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Numerical Simulation of a Non-Newtonian Fluid during the Filling Process of a Die

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Abstract
In this paper, a numerical model is developed which can predict behavior of non-Newtonian fluids. These kinds of fluids have complex rheology and simulation of their behavior has always been a challenge. The present study concentrates on a special type of non-Newtonian fluids called viscoplastic. To investigate their behavior a numerical model is developed in which the free surface is determined by volume-of-fluid method. To validate the model, flow properties of Herschel-Bulkley are modeled and compared with the experimental results reported in the literature. Afterwards, filling of a 2D cavity with Bingham fluid is simulated. Models which are used for Herschel-Bulkley and Bingham fluids are Herschel-Bulkley and Papanastasiou models, respectively. Five flow patterns are observed by changing the Reynolds and Bingham numbers of the flow. It is shown that formation of voids which undesirably occurs during the filling process can be eliminated by controlling the flow velocity. The obtained results well agree with those reported in the literature.

Keywords: non-Newtonian fluids, VOF method, injection molding, die filling

Introduction

Non-Newtonian fluids have complex rheology and it is not possible to explain their behavior by means of Newtonian fluid models. They have wide applications in industrial processes one of which is injection molding. Injection molding is an important process in industry because of its ability to make products in small and large sizes by using polymer melts, suspensions and semi-solid metals [1,2]. Four steps for this process are: preprocessing, filling, solidification and part ejection. Obviously, filling is the most important step because it determines defects and quality of the final part and most problems occur in this step.

Most of previous studies have focused on 3D injection molding [3,4,5] but a few of them have considered complex properties of fluids in the process. Viscoplastic fluids are classified in two groups; Bingham and Herschel-Bulkley which are considered as fluids in injection molding in the literature. Alexandrou et al. [6] estimated properties of semi-solid metals as Herschel-Bulkley and examined their behavior while filling 2D and 3D cavities. They studied the effect of temperature and other fluid properties on the time of filling in 1999. In 2001, by changing flow parameters, different flow patterns were obtained for Bingham fluid when it fills a 2D cavity [1]. Irregularities that result toothpaste effect were modeled for Herschel-Bulkley in 2003 [7]. Rudert et al. [2] studied filling a 3D cavity by viscoplastic fluid, experimentally and theoretically. Roberts et al. [8] investigated the profile of jet while impinging the surface of the shear thinning fluid.

The goal of the present study is to develop a numerical model which simulates non-Newtonian fluid flow. In particular Bingham and Herschel-Bulkley are investigated and results are presented for Bingham fluid in injection molding.

Mathematical Model

Governing Equations

Governing equations are continuity and momentum equations as following:

$$\vec{\nabla}.\vec{V} = 0 \tag{1}$$

$$\frac{\partial \vec{V}}{\partial t} + \vec{\nabla}.\vec{V}\vec{V} = -\frac{1}{\rho}\vec{\nabla}P + \frac{1}{\rho}\vec{\nabla}.\vec{\tau} + \vec{g} + \frac{1}{\rho}\vec{F}_b \tag{2}$$

where $\vec{V}$, ρ, $\vec{\tau}$, $\vec{g}$ and $\vec{F}_b$ are velocity vector, fluid density, stress tensor, gravity and body forces, respectively.

Viscosity of non-Newtonian fluid is not constant and it is a function of shear rate. There are different models for Bingham fluid; the most popular one of which is Bingham model. This model is defined as below [9,10]:

$$\begin{cases} \dot{\gamma} = 0 & \text{For } \tau \le \tau_0 \\ \tau = \left(\mu + \tau_0/\dot{\gamma}\right)\dot{\gamma} & \text{For } \tau > \tau_0 \end{cases} \tag{3}$$

