Journal of Non-Newtonian Fluid Mechanics 241 (2017) 34–42

Contents lists available at ScienceDirect

Journal of Non-Newtonian Fluid Mechanics

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

Multiscale simulations for entangled polymer melt spinning process

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ARTICLE INFO

Article history:
Received 14 December 2016
Accepted 3 February 2017
Available online 4 February 2017

Keywords:
Polymer melt spinning process
Multiscale simulation
Slip-link model
Entangled polymer melt

ABSTRACT

We successfully applied a multiscale simulation method to a spinning process of a well-entangled polymer melt. In the spinning process, the macroscopic dynamics of the polymer melt and microscopic states of polymer chains are tightly connected through the strain rate and stress fields. A macroscopic model for the spinning process is constructed by using the standard and simplified 1D approach, thus ignoring the complex flow conditions near the die exit. In our multiscale simulation method, to evaluate the flow history of the stress, we employ a particle method in the Lagrangian manner at the macroscopic level and use the slip-link model to address entangled polymer dynamics at the microscopic level. Therefore, we can take into account the history effect of polymer melts and quantitatively evaluate the polymer dynamics, such as the entanglements. From our multiscale simulations, the number of entanglements decreases with flow down the spinning line because of the convective constraint release (CCR) effect. Moreover, we found that the number of entanglements generally decreases in the middle section of a polymer chain. This result shows that our multiscale simulation makes it possible to design a polymer melt that has desirable physical properties for producing a sophisticated fiber.

1. Introduction

Polymer melt spinning process is a common technique for manufacturing a polymeric fiber. Physical properties of the fiber made by the melt spinning process depend on both the macroscopic rheological properties and the microscopic structure, such as molecular orientation and entanglements. To produce a desirable fiber, we must study this process from both the macroscopic and microscopic aspects. A number of experimental and/or theoretical studies related to the polymer melt spinning process have been conducted, mostly since the 1960s. One of the pioneering studies involving the development of a mathematical model of the spinning process was performed by Kase and Matsuo [1,2] at relatively low take-up speeds for a Newtonian fluid. Fisher and Denn [3,4] used the Maxwell model as a viscoelastic constitutive equation and analyzed a flow instability of the elongational flow known as the draw resonance phenomenon. Phan-Thien [5] and Gagon and Denn [6] employed the Phan-Thien Tanner (PTT) model as a viscoelastic constitutive equation. After these pioneering studies, research interest was extended to microscopic structures, such as the molecular orientation and crystallization induced by the elongational flow. Zieminski and Spruiell [7] developed a model that included polymer crystallization at high take-up speeds for nylon-66 by using the Newtonian fluid. However, their model of crystallization was not constructed from a molecular viewpoint, and the fluid that they used did not have viscoelastic properties. Subsequently, mathematical models that include crystallization and use the viscoelastic fluid have been developed by many researchers [8–10]. Doufas et al. [8] proposed a mathematical model for the flow-induced crystallization of nylon-66 that involved coupling a semi-crystalline phase described as rigid rods with the Giesekus model as a viscoelastic constitutive equation. Joo et al. [9] proposed a two-dimensional model that included thermally and stress-induced crystallization for polystyrene and nylon-66. Moreover, van Meerveld et al. [10] presented a mathematical model for PET and nylon-66 based on a non-equilibrium thermodynamics analysis of flow induced crystallization. More recently, Dietz [11] focused on a discrete relaxation spectrum of polyester and analyzed the spinning process by using the PTT model.

To the best of our knowledge, a constitutive equation is used to couple the strain rate with the stress tensor in all of the studies about the polymer melt spinning process. However, it is often difficult to uniquely choose an appropriate constitutive equation and obtain a parameter set that fits the experiments on targeting polymer melt because there is no definite method for choosing a proper constitutive equation from among the known ones.

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http://dx.doi.org/10.1016/j.jnnfm.2017.02.001
0377-0257/

