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One-dimensional modeling of flat sheet casting or rectangular fiber spinning process and the effect of normal stresses

Youngdon Kwon*
Department of Textile Engineering
Sungkyunkwan University
300, Chunchun-dong, Jangan-gu, Suwon
Kyunggi-do 440-746, Korea

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Abstract

This study presents 1-dimensional simple model for sheet casting or rectangular fiber spinning process. In order to achieve this goal, we introduce the concept of force flux balance at the die exit, which assigns for the extensional flow outside the die the initial condition containing the information of shear flow history inside the die. With the Leonov constitutive equation that predicts non-vanishing second normal stress difference in shear flow, we are able to describe the anisotropic swelling behavior of the extrudate at least qualitatively. In other words, the negative value of the second normal stress difference causes thickness swelling much higher than width of extrudate. This result implies the importance of choosing the rheological model in the analysis of polymer processing operations, since the constitutive equation with the vanishing second normal stress difference is shown to exhibit the characteristic of isotropic swelling, that is, the thickness swell ratio always equal to the ratio in width direction.

Key words **:** flat sheet casting, rectangular fiber spinning, extrudate swell, Leonov model, force flux balance

1. Introduction

In modern plastics industry, the complexity of flow geometry combined with high Deborah number deformation rate yields highly nonlinear viscoelastic phenomena of polymeric liquid, which until now prohibited thorough interpretation and detailed mathematical modeling in view of fluid mechanics. This limitation in the study of non-Newtonian behavior may result from instability of numerical solutions in high Deborah number flows, computational impracticability under full 3D modeling, and so on. However, in such polymer processing operations as fiber spinning, flat sheet casting and film blowing processes, the flow geometry becomes the simplest due to some symmetry existent in product shape and deformation type.

Even though there have been many attempts to numerically solve those problems employing 2D or 3D formulation under the regime of Newtonian or viscoelastic flow (Crochet and Keunings, 1982; Caswell and Viriyayuthakorn, 1983; Bush *et al.*, 1984; Otsuki, *et al.*, 1997), their 1D modeling can also be found (Tanner, 1970; Pearson and Petrie, 1970). In this work, we model the flat sheet casting or rectangular fiber spinning process employing some simplifying assumptions for 1D formulation.

*Corresponding author: ydkwon@yurim.skku.ac.kr

Major problems associated with sheet or film casting (or rectangular fiber spinning) process are non-uniform distribution of film thickness along its width, instability of the process caused by draw resonance or melt fracture and formation of edge beads (Baird and Collias,1995). For their theoretical explanation, the process should be modeled in terms of full 3D formulation with evolutionary behavior inevitably taken into account in some cases. However, this type of analysis frequently meets with such difficulties as requirement of tremendous computation time and numerical instability especially in modeling high Deborah number flows. However, when one employs 1D formulation of steady state, there is usually no limit in the Deborah number, but he has to sacrifice interpretation of 2D, 3D or transient flow phenomena to this stable 1D solution.

In sheet casting and rectangular fiber spinning processes where the products possess high aspect ratio (width to thickness ratio), there exists another nonlinear viscoelastic phenomenon that the aspect ratio of the die does not always coincide with that of the product. In reality, the width of the sheet or the rectangular fiber does not change much in comparison with the size of the die width, while its thickness increases several times larger than that of the die due to extrudate swelling (it has been reported that the aspect ratio of the rectangular fiber often reduces to one fifth of that of the die (Kikutani *et al.*, 1998). Here we establish 1D formulation that possibly estimates this anisotropic swelling behavior of the extrudate quantitatively. For this purpose we employ the concept of force flux balance at the die exit, which contains the information of shear flow history accumulated inside the die. This idea of using balance equations has been already applied to the analysis of swelling of extrudate in the case of circular die (Choi *et al.*, 1998).

In our opinion, the anisotropy in swelling is caused by the non-vanishing second normal stress difference ($N_2<0$) in shear flow inside the die, i.e., its negative value incurs reduction of the sheet width in comparison with its thickness. In addition, by this simple analysis, we may be able to examine the role of the nonzero second normal stress difference quantitatively in polymer processing operations. For proper estimation of this effect, we choose the constitutive model that describes nonzero N_2 and then compare the result with the vanishing N_2 case. Since many viscoelastic constitutive equations predict the vanishing second normal stress difference in shear flow, on the basis of our result we hopefully evaluate the applicability of rheological models to process modeling.

2. Modeling of sheet extrusion or rectangular fiber spinning process

In order to appropriately describe viscoelastic behavior of polymeric fluid, the simplest version of the Leonov model (Leonov, 1976) is chosen, which has exhibited good coincidence with experimental data (Simhambhatla and Leonov, 1995) as well as sound character in view of mathematical stability (Kwon and Leonov, 1995). Then the total set of equations for incompressible media becomes

$$\rho\frac{d\mathbf{v}}{dt} = \nabla\cdot\boldsymbol{\sigma}+\rho\mathbf{g}, \quad \nabla\cdot\mathbf{v} = 0,$$

$$\boldsymbol{\sigma} = -p\boldsymbol{\delta}+\boldsymbol{\tau} = -p\boldsymbol{\delta}+\sum_{i=1}^{N} G_i\mathbf{c}^{(i)},$$

$$\overset{\nabla}{\mathbf{c}}^{(i)}+\frac{1}{2\theta_i}\left[(\mathbf{c}^{(i)})^2+\frac{I_2^{(i)}-I_1^{(i)}}{3}\mathbf{c}^{(i)}-\boldsymbol{\delta}\right] = \mathbf{0},$$