Where τ is viscous stress tensor, μ is effective viscosity or viscosity of the deformed material, τ_0 and $\dot{\gamma}$ are respectively yield stress of non-Newtonian fluid and rate of strain tensor defined as [2]:

$$\dot{\gamma}_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{4}$$

$$\dot{\gamma} = \sqrt{\dot{\gamma}_{ij}\dot{\gamma}_{ji}} \tag{5}$$

Equation 3 characterizes two different flow regimes: when $\tau \le \tau_0$ the material behaves as a rigid solid, when $\tau > \tau_0$ it flows and its apparent viscosity will be:

$$\mu_{app} = \mu + \tau_0/\dot{\gamma} \tag{6}$$

Using the Bingham model makes some difficulties, one of which is infinite apparent viscosity at vanishing shear rates. To overcome this problem another model is used which called Papanastasiou and defined as below [11]:

$$\tau = \left(\mu + \tau_y \frac{1-\exp(-m|\dot{\gamma}|)}{|\dot{\gamma}|}\right)\dot{\gamma} \quad (7)$$

where m is a parameter which has dimension of time and it controls the exponential rise at low strain rate. In Papanastasiou model for $\dot{\gamma} = 0$, apparent viscosity will be $\mu_{app} = \mu + m\tau_y$ which is finite. Based on equation7, the parameter m has dimension of time and the value of m is considered 200 in this study. More discussions about m and its effect on the results can be found in previous studies [12,13].
For Herschel-Bulkley fluid the shear stress versus shear rate relationship is reasonably well described by the Herschel-Bulkley model [14]:

$$\tau = \tau_y + k\dot{\gamma}^n \quad (8)$$

where τ_y is the yield stress (dynamic), k is the consistency and n is the flow index.

Numerical Model

The developed numerical model is capable to simulate incompressible two phase flow of Bingham and Herschel-Bulkley fluids. Convective, gravity and body force terms are calculated explicitly. If we use explicit method to calculate viscous term, because of high viscosity in solution domain, time step will be decreased and governing equations will need long time to be solved. Therefore an implicit method developed by Mirzaii and Passandideh-Fard [15] is used for solving the viscous term.
To determine the location of liquid interface, volume of fluid (VOF) method is applied in which by using a scalar parameter (f), the interface is captured. The function f is defined as:

$$f = \begin{cases} 0 & \text{in gas} \\ 0 < f < 1 & \text{at gas-liquid interface} \\ 1 & \text{in liquid} \end{cases} \quad (9)$$

In fact, value of f shows the fraction of liquid volume in every computational cell. This value is not used in momentum equation directly, but it affects density and viscosity.

$$\rho = f\rho_L + (1-f)\rho_g \quad (10)$$

$$\mu = f\mu_L + (1-f)\mu_g \quad (11)$$

Values of f move in solution domain according to the following equation:

$$\frac{\partial f}{\partial t} + (\vec{V}.\nabla)f = 0 \quad (12)$$

Two considered fluids are air and non-Newtonian fluids.

Validation of the Numerical Code

Two non-Newtonian fluids are simulated; Herschel-Bulkley and Bingham. For Bingham fluid, results are compared with those obtained by Alexandrou et al. [1] in the next section. For Herschel-Bulkley, results are compared with experimental and analytical results which have been obtained by Sutalo et al. [14]. The flow of Herschel-Bulkley fluid down an inclined plane is simulated. Inclined angle is 45° and properties of fluid which is 0.15 wt.% Ultrez 10 solution, are listed in Table 1. Our results show that the thickness of film layer for flow rate = 56.5 L.min^{-1}at 100 mm distance from the plate tip agrees with those reported in previous studies [14]. The film layer thickness obtained by the present study is 20 mm as shown in the last image of Figure 1.

