International Journal of Heat and Mass Transfer 104 (2017) 374–391

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Three-dimensional simulations of non-isothermal transient flow and flow-induced stresses during the viscoelastic fluid filling process

Xin Zhuang, Jie Ouyang *, Wuming Li, Yanggui Li

Department of Applied Mathematics, Northwestern Polytechnical University, Xi'an 710129, China

A R T I C L E I N F O

Article history:
Received 29 October 2015
Received in revised form 21 July 2016
Accepted 19 August 2016
Available online 28 August 2016

Keywords:
Non-isothermal
XPP fluid
Flow-induced stresses
3D filling process
Two-phase flow

A B S T R A C T

The three-dimensional (3D) viscoelastic polymer melt filling process in injection molding has always been regarded as a challenging two-phase flow problem. Numerical investigations concerning it are very limited, especially under the non-isothermal condition. Thus, this article presents a 3D non-isothermal two-phase model to investigate the flow-induced stresses during the viscoelastic fluid filling process. The viscoelastic behavior of polymer melt is predicted by the eXtended Pom–Pom (XPP) model, in which the temperature dependence of polymeric viscosity and relaxation times are described using the Arrhenius equation. The 3D governing equations are solved by a collocated finite volume method. The high resolution revised level set method coupled with a domain extension technique is extended to capture the 3D melt front interface in an irregular cavity. The collocated finite volume method and the revised level set solver are respectively validated using the XPP melts past a cylinder and the single vortex flow. Then the ability of the presented 3D two-phase model is verified by the isothermal Newtonian fluid filling process in a thin rectangular cavity. The numerical results are in good agreement with those reported in literature. Finally, the challenging problem of non-isothermal XPP fluid filling process in a 3D rectangular cavity with one cylindrical insert is investigated. The temperature field, flow-induced stresses and the corresponding rheological behaviors of polymer melt during 3D filling process are quantitatively predicted. Especially, the effects of processing conditions and energy source term on the two normal stress differences are discussed. It is found that melt temperature and injection velocity are the main factors that affect the normal stress differences. The obtained results should be helpful for improving the product properties in practical production.

1. Introduction

Injection molding is one of the most widely used manufacturing processes for producing high quality polymer products. The typical injection molding is a cycle process which including filling, packing and cooling. In fact, the filling process is a very important stage in injection molding, which is a rather complex non-isothermal viscoelastic fluid flow process. Since the polymer melt experiences high deformations as well as the temperature and pressure variations during the filling process, generating complex flow-induced stresses in cavity [1]. It has been known that the anisotropy of the mechanical, thermal and optical properties of the final products are directly determined by the flow-induced stresses [2]. In recent years, with the rapid development of processing technology and the extensive application of plastic products, the effects of the flow-induced stresses on the final product properties have attracted considerable attention. However, both the understanding of the heat transfer and the effects of the processing conditions on the flow-induced stresses are far behind the requirements of engineering applications. Therefore, the investigation of non-isothermal viscoelastic fluid filling process has important scientific meaning and engineering practical value for improving the mechanical and thermal properties of products. However, it is nearly impossible to handle this complex problem only through analytical and experimental methods. Alternatively, the numerical simulation therefore becomes a powerful tool to accurate predict the flow-induced stresses and control the manufacturing processes.

In the past decades, studying the 3D filling process through numerical simulation has become a significant research subject. Kim and Turng [3] and Cardozo [4] have given detailed description of the developments of 3D filling simulation for polymer injection molding. The finite element method [5–8] and finite volume method [9–11] were mainly employed to simulate the 3D filling

* Corresponding author.
E-mail addresses: zhuangxin1983@126.com (X. Zhuang), jieouyang@nwpu.edu.cn (J. Ouyang), liwum0626@126.com (W. Li), liyanggui@126.com (Y. Li).

http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.08.064
0017-9310/

Nomenclature

a_T	shift factor
$\mathbf{B}$	slip tensor
Br	Brinkman number
C	specific heat, $\mathrm{J \cdot kg^{-1} \cdot K^{-1}}$
$\mathbf{d}$	deformation rate tensor
E_0	activation energy constant, $\mathrm{J \cdot mol^{-1}}$
H_ε	Heaviside function
L	length scale, m
p	pressure, Pa
Pe	Peclet number
q	number of arms
r	ratio of orientation to stretch relaxation time
R	ideal gas constant, $\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$
Re	Reynolds number
T	temperature, K
T_0	temperature scale, K
T_r	reference temperature, K
U	velocity scale, $\mathrm{m \cdot s^{-1}}$
$\mathbf{u}$	velocity vector, $\mathrm{m \cdot s^{-1}}$
We	Weissenberg number