$$I_1^{(i)} = \mathrm{tr}\mathbf{c}^{(i)}, \quad I_2^{(i)} = \mathrm{tr}(\mathbf{c}^{(i)})^{-1}d, \quad \det\mathbf{c}^{(i)} = 1,$$

$$\overset{\nabla}{\mathbf{c}}^{(i)}+\frac{d\mathbf{c}^{(i)}}{dt}-(\nabla\mathbf{v})^T\cdot\mathbf{c}^{(i)}-\mathbf{c}^{(i)}\cdot(\nabla\mathbf{v}), \tag{1}$$

where ρ is the density, $\mathbf{v}$ the velocity vector, $\mathbf{g}$ the gravity, $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ are total and deviatoric stress tensors respectively, p is the isotropic pressure, $\boldsymbol{\delta}$ a unit tensor, $\mathbf{c}^{(i)}$ an elastic strain tensor in the i-th Maxwellian mode, *N* the total number of nonlinear Maxwell elements, $\overset{\nabla}{\mathbf{c}}^{(i)}$ an upper convected time derivative of $\mathbf{c}^{(i)}$, G_i and θ_i are elastic modulus and relaxation time of the i-th mode and tr is the trace operator. Note that this constitutive equation does not include any nonlinear parameter. In addition, it allows instantaneous elastic response or propagation of elastic shear wave, since it contains no retardation term.

The geometry of the flow considered herein is depicted in Fig.1, and it is supposedly divided into three deformation types: shear flow inside the die (region I), transitional flow near the die exit (region II), and extensional flow outside the die (region III). In this simple formulation, we assume that inside and outside the die the flow is isothermal, inertialess, incompressible and steady. The die is long enough for the flow to be fully developed ($L>>H_0$), i.e. entrance effect can be neglected. We also consider only the case where the width of the die is much greater than its height ($W_0>>H_0$) and thus the secondary flow near the edge of the die is assumed to be negligible. In the extensional flow outside the die, for the simple 1D approach we suppose that the extrudate profile varies slowly along the flow direction. Effects of gravity, surface tension and air drag outside the die are also ignored. However, effects of gravity, air drag and non-isothermality can be easily included in the formulation, and such inclusion has already been demonstrated for modeling fiber spinning process (Choi *et al.*, 1998).

In region II, the velocity distribution along the height starts to change just before the die exit. Then rapid rearrangement occurs immediately outside the die, and the velocity becomes almost uniform across the extrudate cross-section. The length of this transitional flow region is thought to be in the order of height ($2H_0$) of the die, and here by assumption the shear flow instantly transforms to the extensional flow. In order to take into account such transition, we employ and modify the procedure proposed by Choi *et al.* (1998).

2.1 Shear flow inside a wide slit die

When the Poiseuille flow through a wide slit die is steady and fully developed, the equation of motion determines non-vanishing components of the stress tensor as follows in a typical coordinate system shown in Fig.1:

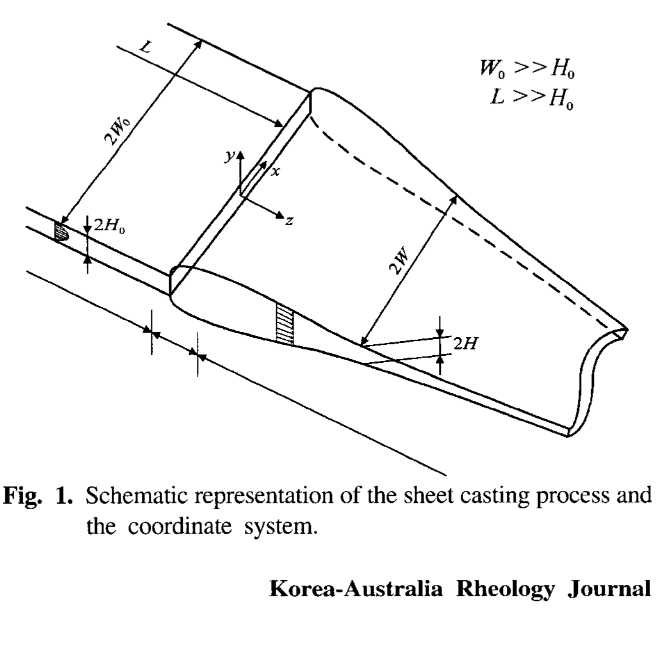


Fig. 1. Schematic representation of the sheet casting process and the coordinate system.

$$\tau = \begin{bmatrix} \tau_{zz} & \tau_{yz} & 0 \\ \tau_{yz} & \tau_{yy} & 0 \\ 0 & 0 & \tau_{xx} \end{bmatrix}, \quad \tau_{yz} = -\frac{P_0+\sigma_0}{L}y, \quad \left(\sigma_0 = \frac{F_0}{4W_0H_0},\right) \tag{2}$$

where z, y and x are flow, thickness and width directions respectively, P_0 is the pressure applied at the entrance to the slit, L the length of the die, and F_0 the applied stretching force.