Table 1: Ultrez 10 solution 0.15 wt.% properties

Material	τ_y (Pa)	k (Pa.s^n)	n	ρ (kg/m^3)
0.15 wt.% Ultrez 10 solution	4.12	13.75	0.412	1000

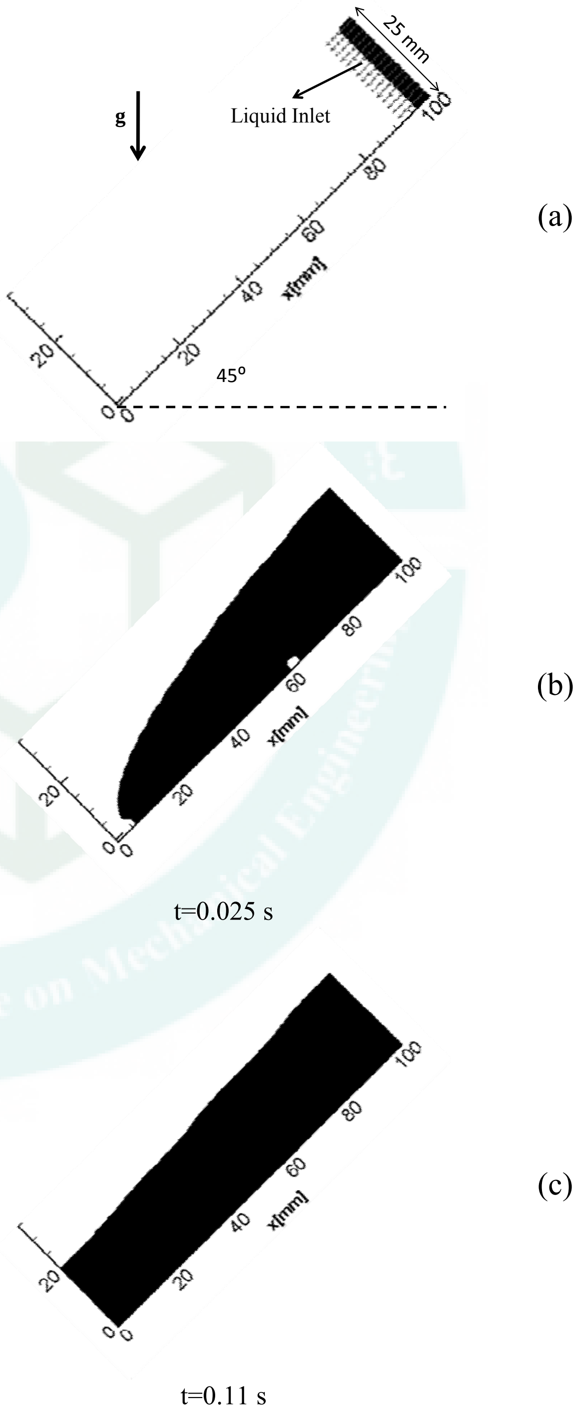

Figure 1: results obtained in the present study for the flow of Ultrez 10 solution 0.15 wt.% down an inclined plane

Table 2 shows the results of the present study and those obtained by Sutalo et al. [14].

Table 2. Film layer thickness for Ultrez 10 solution 0.15 wt.% obtained in the present study and reported by Sutalo et al. [14]

	Numerical results of the present study	Analytical result reported by Sutalo et al. [14]	Experimental measurement reported by Sutalo et al. [14]
Distance from Plate tip (mm)	100	100	100
Film thickness (mm)	20	19.2	19.5-20

Results and Discussion

A 2D cavity as shown in Figure 2 is investigated. Jet velocity V is constant and it fills the cavity from the top of the mold. No-slip condition is applied to the right and bottom boundaries. There is symmetric boundary for symmetric axis of the mold. We have considered the effect of air in the cavity. Results are obtained for half of domain.

