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Modeling and simulation of the viscoelastic fluid mold filling process by level set method

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ABSTRACT

A model for unifying a viscoelastic fluid and a Newtonian fluid is established, in which the governing equations for the viscoelastic fluid and the Newtonian fluid are successfully united into a system of generalized Navier–Stokes equations. A level set method is set up to solve the model for capturing the moving interface in the mold filling process. The physical governing equations are solved by the finite volume method on a non-staggered grid and the interpolation technique on the collocated grid is used for the pressure-velocity and the stress-velocity decoupling problems. The level set and its reinitialization equation are solved by the finite difference method, in which the spatial derivatives are discretized by the 5th-order Weighted Essentially Non-Oscillatory (WENO) scheme, and the temporal derivatives are discretized by the 3rd-order Total Variation Diminishing Runge–Kutta (TVD-R–K) scheme. The validity of the method is verified by some benchmark problems. Then a simulation of viscoelastic fluid mold filling process is pursued with the method. The moving interface and all the information of the physical quantities during the injection process are captured. The die swelling phenomenon is found in the simulation. The influences of elasticity and viscosity on the physical quantities such as stresses etc. in the mold filling process are analyzed. Numerical results show that elastic characteristics such as the stretch and die swelling etc. reinforce accordingly as Weissenberg number increases. Pressures increase continuously in the mold filling process and the pressure maintains the maximum value at the inlet. Injection velocity is proportional to injection pressure. A higher viscosity leads to a higher pressure distribution, that is, the pressure decreases as Reynolds number increases.

1. Introduction

Fluid flows of viscoelastic materials, such as polymer melts in mold filling process, are frequently used in industrial production and often involve multiple moving free surfaces. Many numerical techniques for simulating viscoelastic free surface flows have been developed. Keunings and co-workers did some early studies on viscoelastic two-dimensional free surface flows in 1980s [5,6,13,14]. Tomé and co-workers did many studies on simulations of viscoelastic free surface flows in 2D [33–35] and 3D [31,32,36], using finite difference methods on staggered grids and Marker-and-Cell method. Picasso and co-workers presented a numerical model for the simulation of viscoelastic flows with complex free surfaces in 3D [4,10]. Eriksson et al. studied the effects of polymer melt rheology on the replication of surface microstructures in isothermal molding [8]. Rasmussen and Eriksson also did some experiments and viscoelastic simulations of gas displacement of polymer melts in a cylinder [19].

The papers mentioned above considered only the viscoelastic fluid phase and the constitutive equations adopted are UCM, Oldroyd-B or PTT etc., which are developed based on phenomenological theory. The extended pom–pom (XPP) constitutive equation developed by Verbeeten et al. [37,38] is based on molecular theory of rheology and can provide a good fitting to the rheology of polymer melts and concentrated solutions. Moreover, the XPP model reduces the influences of stress singularity to some extent that Weissenberg numbers can reach higher values than those in some models developed based on phenomenological theory. However, as far as we know, its application to free surface flows has not yet been demonstrated. There are single equation version and double equation version of the XPP model. As pointed in [2], the two versions have been shown to be mathematically equivalent involving a constitutive equation for the orientation tensor and an evolution equation for the stretch. In this paper, we use the single equation version of the XPP (SXPP) model as the constitutive equation since it is easier to deal with than double equation mode.

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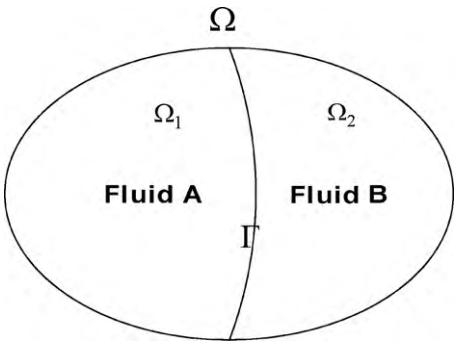

Fig. 1. Schematic plot of level set method.

Moreover, as for the Newtonian fluid, the free surface problems for two-phase cases have already been studied for many years [26–29,41], in which the governing equations for two different Newtonian fluid flows can be unified by the definition of the Heaviside function. This paper tries to do some research on the free surface problem for the viscoelastic-Newtonian fluid flows inspired by the Newtonian-Newtonian case. We focus on the mold filling problem that has been studied with only viscoelastic fluid phase considered in [4,9,32]. The Level set method proposed by Osher and Sethian [17] is used to capture the interface. When only the melt phase in the cavity is considered, one must devise appropriate extension velocities, for example, the Ghost Fluid Method (GFM), to transport the neighboring level set functions in tandem with the one corresponding to the zero level set because both the level set function and the velocity field defined at the interface are defined throughout all of space [21–23]. This paper successfully unifies the governing equations of the viscoelastic fluid described by an SXPP constitutive model and those of a Newtonian fluid, and then the mold filling process is simulated numerically. The motion of the interface in the mold filling process is captured. The finite volume method is used to discretize the governing equations on a non-staggered grid. The level set equation and the reinitialization equation are spacial discretized by 5th-order Weighted Essentially Non-Oscillatory (WENO) scheme and temporal discretized by Total Variation Diminishing Runge–Kutta (TVD-R–K) method. The influences of physical quantities, such as the Reynolds number and the Weissenberg number, on the interface motion are studied. The influences of the viscosity and the elasticity on the first normal-stress difference and the stretch are discussed. The relationship between the viscosity and the injection pressure under different flow rates are discussed as well.