The kinetic tensor relation in eqs.(1) yields simple algebraic solutions for $\mathbf{c}^{(i)}$tensor, whose explicit form for steady state can be written as

$$c_{zz}^{(i)} = \left[\frac{2\{1+(2\theta_i\dot{\gamma})^2\}}{1+\sqrt{1+(2\theta_i\dot{\gamma})^2}}\right]^{\frac{1}{2}},$$

$$c_{yy}^{(i)} = \left[\frac{2}{1+\sqrt{1+(2\theta_i\dot{\gamma})^2}}\right]^{\frac{1}{2}},$$

$$c_{yz}^{(i)} = \frac{2\theta_i\dot{\gamma}}{1+\sqrt{1+(2\theta_i\dot{\gamma})^2}}, \qquad c_{xx}^{(i)} = 1. \tag{3}$$

Here $\dot{\gamma} = dv_z/dy$ ($\dot{\gamma} < 0$) is the shear rate.

For simplicity, now we introduce dimensionless variables and parameters defined as

$$\xi = \frac{y}{H_0}, \quad \Gamma = \theta_1\dot{\gamma}, \quad \kappa_i = \frac{\theta_i}{\theta_1}, \quad \nu_i = \frac{G_i}{G_1},$$

$$\hat{v} = \frac{v_z\theta_1}{H_0}, \quad \langle\hat{v}\rangle = \frac{Q\theta_1}{4W_0H_0^2}, \quad \hat{\tau}_{yz} = -\frac{\tau_{yz}}{G_1},$$

$$\hat{\tau}_w = \hat{\tau}_{yz}\big|_{\xi=1}, \quad \hat{\tau}_{zz} = \frac{\tau_{zz}}{G_1}, \quad \hat{\tau}_{yy} = \frac{\tau_{yy}}{G_1}, \quad \hat{\tau}_{xx} = \frac{\tau_{xx}}{G_1} \tag{4}$$

where Q is the volumetric flow rate. Then, we can readily obtain the extrastress components in dimensionless form

$$\hat{\tau}_{zz} = \sum_i \hat{\tau}_{zz}^{(i)} = \sum_i \nu_i\left[\frac{2\{1+4\kappa_i^2\Gamma^2\}}{1+\sqrt{1+4\kappa_i^2\Gamma^2}}\right]^{\frac{1}{2}},$$

$$\hat{\tau}_{yy} = \sum_i \hat{\tau}_{yy}^{(i)} = \sum_i \nu_i\left[\frac{2}{1+\sqrt{1+4\kappa_i^2\Gamma^2}}\right]^{\frac{1}{2}},$$

$$\hat{\tau}_{yz} = \sum_i \hat{\tau}_{yz}^{(i)} = \sum_i \frac{2\nu_i\kappa_i\Gamma}{1+\sqrt{1+4\kappa_i^2\Gamma^2}},$$

$$\hat{\tau}_{xx} = \sum_i \hat{\tau}_{xx}^{(i)} = \sum_i \nu_i. \tag{5}$$

As one can see in eqs.(5), neither the first ($N_1 = \tau_{zz}-\tau_{yy}>0$) nor the second normal stress difference ($N_2 = \tau_{yy}-\tau_{xx}>0$) vanishes for this Leonov model.

In this approach to determine the flow history accumulated inside the die, we define following average quantities:

$$\langle\hat{v}\rangle = \int_0^1 \hat{v}_z(\xi)d\xi, \quad \langle\hat{v}_z\hat{\Psi}\rangle = \int_0^1 \hat{\Psi}\hat{v}_z(\xi)d\xi. \tag{6}$$

Here $\langle \hat{v}_z \hat{\Psi} \rangle$ is the dimensionless average flux of some dimensionless physical quantity $\hat{\Psi}$.

Eqs.(2), (4) and (5) substitute functions of dimensionless shear rate Γ for ξ and its differential

$$\xi = \frac{\hat{\tau}_{yz}(\Gamma)}{\hat{\tau}_w}, \quad \xi d\xi = \frac{\hat{\tau}_{yz}(\Gamma)}{\hat{\tau}_w^2}\varphi(\Gamma)d\Gamma, \tag{7}$$

where $\varphi(\Gamma)$ is in the form of

$$\varphi(\Gamma) = 2\sum_i \nu_i\kappa_i(1+4\kappa_i^2\Gamma^2)^{-1/2}(1+\sqrt{1+4\kappa_i^2\Gamma^2})^{-1}. \tag{8}$$

Then eqs.(6) become

$$\langle\hat{v}\rangle = \frac{1}{2}\left[\Gamma_w - \frac{1}{\hat{\tau}_w^3}\int_0^{\Gamma_w}\hat{\tau}_{yz}^3 d\Gamma\right],$$

$$\langle\hat{v}_z\hat{\Psi}\rangle = \frac{1}{\hat{\tau}_w}\int_0^{\Gamma_w}\hat{\Psi}(\Gamma)\hat{v}_z^*(\Gamma)\varphi(\Gamma)d\Gamma, \tag{9}$$

where Γ_w is the dimensionless shear rate at the die wall ($\xi = \pm 1$). The velocity distribution expressed in terms of Γ is

$$\hat{v}_z(\xi) = \hat{v}_z^*(\Gamma) = \frac{1}{2\hat{\tau}_w}\sum_i \frac{\nu_i}{\kappa_i}\ln\left(\frac{1+\sqrt{1+4\kappa_i^2\Gamma_w^2}}{1+\sqrt{1+4\kappa_i^2\Gamma_w^2}}\right). \tag{10}$$

Hence, we can calculate some average quantity of flow history inside the die, whenever the shear rate is given.

