a fluid, pooling at the center of the mold is seen and the desired mold shape is not achieved.

In mold filling of a Newtonian fluid, such as an uncured epoxy, in a complex mold with obstacles, a void can be seen forming as knit lines come together. The knit lines are formed as the flow field is split into two streams by the posts. These voids are very difficult to remove and will result in a defect in the final part. Figure 2 shows a representative geometry for encapsulation. The filling profiles show that a void is left at the center of the four posts. This void persists even after long times.

Fig. 2. Mold filling with a viscous liquid shows void formation as knit lines come together to entrap

a gas in a complex geometry with inclusions [Mondy et al, 2007].

Even if the bubble escapes from the mold or diffuses into the fluid, the knit lines themselves are defects that can lead to cracking in the epoxy as it experiences thermal cycling.

During bottle filling of non-Newtonian fluids (Figure 3), there exist several different flow regimes from the ideal case of steady filling to flow instabilities such as mounding, buckling, coiling, and delayed die swell to high speed filling processes where air is entrained and bubbly flows can result. The flow behavior depends on the fluid rheology, nozzle geometry, nozzle height, among other things [Roberts and Rao, 2011].

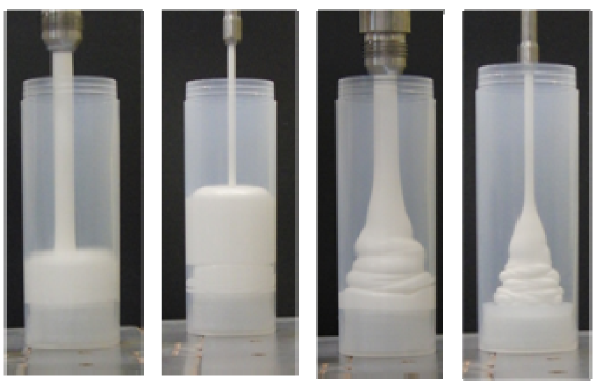

Fig. 3. Bottle filling of a non-Newtonian liquid for various nozzle diameters and filling speeds.

In all these flows, computational fluid dynamics (CFD) can be a useful tool for predicting flow instabilities and defects, such as voids and knit lines. CFD can also be useful for optimizing filling processes with respect to processing parameters (e.g. flow rate, temperature, and rheology) and mold design (e.g. gate and vent location).

In this paper, we investigate the physics of the filling process with numerical simulations. Here, the finite element method is used to understand the interaction of the extrusion jet with the geometry and the fluid pool. Filling dynamics are moving boundary problems, where the location of the fluid-gas interface is unknown a priori and must be solved as part of the numerical method. Here we use an Eulerian technique, where the mesh is stationary and at the interface is captured using a level set method [Sethian 1999].

The paper is organized in the following manner. First we discuss the experimental method used to provide experiments for validation of the numerical method. Next we present the equations and numerical method. In the following section, we give results for three different flow problems: 1) Injection loading of a Newtonian fluid into a coat hanger die, where the 3D level set simulations are compared to validation experiments 2) Mold filling of a Newtonian fluid into a complex mold with obstacles, where 3D level set simulations are also compared to validation experiments. 3) 2D bottle filling of a Carreau fluid using the level set method. We conclude by summarizing the results and discussing future efforts.

Experimental

We recorded the flow of a Newtonian liquid through transparent molds to validate the front tracking and wetting models used in the computations. The liquid used was a lubricant, UCON 75-H-90,000, an oxyethylene/ oxypropylene. Before this liquid was injected, it was held in a water bath at a constant temperature of 23.5oC. The viscosity, surface tension, and wetting properties of the UCON lubricant were determined at this temperature. The viscosity of the lubricant was measured with a Rheologica™ constant stress rheometer and was equal to 39 Pa-s over a shear rate ranging from 0.1 - 10 sec-1. The surface tension measured with a Du Noüy ring (mean circumference of 5.935 cm) was 42.4±0.1 dyne/cm. The dynamic contact angle on acrylic was measured with a feed-through goniometer [Mondy, 2007], in which liquid can be continuously injected to achieve "high" velocities, or the sessile drop can be allowed to relax to obtain "low" velocities.