Moreover, to use the constitutive equation prohibits one from directly obtaining microscopic information that is tightly related to the macroscopic flow and physical properties of the resultant product. In fact, to develop well-controlled polymeric products, it is significantly important to know the correlation between the macroscopic flow behaviors and the state of polymer chains at a local place. Despite the recent rapid development of computational ability, it is still difficult to solve flow problems of polymeric liquids by using solely a molecular dynamics (MD) simulation because of its high computational cost. To overcome these difficulties, increasing attention has been paid to a multiscale approach that directly combines the macroscopic model with the microscopic model. For a pioneering study on the multiscale simulation method, Calculation of Non-Newtonian Flow: Finite Elements and Stochastic Simulation Technique (CONNFFESSIT) [12,13] was proposed by Laso and Öttinger. In the CONNFFESSIT, microscopic information obtained from the multiscale simulation is limited because the dumbbell model was used as a microscopic polymer model. Ren and E [14] proposed another type of the multiscale approach known as the Heterogeneous Multiscale Method (HMM). The HMM variation of the multiscale method can be applied to many flow problems because of its general methodology. Yasuda and Yamamoto [15,16] developed a multiscale simulation method similar to the HMM and applied it to polymeric liquids with the memory effect but without entanglement. More recently, Yasuda and Yamamoto [17] extended their model for the coupled heat and momentum transfer of complex fluids. De et al. [18] proposed a multiscale simulation method based on a scale-linking scheme that can correctly address the memory effect. Halin et al. [19] introduced a different multiscale approach, a Lagrangian Particle Method (LPM), to calculate time-dependent viscoelastic flows. In the LPM, the extra-stress originating from the polymer dynamics was calculated on convected particles, and the conservation laws were solved in the Eulerian manner. After that, Wapperom et al. [20] developed the LPM into more accurate and efficient method, a Backward-tracking Lagrangian Particle Method (BLPM), by introducing the backward-tracking process. By using a particle-based Lagrangian method similar to the LPM, Murashima and Taniguchi developed a multiscale simulation method of viscoelastic fluids that used the dumbbell model [21] and the slip-link model for a well-entangled monodisperse polymer melt [22,23]. Although many researchers have developed the multiscale simulation method, the application examples are limited to rather simple cases such as flows between two parallel plates, flows around an infinitely long cylinder and so on. In addition, it is discussed whether these multiscale simulation methods are consistent with a framework of non-equilibrium thermodynamics called “GENERIC” [24,25].

The authors developed a multiscale simulation method for the spinning process by using the particle-based Lagrangian method and the dumbbell model recently [26]. However, realistic polymer melts used in the spinning process are more complex due, for example, to the effect of entanglements. In fact, entangled polymer melts are used to enhance the strength of the product in industrial cases. Based on the current situation mentioned above, the aim of this paper is to establish a multiscale simulation method for the spinning process of well-entangled polymer melts. In the present work, we therefore employ a more complex microscopic polymer model that describes well-entangled polymer melts called the slip-link model [27] and analyze the spinning process from both the macroscopic and microscopic viewpoints.

The content of this paper is as follows. In the next section, we describe our model for the melt spinning process at the macroscopic level (Section 2.1), the microscopic level (Section 2.2) and the multiscale simulation method (Section 2.3) separately. In Section 3, we present the result of our multiscale simulation. Finally, we give a conclusion in Section 4.

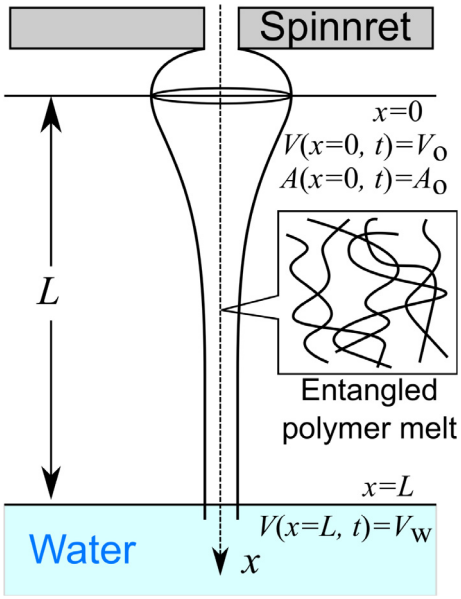

Fig. 1. Schematic view of the polymer melt spinning process.

2. Model of melt spinning

2.1. Macroscopic model

In the multiscale simulation of the polymer melt spinning process, we must connect the macroscopic flow behavior of the filament and the microscopic molecular motions. A schematic view of the polymer melt spinning process considered in this study is shown in Fig. 1. Here we briefly explain macroscopic equations; see our previous study for details [26]. To set up the macroscopic equations, we made the following assumptions.

(i) The shape of the filament is axi-symmetric.
(ii) The polymer chains are relaxed at the location where the diameter of the filament shows a maximum due to the die swelling effect.
(iii) The filament in the air gap region is isothermal.
(iv) The gravitational force, the surface tension between the polymer melt and the air, and the friction of the filament with the air are all neglected.
(v) The polymer filament is in the melt state just before reaching the surface of the cooling-water; just after it has gone into the water bath, it is solidified instantaneously by cooling.

A number of previous studies made assumptions (i) and (ii), (v) particularly in isothermal condition. However, the initial condition originating from assumption (ii) does not exactly fit with the condition in the real process because the flow history in the die is neglected. To obtain more practical solution, we must consider the shear flow in the die as shown in Refs [9,11]. Assumptions (iii) and (iv) appear to be strong for industrial applications. In particular, we should replace the isothermal assumption (iii) with the non-isothermal one to discuss crystallization and/or solidification. In principle, it is possible to consider the non-isothermal condition in our multiscale method by employing a microscopic polymer model that takes into account temperature change. However, the aim of this study is to assess the present multiscale simulation method because the industrial application of the multiscale simulation method has not yet been established. Therefore, it is suitable to make these assumptions in the present work.