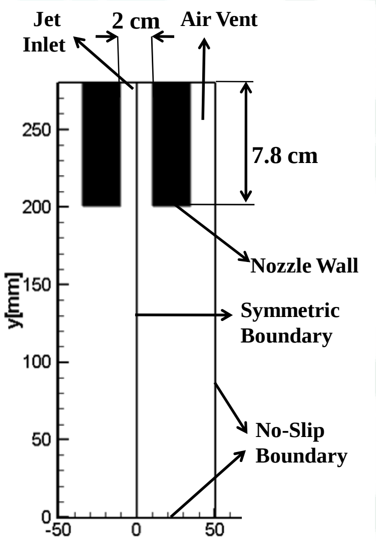

Figure 2: Geometry of 2D cavity, sizes and boundary conditions

By changing τ_0, μ and V in the governing equation for viscosity of Bingham fluid, the flow pattern in die filling step of injection molding will change and five different flow patterns will be obtained which are mound filling, transition filling, disk filling, bubble filling and shell filling. Previous studies show that these flow patterns depend on two non-dimensional numbers which are Reynolds and Bingham numbers and defined as below for Bingham fluid:

$$Re = \rho VH/_{\mu} \quad , \quad Bi = \tau_0 H/_{\mu V} \qquad (13)$$

where ρ, V, H, μ and τ_0 are respectively density, jet velocity, jet diameter, effective viscosity and yield stress.

For Herschel-Bulkley Reynolds and Bingham numbers are as following:

$$Re = \rho V^{(2-n)} H^n/_{k} \quad , \quad Bi = \tau_0 H^n/_{kV^n} \qquad (14)$$

where k and n are respectively consistency and flow index. The parameter k or consistency is a coefficient in power-law model which has a dimension of $[M.T^{n-2}/L]$.

Results which are shown in Figure 4 to Figure 8 are obtained for properties of Bingham fluid in Table 3.

The parameter t* in the figures which is called non-dimensional time is defined as following:

$$\bar{t} = H/V \quad , \quad t^* = t/\bar{t} \qquad (15)$$

t is the time for each step, $\bar{t}$ is characteristic time and H and V are respectively diameter and velocity of the jet. Choosing of properties is based on obtaining five different flow patterns. Reynolds and Bingham numbers are also mentioned in Table 3. In all the results, jet inlet velocity is considered 1 m/s and density is 2500 kg/m^3. Results are mesh- independent. Mesh size is considered 30×168 and Figure 3 shows the appropriate mesh size. In Figure 3 the vertical axis indicates fluid height for disk filling flow pattern at t*=25.

Table 3: Reynolds number, Bingham number, yield stress and effective viscosity for obtained results

	Figure4	Figure5	Figure6	Figure7	Figure8
Re	1	12.5	50	50	1000
Bi	0.001	9.35	10	200	50
τ_0(Pa)	2.5	1870	500	10000	125
μ(Pa.s)	50	4	1	1	0.05

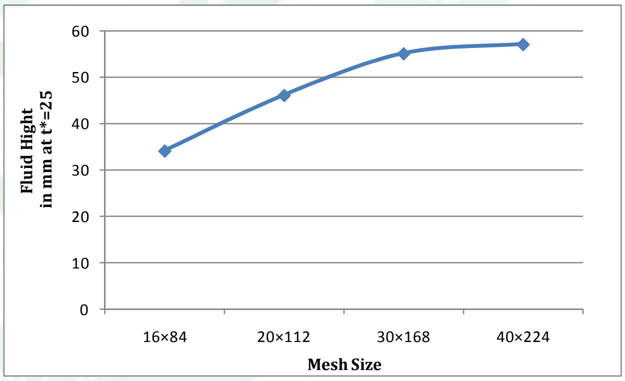

Figure 3: Fluid height inside the cavity in different mesh sizes at t*=25

Mound filling is shown in Figure 4. When the liquid jet strikes the bottom of cavity it does not split into two parts and central column of liquid grows slowly. This kind of filling is obtained in low Reynolds numbers. Mound filling produces parts without gas-induced porosity but low production rate makes it undesirable.

Figure 5 shows transition filling. In this kind of flow pattern liquid jet starts to grow from the bottom of cavity and after receiving the top of cavity, a bubble develops and air will trap in the middle of mold.