2.2 Extensional flow of the extrudate

The coordinate axes and the variables specified in this formulation are illustrated in Fig.1. We again define following new variables and parameters necessary for description of the state outside the die:

$$w = \frac{W}{W_0}, \quad h = \frac{H}{H_0}, \quad \hat{z} = \frac{z}{L}, \quad \langle\hat{v}\rangle = \frac{Q\theta_1}{4W_0H_0^2},$$

$$\hat{v}_z = \frac{\theta_1}{H_0}v_z = \frac{4\langle\hat{v}\rangle}{wh}, \quad \hat{\sigma}_{zz} = \hat{\tau}_{zz} - \hat{\tau}_{yy} = \frac{\hat{\sigma}_0}{hw},$$

$$\hat{\sigma}_0 = \frac{F_0}{4G_1W_0H_0}. \tag{11}$$

Here w and h express width and thickness variations along the flow direction respectively, v_z is the axial velocity, and $\hat{\sigma}_{zz}$ actual dimensionless normal stress on the extrudate cross-section acting in flow direction.

Due to assumed uniformity of variables over the cross-section of extrudate and negligible variation of extrudate profile along the flow direction ($|dW/dz| \ll 1$ and $|dH/dz| \ll 1$), $\mathbf{c}^{(i)}$ can be approximated to be diagonal and all the quantities may be represented as functions only of axial distance z. Then the relations (1) reduce to

$$\mathbf{c}^{(i)} = \begin{bmatrix} c_{zz}^{(i)} & 0 & 0 \\ 0 & c_{yy}^{(i)} & 0 \\ 0 & 0 & c_{xx}^{(i)} \end{bmatrix}, \quad \begin{matrix} \hat{\sigma}_{zz} = \sum_i \nu_i (c_{zz}^{(i)} - c_{yy}^{(i)}) = \dfrac{\hat{\sigma}_0}{hw}, \\ \hat{\sigma}_{xx} = \sum_i \nu_i (c_{xx}^{(i)} - c_{yy}^{(i)}) = 0, \end{matrix}$$

$$\hat{v}_z \frac{dc_{zz}^{(i)}}{d\hat{z}} + 2\hat{v}_z c_{zz}^{(i)} \left(\frac{1}{w}\frac{dw}{d\hat{z}} + \frac{1}{h}\frac{dh}{d\hat{z}} \right) + \frac{L}{2H_0\kappa_i} \times$$

$$\left[(c_{zz}^{(i)})^2 + \frac{I_2^{(i)} - I_1^{(i)}}{3} c_{zz}^{(i)} - 1 \right] = 0,$$

$$\hat{v}_z \frac{dc_{yy}^{(i)}}{d\hat{z}} - 2\hat{v}_z c_{yy}^{(i)} \frac{1}{h}\frac{dh}{d\hat{z}} + \frac{L}{2H_0\kappa_i} \times$$

$$\left[(c_{yy}^{(i)})^2 + \frac{I_2^{(i)} - I_1^{(i)}}{3} c_{yy}^{(i)} - 1 \right] = 0,$$

$$\hat{v}_z \frac{dc_{xx}^{(i)}}{d\hat{z}} - 2\hat{v}_z c_{xx}^{(i)} \frac{1}{w}\frac{dw}{d\hat{z}} + \frac{L}{2H_0\kappa_i} \times$$

$$\left[(c_{xx}^{(i)})^2 + \frac{I_2^{(i)} - I_1^{(i)}}{3} c_{xx}^{(i)} - 1 \right] = 0, \tag{12}$$

where $I_1^{(i)} = c_{xx}^{(i)} + c_{yy}^{(i)} + c_{zz}^{(i)}$, $I_2^{(i)} = \dfrac{1}{c_{xx}^{(i)}} + \dfrac{1}{c_{yy}^{(i)}} + \dfrac{1}{c_{zz}^{(i)}}$ and

$c_{xx}^{(i)} c_{yy}^{(i)} c_{zz}^{(i)} = 1.$

The above three differential equations combined with two stress relations in (12) constitute a closed set for this problem. Hence, as soon as initial values $c_{xx}^{(i)}$ $(\hat{z} = 0)$, $c_{yy}^{(i)}$ $(\hat{z} = 0)$, $c_{zz}^{(i)}$ $(\hat{z} = 0)$, and $w(\hat{z} = 0)$, $h(\hat{z} = 0)$ are assigned, we can determine subsequent profile of the extrudate and stress variation along the flow direction. Now we establish the scheme for obtaining the initial condition, using some concept of force flux balance.

2.3 Formulation of initial conditions

In this section, we take the transitional flow into consideration. The initial condition that has to be supplied for solving eqs.(12) still remains unknown. For convenience, we denote the initial values of variables at die exit as

$$w|_{z=0} = w_0,\ h|_{z=0} = h_0,\ c_{xx}^{(i)}|_{z=0} = (c_{xx}^{(i)})_0,\ \ c_{yy}^{(i)}|_{z=0} = (c_{yy}^{(i)})_0,$$

$$c_{zz}^{(i)}|_{z=0} = (c_{zz}^{(i)})_0. \tag{13}$$

w_0 and h_0 which are not unit in general, designate sudden changes in width and thickness of extrudate at die exit due to instantaneous elastic response. This instantaneous deformation of extrudate can be justified by the following argument. Since the constitutive equation does not include any retardation term, it allows immediate elastic response. Therefore when the material is released from its constraint (the die wall) at the exit, on the basis of this hypothesis it instantaneously expands (or may shrink) to achieve $w = w_0$ and $h = h_0$. In the real situation, this kind of instant elasticity is suppressed due to the existence of surface tension and inertia. When the material shows much slower elastic response, we think its behavior has to be described by the constitutive equation with a retardation term. Then the above type of quick elastic response will be restrained. With little modification, the procedure developed hereafter can also be used for the viscoelastic model with a Newtonian viscous term. From now on, modifying the method employed in the paper by Choi *et al.* (1998), we develop mathematical procedure, which provides the initial values to express the information of shear flow history.