2. Level set method

Assume that two sub-domains Ω_1 and $\Omega_2$of the domain Ω are filled with two different fluids which is shown in Fig. 1.

To describe the interface Γ between the two sub-domains, we use the level set method, which is based upon an implicit representation of the interface Γ by a smooth, scalar function φ called the level set function. The function usually takes the form of a signed distance to the interface, whereby the zero level set $\varphi = 0$ represents the points $\mathbf{x}(\mathbf{x} = (x, y))$ on the actual interface Γ. And φ satisfies the following formula [16].

$$\varphi(\mathbf{x}, t) = \begin{cases} \text{distance}\,(\mathbf{x}, \Gamma(t)) & \mathbf{x} \in \Omega_1(t) \\ 0 & \mathbf{x} \in \Gamma(t) \\ -\,\text{distance}(\mathbf{x}, \Gamma(t)) & \mathbf{x} \in \Omega_2(t) \end{cases} \tag{1}$$

And the interface can be written as follows [16]

$$\Gamma(t) = \{\mathbf{x} \in \Omega | \varphi(\mathbf{x}, t) = 0\} \tag{2}$$

Then the interface is evolved by the velocity (u, v). It can be described by the advection equation in the Eulerian coordinate [16].

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = 0 \tag{3}$$

A high velocity gradient can produce wide spreading and stretching of the level sets when the level set method is developed, which leads to the result that φ will no longer remain a distance function after one or more time steps. A reinitialization algorithm must be applied to keep φ as the algebraic distance to the interface. The algorithm is based on the iterative solution of the following initial value problem [16].

$$\begin{cases} \dfrac{\partial \varphi}{\partial t_r} = sign(\varphi_0)(1 - |\nabla \varphi|) \\ \varphi(x, y, 0) = \varphi_0(x, y) \end{cases} \tag{4}$$

where t_r is a pseudo time and $sign(\varphi_0)$ is the sign function of φ which is defined as

$$sign(\varphi_0) = \frac{\varphi_0}{\sqrt{{\varphi_0}^2 + [\min(\Delta x, \Delta y)]^2}}$$

Here, Δx and Δy are the grid widths along x and y direction respectively, and $[\min(\Delta x, \Delta y)]^2$ is used to avoid denominator's dividing by zero.

Reinitialization equation (4) does not change the position of the zero level set of φ. Unfortunately in numerical computation this may not be true [26]. We use the method presented by Sussman et al. [26] to improve the accuracy of solving the reinitialization equation. A local correction item, $\omega\delta_\varepsilon(\varphi)|\nabla\varphi|$, is added to the reinitialization equation. The revised reinitialization equation can be described as

$$\frac{\partial \varphi}{\partial t_r} + sign(\varphi_0)(|\nabla \varphi| - 1) = \omega \delta_\varepsilon(\varphi)|\nabla \varphi| \tag{5}$$

where ω is the weight coefficient, $\delta_\varepsilon(\varphi)$ is the Dirac function defined in (18). See [26] for more details.

3. A unified model for viscoelastic-Newtonian fluid flows

In this section, the unified model for voscoelastic-Newtonian fluid flows will discuss in detail.

In mold filling process, since the gas phase and the liquid-phase are immiscible and the Mach number of the gas is very small, both the gas phase and the liquid-phase can be regarded as incompressible flows.

The governing equations for the gas phase in the cavity are

$$\text{continuity} \quad \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{6}$$

$$u\text{-momentum} \quad \frac{\partial(\rho_g u)}{\partial t} + \frac{\partial(\rho_g u u)}{\partial x} + \frac{\partial(\rho_g v u)}{\partial y} = -\frac{\partial p_g}{\partial x} + \frac{\partial^2(\mu_g u)}{\partial x^2} + \frac{\partial^2(\mu_g u)}{\partial y^2} \tag{7}$$

$$v\text{-momentum} \quad \frac{\partial(\rho_g v)}{\partial t} + \frac{\partial(\rho_g u v)}{\partial x} + \frac{\partial(\rho_g v v)}{\partial y} = -\frac{\partial p_g}{\partial y} + \frac{\partial^2(\mu_g v)}{\partial x^2} + \frac{\partial^2(\mu_g v)}{\partial y^2} \tag{8}$$

where u, v are the velocities along x, y directions respectively, ρ is the density, μ is the viscosity and the subscript g denotes the gas phase.

The continuity equation for the viscoelastic flow with SXPP constitutive model is the same as Eq. (6). The momentum equations