To mimic an actual injection process we were exploring, we used a pressure driven syringe held at a constant pressure of 29.95 ± 0.10 psig during injection. The resulting typical Reynolds numbers were in the Stokes regime of much smaller than one. The syringe plunger was modified with an extra o-ring to minimize air leakage around the seal. The time to fill the molds varied from test to test, but was determined and recorded for each test. The frame numbers of the video recorded at 30 f/s gave us times for each frame used to compare the results with numerical predictions.

Equations and Numerical Method

The fluids of interest are incompressible, meaning that the velocity field will be solenoidal and the continuity equation contains no density or pressure.

$$\nabla \bullet v = 0 \qquad (1)$$

Conservation of momentum takes into account gradients in the fluid stress, π, and pressure, p, as well as gravitational effects. Note that gravity, g, can be an important body force in filling processes.

$$\rho \frac{\partial v}{\partial t} + \rho v \bullet \nabla v = \nabla \bullet \underline{\underline{\pi}} - \nabla p + \rho \underline{g} \qquad (2)$$

The stress tensor can be written in generalized Newtonian terms.

$$\underline{\underline{\pi}} = \eta(\nabla v + \nabla v^t) \qquad (3)$$

The shear viscosity, η, can be either Newtonian or a function of shear rate as described by a Carreau-Yasuda model [Bird et al, 1987].

$$\eta = \eta_\infty + (\eta_0 - \eta_\infty)(1 + (\lambda \dot{\gamma})^a)^{\frac{(n-1)}{a}} \qquad (4)$$

The equations of motion are discretized with the finite element method. For these problems, we use the level set method of Sethian [1999], a front capturing scheme, which is used to determine the evolution of the interface with time. The level set is a scalar distance function, the zero of which coincides with the free surface or fluid-gas interface, e.g.

$$\phi(x, y, z) = 0 \,. \qquad (5)$$

We initialize this function to have a zero value at the fluid-gas interface, with negative distances residing in the fluid phase and positive distances in the gas phase. An advection equation is then used to determine the location of the interface over time.

$$\frac{\partial \phi}{\partial t} + v \bullet \nabla \phi = 0 \quad (6)$$

Derivatives of the level set function can give us surface normals, n, and curvature, κ, at the interface useful for applying boundary conditions.

$$n = \nabla \phi$$
$$\kappa = \nabla \bullet \nabla \phi \qquad (7)$$

Material properties vary across the phase interface from the properties of the fluid to the properties of the displaced gas. This variation is handled using a smooth Heaviside function that modulates material properties to account for the change in phase.

$$H_\alpha(\phi) = \frac{1}{2}(1 + \frac{\phi}{\alpha} + \frac{1}{\pi}\sin(\frac{\pi\phi}{\alpha})) \qquad (8)$$

This is a diffuse interface implementation of the level set method, which allows for an interfacial zone of length 2α, in which the properties will vary from fluid to gas values. Note that this method can be applied to both Newtonian and non-Newtonian fluids. We have also implemented another level set method where equation averaging is done using a Heaviside.

The momentum equation, including property modulation, becomes

$$(H_A\rho_A + H_B\rho_B)(\frac{\partial u}{\partial t} + u \bullet \nabla u) =$$
$$H_A \nabla \bullet \underline{\underline{\pi_A}} + H_B \nabla \bullet \underline{\underline{\pi_B}} + (H_A\rho_A + H_B\rho_B)\underline{g}$$
$$\underline{\underline{\pi_i}} = \eta_i(\nabla u + \nabla u^t) - p\underline{\underline{I}} \text{ where } i\text{=A,B}$$
$$\nabla \bullet u = 0 \qquad (9)$$

Boundary conditions for the dynamic contact line where the free surface and wall intersects are handled with a Blake wetting condition [Blake and Haynes, 1969]. Parameters for the model are informed by goniometer experiments that determine the wetting speed as a function of dynamic contact angle for the various fluids and surfaces of interest.

$$v_{wall} = v_o \sinh(\bar{\gamma}(\cos\theta_s - \cos\theta)) - \tau \frac{\partial v_{wall}}{\partial t} \quad (10)$$

Both Galerkin-least squares [Hughes, 2000] and Dohrmann-Bochev pressure stabilization [Dohrmann and Bochev, 2004] are used to reduce the condition number of the matrix, allow for equal order interpolation, and enable the use of Krylov-based iterative solvers. Further details of the modeling approach and equations, the numerical methods used and the finite element implementation can be found in a report by Rao et al. [2008].