In the Leonov model, the extra-stress tensor implies the elastic strain assigned during the flow. Hence, we here assume that via instantaneous elastic swelling near die exit the rheological stress in shear flow is transformed to the stress in extensional flow and the isotropic pressure relaxes independently. Following transformation of the force flux that has been formulated in the work by Choi *et al.* (1998), is now introduced:

$$\hat{v}_z \hat{\tau}^- = \langle \hat{v} \rangle \mathbf{F} \cdot \hat{\tau}^+ \cdot \mathbf{F}^T. \tag{14}$$

Here $\hat{\tau}^- = \sum_{i=1}^{N} (\hat{\tau}^{(i)})^-$ and $\hat{\tau}^+ = \sum_{i=1}^{N} (\hat{\tau}^{(i)})^+$ are the stress tensors in the shear flow inside the die and in the extensional flow outside it, respectively. In order to describe equilibrium swell ratio of cylindrical extrudate, similar transformation was introduced by Tanner (1970) not for force flux but for force balance. **F** and $\mathbf{F}^T$ are appropriate transformation matrix and its transpose.

In the most general axisymmetric (non-twisting) deformation, when we denote {z', y', x'} and {z, y, x} as the coordinate systems before and after instantaneous swelling respectively, the relation between the coordinates and **F** become

$$\left\{ \begin{matrix} z' = w_0 h_0 z + b(y) \\ y' = y/h_0 \\ x' = x/w_0 \end{matrix} \right\}, \quad F = \begin{bmatrix} w_0 h_0 & b'(y) & 0 \\ 0 & 1/h_0 & 0 \\ 0 & 0 & 1/w_0 \end{bmatrix},$$

$$\begin{bmatrix} \hat{v}_z \hat{\tau}_{zz}^- & \hat{v}_z \hat{\tau}_{yz}^- & 0 \\ \hat{v}_z \hat{\tau}_{yz}^- & \hat{v}_z \hat{\tau}_{yy}^- & 0 \\ 0 & 0 & \hat{v}_z \hat{\tau}_{xx}^- \end{bmatrix} = \langle \hat{v} \rangle \begin{bmatrix} w_0 h_0 & b'y & 0 \\ 0 & 1/h_0 & 0 \\ 0 & 0 & 1/w_0 \end{bmatrix} \times$$

$$\begin{bmatrix} \hat{\tau}_{zz}^+ & 0 & 0 \\ 0 & \hat{\tau}_{yy}^+ & 0 \\ 0 & 0 & \hat{\tau}_{xx}^+ \end{bmatrix} \begin{bmatrix} w_0 h_0 & 0 & 0 \\ b'(y) & 1/h_0 & 0 \\ 0 & 0 & 1/w_0 \end{bmatrix}. \tag{15}$$

Here b(y) takes account of shearing deformation during transition, and b' = db/dy. In the case of extrudate swell for a capillary die (Choi *et al.*, 1998), the above type of transformation was not possible since $\tau_{xx}^- \neq \tau_{yy}^-$. However, it is not only valid for this geometrical system but also naturally gives rise to anisotropy of swelling in width and thickness directions (that is, $w_0 \neq h_0$ in general, and subsequently

$w \neq h$). Just for the comparison with the constitutive equation that predicts $N_2=0$ in shear flow, we intentionally modify the tensor $\mathbf{c}^{(i)}$ under the condition of incompressibility det $\mathbf{c}^{(i)}=1$ to give $\tau_{xx}^{-} = \tau_{yy}^{-}$. Then, we have

$$\det\begin{bmatrix} c_{zz}^{(i)} & c_{yy}^{(i)} & 0 \\ c_{yy}^{(i)} & \bar{c}^{(i)} & 0 \\ 0 & 0 & \bar{c}^{(i)} \end{bmatrix} = 1, \quad (\bar{\tau}^{(i)} = v_i \bar{c}^{(i)}). \tag{16}$$

Here $\bar{\tau}^{(i)}$ is the modified dimensionless stress component for normal stresses $(\tau_{yy}^{(i)})^{-}$ and $(\tau_{xx}^{(i)})^{-}$ in the *i*-th Maxwellian mode, and its explicit form becomes

$$\bar{\tau}^{(i)} = \frac{1}{2(\hat{\tau}_{zz}^{(i)})^{-}}\{[(\hat{\tau}_{yz}^{(i)})^{-}]^2 + \sqrt{[(\hat{\tau}_{yz}^{(i)})^{-}]^4 + 4v_i^3(\hat{\tau}_{zz}^{(i)})^{-}}\},$$

$$\bar{\tau} = \sum_{i=1}^{N}(\bar{\tau}^{(i)}). \tag{17}$$

Hence, we imply that $\bar{\tau}$ is substituted for both $\hat{\tau}_{yy}^{-}$ and $\hat{\tau}_{xx}^{-}$ in eq.(15), when we mention the formulation with the constitutive model that predicts $N_2=0$ in shear flow.