Greek symbols

α	anisotropy parameter
β	ratio of solvent viscosity to total viscosity
$\dot{\gamma}$	shear rate, $\mathrm{1 \cdot s^{-1}}$
η	viscosity, $\mathrm{Pa \cdot s}$
κ	thermal conductivity, $\mathrm{W \cdot m^{-1} \cdot K^{-1}}$
Λ	backbone stretch
λ	orientation relaxation time, s
λ_s	tube stretch relaxation time, s
ρ	density, $\mathrm{kg \cdot m^{-3}}$
$\boldsymbol{\sigma}$	extra stress tensor, Pa
$\boldsymbol{\tau}$	polymeric contribution to extra stress, Pa
ϕ	level set function
ϕ_0	initial value of level set function
ω	energy partitioning coefficient

Subscripts

g	gas phase
m	melt phase

process of injection molding. Unfortunately, all of these 3D simulations were confined to the Newtonian or non-Newtonian viscous fluids, and the non-Newtonian viscoelastic fluid was not considered. To date, the numerical simulations of flow-induced stresses have still been limited to two-dimensional (2D) and 2.5-dimensional (2.5D) in which the variations of stress, temperature, velocity and pressure in the gap-wise (thickness) direction are neglected. Isayev and Hieber [12] firstly predicted the flow-induced stresses using the finite element method and applied the traditional incompressible version of the Leonov model in one-dimensional (1D) viscoelastic fluid filling process. Baaijens [13] used a compressible version of the Leonov model to calculate the flow-induced stresses in 2D injection molding for a strip cavity. Isayev et al. [14] simulated the temperature field and the flow-induced stresses in a center-gated disk during the filling and packing stages based on the compressible Leonov model. Moreover, Kamal et al. [15] and Goyal et al. [16] investigated the 2D viscoelastic polymer fluids filling processes, and the flow-induced stresses in filling processes were predicted using the White–Metzner model. More recently, Dou et al. [17] successfully simulated the distributions of flow-induced stresses based on the fiber stress constitutive model during 2D filling process using level set method and projection method. As for the calculation of the flow-induced stresses in non-isothermal viscoelastic melt filling and packing stages based on the PTT model, one notable work was presented by Cao et al. [18]. They introduced a 2.5D semi-analysis method and studied the flow-induced stresses in regular cavities.

It is generally accepted that the Pom–Pom model, originally proposed by McLeish and Larson [19] based on the tube theory can characterize the non-linear rheological behavior of branched polymer melts in both shear and extension flows. To overcome some shortcomings of the original Pom–Pom model, Verbeeten et al. [20] firstly introduced the eXtended Pom–Pom (XPP) model, an improvement of the original differential Pom–Pom model. The XPP model not only can predict a non-zero second normal stress difference in shear flow but also can remove discontinuities solutions in steady state elongation flow. From then on, this improved model has been widely used to investigate the benchmark problems [21–24]. As a promising constitutive model, the XPP model also has been employed by various research groups [25–28] to simulate the viscoelastic free surface flows, such as extrudate swell, jet buckling and rob-climbing effect. However, until now, the numerical prediction of viscoelastic fluid filling process in injection molding based on the XPP model has received less attention. Yang et al. [29] simulated the 2D viscoelastic fluid filling process using finite volume method based on the XPP model. More recently, Ren et al. [30] applied an improved smoothed particle hydrodynamics (SPH) method to simulate the 2D non-isothermal XPP fluid filling process. The physical model and numerical method in the two aforementioned simulations were based on the 2D approximation and the 2D flow-induced stresses were simulated. Although the assumptions of 2D flow simplifies the non-linear model and greatly reduces the computation complexity, the simulation of non-isothermal viscoelastic fluid filling process in 3D case would be more significant to the industrial applications. However, the 3D calculation of the flow-induced stresses during non-isothermal viscoelastic fluid filling process is an extremely difficult task. Because such flow involves highly non-linear interaction between complex viscoelastic free surface and transient heat transfer, which challenges the accuracy and stability of the numerical method. To the best of our knowledge, there is almost no numerical research on 3D flow-induced stresses in non-isothermal viscoelastic fluid filling process.

Therefore, the aim of this article is to propose a 3D non-isothermal two-phase flow model based on the level set function to simulate transient flow and flow-induced stresses in a rectangular cavity with a cylindrical insert during the viscoelastic fluid filling process. The viscoelastic behavior of polymer melt is described by the XPP model, in which the temperature dependence of polymeric viscosity and relaxation times are described using the Arrhenius equation. The 3D governing equations are successfully solved by a collocated finite volume method with an interpolation technique. In addition, a high resolution revised level set method is extended to capture the 3D complex melt interface, which avoids the complex reconstruction of the interface. A domain extension technique is presented to deal with the irregular cavities, which is very easy to implement in irregular cavities. To effectively improve the numerical stability, both additional diffusion term [31] and artificial stress [32] are particularly incorporated into the momentum and XPP constitutive equations. An enhanced treatment of the viscoelastic stress solid boundaries and the second-order Runge–Kutta are employed to obtain accurate stress results on solid walls.