Results and Discussion

Results and Validation for Injection Loading in a Coat Hanger Die

A diffuse interface method was used to study the mold design for an injection loading system. The mold is designed to produce a rectangular bar of green ceramic material, which is later heated to burnout the polymeric solvent, and then sintered to produce the final ceramic part. The inflow to the mold is a coat hanger die, which tends to pool material in the middle of the mold, potentially leaving voids in the corners. A redesign of the injection die was undertaken to reduce the chances of void formation.

Figure 4 shows three different mold designs: the original mold from the manufacturer (A), a longer die (B), and a longer, taller die (C). Validation experiments were performed for all three dies as well, and these results are also shown in figure 4.

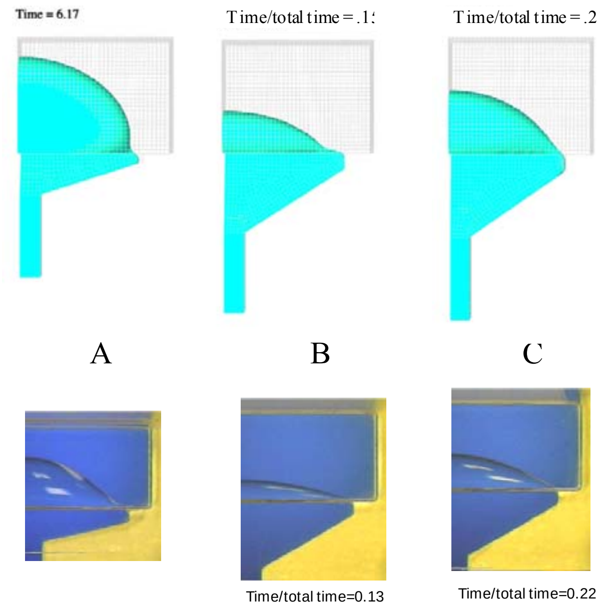

Fig. 4. Simulations (top) and experiments (bottom) for Ucon oil filling a coat hanger die. Only have the geometry is shown.

From figure 4, we can see that the simulations show similar trends to the experiments, though the details of the shape of the meniscus are different.

Results for Injection Loading of a Carreau Fluid

Simulation using a Carreau model, show Newtonian behavior since the shear rates are so high in the injection loader it shear thins to the infinite shear-rate viscosity.

Results for Mold Filling of a Newtonian Fluid in a Mold with Obstacles

We have also investigated the mold filling of a Newtonian fluid into a mold with obstacles using a diffuse interface level set method. Results from the simulations and experiments are shown in figure 5.

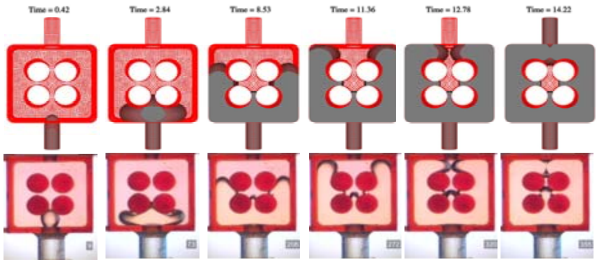

Fig. 5. Real parameters: μ = 390 Poise, θ_{eq} = 39.8^o, v_o = 0.0013 cm/s, σ = 42.4 dyne/cm (Ucon 95-H-90000 measured parameters); fill time=12 s. Model parameters: μ = 390 Poise, θ_{eq} = 39.8^o, v_o = 0.0026 cm/s, σ = 42.4 dyne/cm, fill time=14 s.