With the aid of eqs.(15), we are now able to compute $\hat{\tau}_{xx}^{+}$, $\hat{\tau}_{yy}^{+}$, $\hat{\tau}_{zz}^{+}$, w_0 and h_0, all of which contain the information of the flow history inside the die. However, we require that they be independent of y. Hence, we make an average of the quantities by integrating them over the cross-section of the extrudate (see eqs.(9)) as follows:

$$\langle\hat{\tau}_{xx}\rangle^{+} = \frac{\langle \hat{V}_z\hat{\tau}_{xx}\rangle^{-}}{\langle\hat{v}\rangle}w_0^2,\ \langle\hat{\tau}_{yy}\rangle^{+} = \frac{\langle \hat{V}_z\hat{\tau}_{xx}\rangle^{-}}{\langle\hat{v}\rangle}h_0^2,$$

$$\langle\hat{\tau}_{zz}\rangle^{+} = \frac{1}{\langle\hat{v}\rangle}\left\langle\hat{v}_z\left[\hat{\tau}_{zz} - \frac{\hat{\tau}_{yz}^2}{\hat{\tau}_{yy}}\right]\right\rangle^{-}\frac{1}{w_0^2h_0^2} \tag{18}$$

$$\text{with}\quad b'(y) = \frac{\hat{\tau}_{yz}^{-}}{\hat{\tau}_{yy}^{-}}\frac{1}{h_0}. \tag{19}$$

There also exist outside the die force balance relations such as

$$\langle\hat{\tau}_{zz}\rangle^{+} - \langle\hat{\tau}_{yy}\rangle^{+} = \frac{\hat{\sigma}_0}{w_0h_0},\quad \langle\hat{\tau}_{zz}\rangle^{+} - \langle\hat{\tau}_{yy}\rangle^{+} = 0. \tag{20}$$

Now, eqs.(18) and (20) constitute a nonlinear relation for w_0 and h_0 which express the instantaneous swelling of extrudate in the inertialess approach. However, we require *N* more sets of relations to calculate 3*N* unknown initial values $(c_{xx}^{(i)})_0$, $(c_{yy}^{(i)})_0$, $(c_{zz}^{(i)})_0$. They may be established if we introduce additional assumption of force flux balance valid in each Maxwellian element. We repeat the above procedure for the individual Maxwell element. Note that at the die lip after the instantaneous swelling (hence the flow is approximated to be extensional) the shear stress component in the individual Maxwell element may become non-zero in general, even though the total shear stress vanishes, i.e., $(\hat{\tau}_{yz}^{(i)})^{+} = 0$ or, $(\hat{\tau}_{yz}^{(i)})^{+} \neq 0$, but $\hat{\tau}_{yz}^{(+)} = \sum_i(\hat{\tau}_{yz}^{(i)})^{+} = 0$.

Applying the previous transformation, we have

$$\hat{v}_z(\hat{\tau}^{(i)})^{-} = \langle\hat{v}\rangle\mathbf{F}\cdot(\hat{\tau}^{(i)})^{+}\cdot\mathbf{F}^{T} \tag{21}$$

where $\mathbf{F}$ has the same form with that in eq.(15). Then, after integration over the cross-section, the resultant relations of assumed force flux balance in each mode reduce to

$$\langle\hat{\tau}_{xx}^{(i)}\rangle^{+} = \frac{w_0^2}{\langle\hat{v}\rangle}\langle\hat{v}_z\hat{\tau}_{xx}^{(i)}\rangle^{-},\quad \langle\hat{\tau}_{yy}^{(i)}\rangle^{+} = \frac{h_0^2}{\langle\hat{v}\rangle}\langle\hat{v}_z\hat{\tau}_{yy}^{(i)}\rangle^{-},$$

$$\langle\hat{\tau}_{yz}^{(i)}\rangle^{+} = \frac{1}{w_0\langle\hat{v}\rangle}\langle\hat{v}_z(\hat{\tau}_{yz}^{(i)} - h_0b'\hat{\tau}_{yy}^{(i)})\rangle^{-},$$

$$\langle\hat{\tau}_{zz}^{(i)}\rangle^{+} = \frac{1}{w_0^2\langle\hat{v}\rangle}\left\langle\hat{v}_z\left(\frac{\hat{\tau}_{zz}^{(i)}}{h_0^2} - 2\frac{b'}{h_0}\hat{\tau}_{yz}^{(i)} + (b')^2\hat{\tau}_{yy}^{(i)}\right)\right\rangle^{-},$$

$$v_i[(c_{zz}^{(i)})_0 - (c_{yy}^{(i)})_0] \approx \langle\hat{\tau}_{zz}^{(i)}\rangle^{+} - \langle\hat{\tau}_{yy}^{(i)}\rangle^{+},$$

$$v_i[(c_{yy}^{(i)})_0 - (c_{xx}^{(i)})_0] \approx \langle\hat{\tau}_{yy}^{(i)}\rangle^{+} - \langle\hat{\tau}_{xx}^{(i)}\rangle^{+},$$

$$\hat{\tau}_{yz}^{(i)} \approx 0,\ (c_{xx}^{(i)})_0(c_{yy}^{(i)})_0(c_{zz}^{(i)})_0 = 1$$

$$\text{for } i=1, \cdots, N. \tag{22}$$

Here b' is written in eq.(19). The solution of eqs.(12) with initial conditions (13) given by eqs.(18-20) and (22) now provides the extrudate profile $w(\hat{z})$ and $h(\hat{z})$ as well as stress distribution.