Another kind of filling which is shown in Figure 6 is called disk filling. This kind of flow pattern is desirable because there are no voids and porosity at final part.

When jet strikes the end of cavity it splits into two parts and develops as a disk during filling step.

Bubble filling is shown in Figure 7. This kind of flow pattern is so different from Newtonian flow patterns and the most important reason is yield stress. When the jet hits the end of cavity it does not split and liquid column starts to grow and after a while a bubble develops at the entry. In previous studies [7] it is obtained that bubble pattern leads to unstable jet behavior and forms toothpaste effect while the other patterns are stable and most of transition cases leads to stable jet profiles. This indicates that bubble filling is a critical pattern and it makes instabilities.

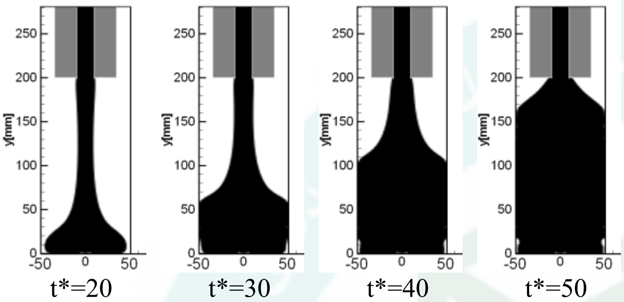

Figure 4: Mound filling, Re=1, Bi=0.001

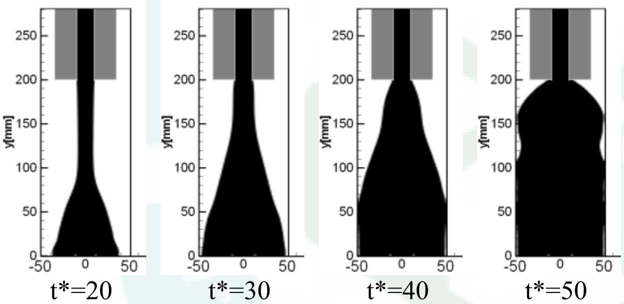

Figure 5: Transition filling, Re=12.5, Bi=9.35

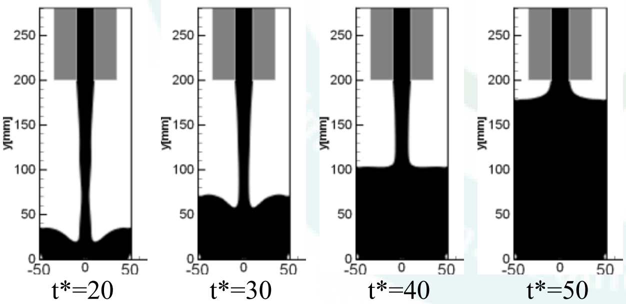

Figure 6: Disk filling, Re=50, Bi=10

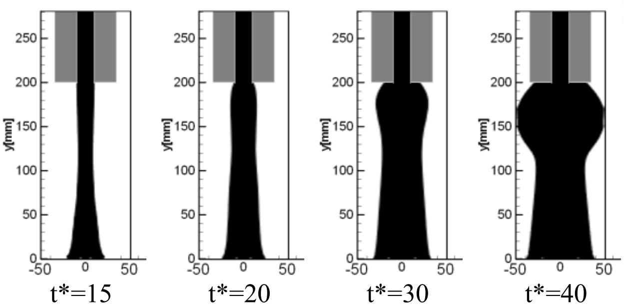

Figure 7: Bubble filling, Re=50, Bi=200

Shell filling is shown in Figure 8. Jet strikes the bottom of cavity and it splits into two layers along the right and left walls. This kind of filling is undesirable because of entrapped gas within the piece.