Figure 6 shows the filling dynamics of a Newtonian fluid as it enters a mold with obstacles as a function of time. Here we can see the shape of the meniscus with time and how it compares to the experimental results. The model and experiments agree well qualitatively, but there are subtle differences between the meniscus shapes especially at early times. Filling times for the experiment are faster than the simulation, using the experimentally determined inflow rate. The wetting speed in the Blake dynamic contact-line model seemed to be faster that what was seen experimentally, when measured in goniometer experiments. Therefore, a slower wetting speed was used to more closely represent the validation experiment. Future work will more closely investigate the wetting model and how it effects the rate of filling.

Results for Bottle Filling of a Newtonian and a Carreau Fluid

We have also investigated the 2D planar bottle filling of both Newtonian and shear-thinning fluids using both the level set method. Figure 7 shows three different flow instabilities seen in bottle filling: buckling, mounding, and entrained flow, where air bubbles are incorporated into the fluid. Even for this simplified geometry, complex physics is observed.

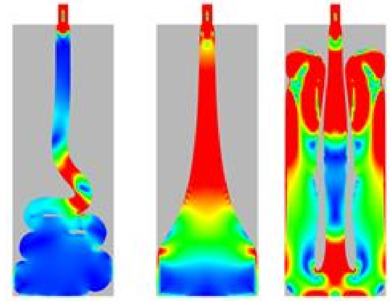

Fig. 6. Level-set simulations of bottle filling with a Newtonian fluid. As the Reynolds number is increased we see a transition from coiling, to mounding, and then breakup flow

We can extend this model to include non-Newtonian rheology as summarized in figure 8.

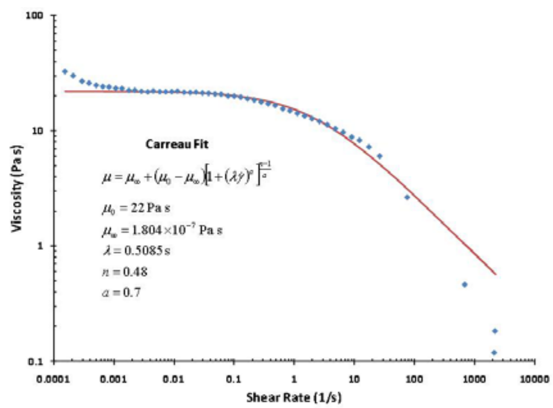

Fig. 7. Carreau fit for bottle filling problem

The results for using this Carreau model with our simulations of bottle filling are given in Figure 9.

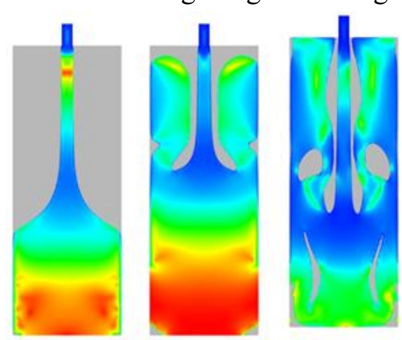

Fig. 8. Level set simulations of bottle filling with a Carreau fluid. As the Reynolds number is increased, we see transition from mounding, to entraining, and then breakup flows.

Here, we still see three flow regimes, but the buckling regime is not seen for the Carreau model, with the parameters shown in figure 8. Instead, we see a mounding regime at low Re, then an entrained regime, and finally a bubbly flow at high Re.

Conclusions and Future Work

A diffuse interface finite element/level set algorithm has been used to investigate filling processes for injection loading, mold filling of a complex mold with obstacles, and bottle filling where an extrudate interacts with a container. The modeling has been successful in matching experimental data qualitatively, but quantitative agreement is still lacking.

For future work, we will investigate an advanced version of the level set method termed the conformal decomposition finite element method (CDFEM). CDFEM is a hybrid moving boundary algorithm, which uses a level set field to determine the location of the fluid-fluid interface and then dynamically adds mesh on the interface to facilitate the application of boundary conditions such as capillarity. This is a sharp interface method, where it is possible to apply jumps in material properties and field variables [Noble et al, 2010]. We believe this algorithm will allow us to agree quantitatively with experiments.

Acknowledgments

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