3. Results and discussion

In this section, we demonstrate the result of model calculation. Since at this point we are not supplied with any complete set of experimental data, its coincidence with experiments is not tested. In the example of computation polyethylene is chosen, of which the standard viscoelastic data have been given by Garcia-Rejon *et al.* (1981), and the linear viscoelastic spectrum has been determined by Choi *et al.* (1998) and it is listed in Table 1.

In Fig. 2, the normal stress differences with respect to shear rate are illustrated. Each values of stress for corresponding shear rate are characteristic of the constitutive equation, and here the Leonov model exhibits monotonic increase of both the quantities (N_1 and $-N_2$). In the region of high shear rate as the shear rate increases, N_1 becomes approximately proportional to shear rate $\dot{\gamma}$, but $-N_2$ approaches the constant value $\sum_i G_i$. Hence the ratio $|N_2/N_1|$ is about 1/10 in the low shear rate, but in the region of high shear it reaches 1/100 and then decreases further to zero. A few experimental observations have reported that $N_1>0$, $N_2<0$, and $|N_2/N_1| \approx 0.1$ possibly in the low shear rate (e.g. see the book by Leonov, 1994). Hence when we assume that these facts are valid in the whole region of deformation rate, the Leonov model may underestimate $-N_2$

Table 1. Linear viscoelastic parameters for polyethylene (Choi *et al.*, 1998).

G_i (Pa)	θ_i (sec)	ν_i	κ_i
1400	22	1	1
4000	5.5	2.86	0.25
10600	0.95	7.57	0.043
26000	0.1698	18.57	0.0077
120000	0.12266	85.71	0.0056

in high shear.

The result of computation is shown in Figs. 3 and 4 in two cases of free swelling ($\sigma_0 = 0$) and stretching the extrudate ($\sigma_0 = 6000$ Pa), respectively. We assigned 1 m and 1 mm for width and height of the die. The shear rate at the wall is 105 sec^{-1}, and thus the volumetric flow rate becomes 4 cm^3/sec. In the figures, solid lines represent the results for the original constitutive model ($N_2<0$), and dotted lines denote the cases for the modified constitutive model ($N_2 = 0$). From Figs. 3(a) and 4(a) it can be clearly seen that the extrudate becomes much wider when the constitutive equation describes the vanishing second normal stress difference.

In Fig. 3(b) and 4(b), the detailed evolutionary behavior of the dimensionless parameters can be examined. When $N_2 = 0$, the value of dimensionless thickness becomes always equal to that of width, and thus the aspect ratio (width to thickness ratio) of the extrudate remains always the same with that of the die. However, when the model predicts nonzero second normal stress difference, the thickness swelling is much higher than the width swelling. Hence the reduction of aspect ratio of the extrudate is clearly manifested. In our case, the aspect ratio of extrudate decreases to about half of that of the die.

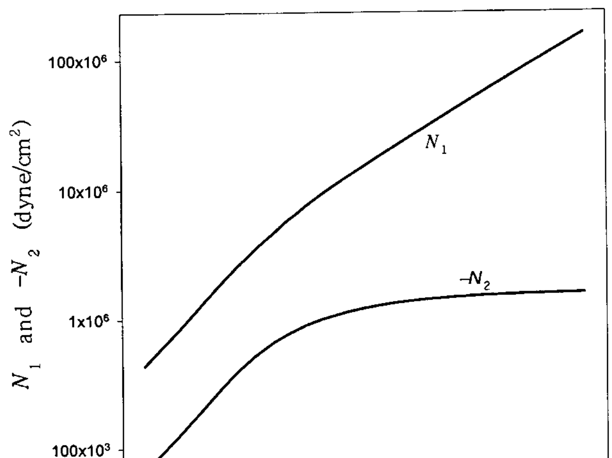
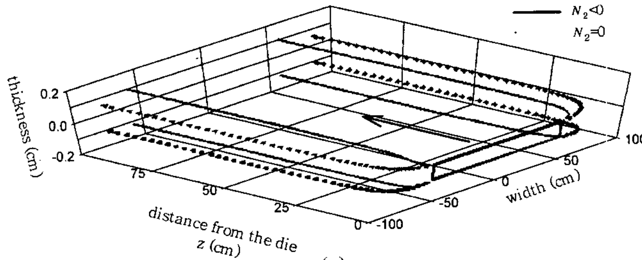
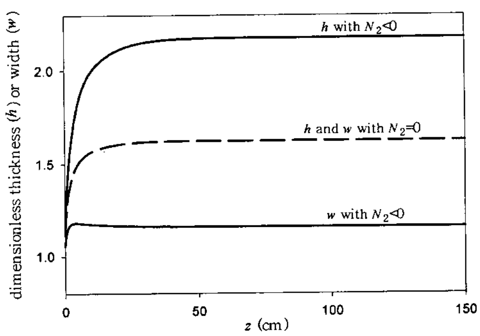


Fig. 2. The first (N_1) and the second normal stress differences ($-N_2$) as functions of shear rate.