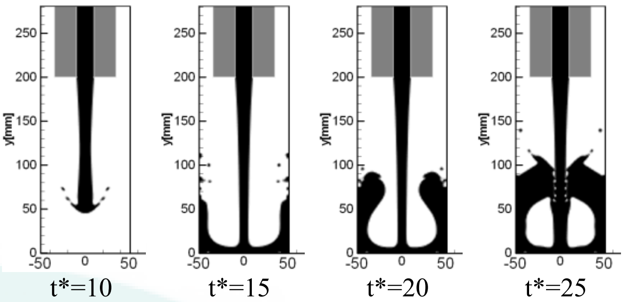

Figure 8: Shell filling, Re=1000, Bi=50

Obtained results well agree with those reported in previous experimental and numerical studies [1,2]. For Bingham fluid, results are compared with those reported by Alexandrou et al. [1]. For a special kind of flow pattern, Bubble filling, in which properties are defined in Figure 9, results are shown. In Figure 9 the first row indicates bubble filling reported in the previous study [1] and the second row shows results of the present study.

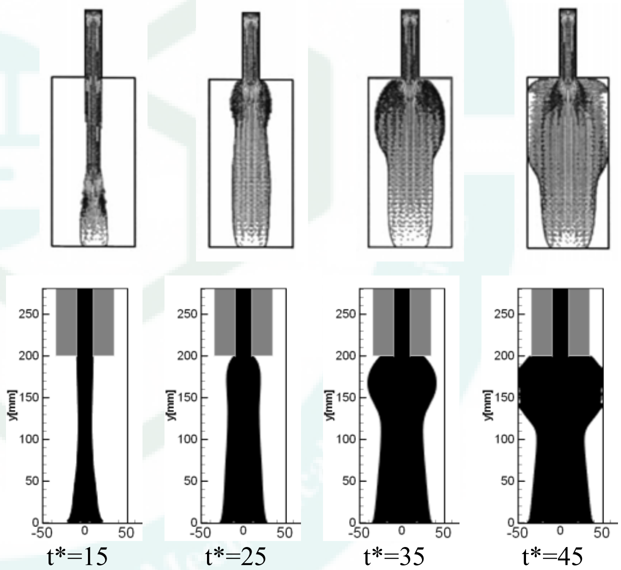

Figure 9: Results obtained in the present study (second row) as compared to the results reported in the literature [1] (first row) τ_0=10000(Pa) and μ=1(Pa.s)

For a constant Reynolds number, with changing Bingham number, results which are reported in Table 4 obtained. These results show the importance of non-Newtonian fluid yield stress which can make bubble filling and cause instabilities.

Table 4. Flow patterns by changing Bi when Re is constant

Re=50	Re=50	Re=50
Bi=10	Bi=45	Bi=200
Disk filling	Transition filling	Bubble filling

Figure 10 shows the stream lines and velocity vectors for disk filling. As shown in the figure, air leaves the cavity through the vents which are on the upper side of the mold.

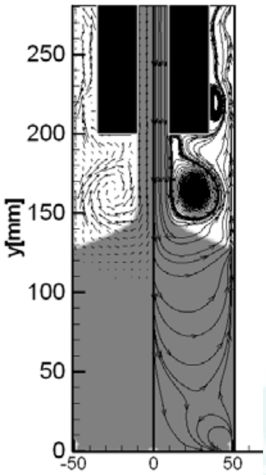

Figure 10: stream lines on the right and velocity vectors on the left

Conclusions

A numerical model is developed which can predict behavior of non-Newtonian fluids. First, the flow of Herschel-Bulkley down an inclined plane is compared with experimental and analytical results. Second, five different flow patterns in injection molding are obtained for Bingham fluid. By analyzing the results it is found that the main reason for some flow patterns like bubble and transition filling is the yield stress of non-Newtonian fluid. On the other hand, the filling pattern determines the final part quality; therefore more studies about filling step and controlling the process parameters like jet velocity can lead to an optimum process with high quality products.

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