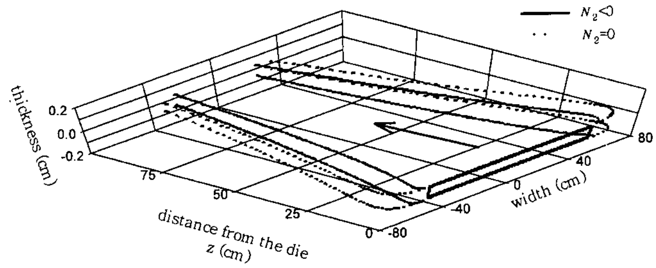


(a)

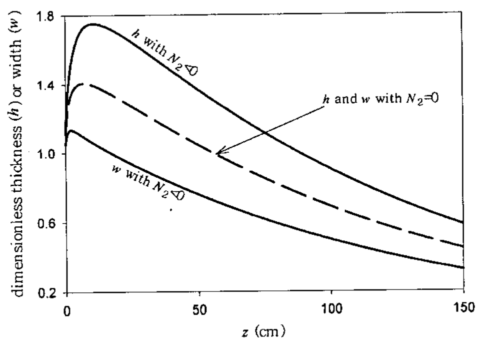


(b)

Fig. 3. Extrudate profile (a) and dimensionless thickness and width (b) in the case of free swelling.



(a)



(b)

Fig. 4. Extrudate profile (a) and dimensionless thickness and width (b) in the case of stretching ($\sigma_0 = 6000$ Pa)

Fig.5 shows equilibrium swell ratios ($\sigma_0 = 0$) of extrudate thickness and width with respect to shear rate at the wall. While the thickness exhibits strong dependence on shear rate, the width of the extrudate varies little. Hence this anisotropy of swelling becomes more severe as the shear rate or the flow rate increases. From the previous results depicted in Figs.3 and 4, it can be stated that the negative value of the second normal stress difference incurs this anisotropic behavior. Therefore, the significant reduction of the aspect ratio in manufacturing rectangular fibers can also be explained at least qualitatively. In our modeling we employed the simplest version of the Leonov model, and it may assign too low value for $-N_2$ in high shear rate region as shown in Fig.2. If the real polymeric fluid exhibits higher $-N_2$, then this anisotropic swelling is expected to be more dominant and thus the reduction of the aspect ratio of the sheet becomes more distinct.

The description of N_2 becomes different for every rheological model, and many viscoelastic constitutive equations predict even vanishing second normal stress difference in shear flow. Thus the behavior of extrudate swelling in sheet casting or rectangular fiber spinning process is strongly dependent on the nature of the constitutive model chosen for analysis. This again reflects the importance of the proper choice of the rheological model for process modeling.

The model developed in this study to account for evolutionary behavior of extrudate swelling in sheet casting and rectangular fiber spinning processes can easily be extended to include such effects as gravity, inertia, non-isothermality and air friction, when we employ the same procedure presented in the work by Choi *et al.* (1998). Therefore this formulation can be readily applied to the analysis of real polymer processing or fiber manufacturing operations (presumably in some restricted type of flow geometry). In addition, it may be utilized to indirectly estimate the approximate value of N_2 in the viscoelastic flow through a wide slit channel.

4. Conclusions

Here we suggest 1D simple model to describe the evolution of extrudate in the flat sheet casting or rectangular fiber spinning process. For proper expression of viscoelastic behavior of polymeric fluid, it employs the simplest Leonov constitutive equation, which predicts the non-vanishing second normal stress difference in shear flow. For 1D modeling we assume that the flow is extensional outside the die. Then in order to obtain initial values that contain the information of deformation history inside the die, we use the concept of force flux balance at the die exit where the transition from shear to extensional flow occurs.

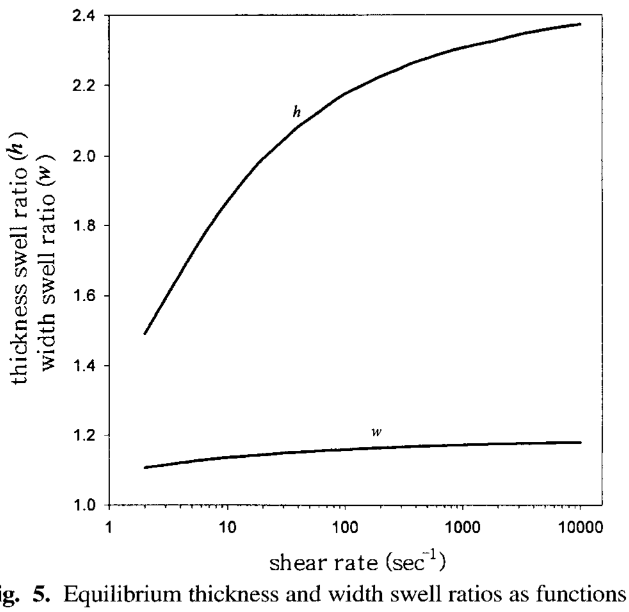


Fig. 5. Equilibrium thickness and width swell ratios as functions of shear rate at the wall.

The calculation of equations shows strong effect of the second normal stress difference on the evolution of extrudate profile. The result describes large increase in sheet thickness and small increase in width, and the second normal stress difference induces this relative reduction of width swell ratio. Such anisotropy in swelling is manifested for both cases of free swelling and stretching of extrudate, and it coincides with real observations in film casting and rectangular fiber spinning at least qualitatively. Many viscoelastic constitutive equations predict the vanishing second normal stress difference in shear flow. Hence on the hypothesis of our formulation, such models will predict no change in aspect ratio of extrudate, which contradicts experimental facts. Therefore, it can be stated that the appropriate choice of the constitutive model seems crucial for successful analysis of complex industrial processes.

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