Numerical Simulation of Viscoelastic Flow in Three-Dimensional Rectangular Abrupt Contraction Channels

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Abstract

Numerical simulation of viscoelastic flow in two three-dimensional (3-D) rectangular abrupt contraction channels was carried out using the Giesekus model. The HSMAC (Highly Simplified Marker and Cell) scheme was applied to solve the discretized basic equations. 3-D flow patterns and the distribution of vortex size were investigated to elucidate 3-D flow property. Several 3-D flow phenomena such as a spiral flow were predicted. The effect of wall was strong when the aspect ratio of the channel (width/height) was small, and the 3-D flow behavior was notable near the channel wall: the vortex size drastically changed near the wall.

Keywords: viscoelastic fluid; three-dimensional flow; Giesekus model; abrupt contraction; numerical simulation

1. Introduction

Viscoelastic flows frequently appear in industrial process, and sometimes the flow behavior in three-dimensional geometry is important. For example, three-dimensional flow is often observed in polymer processing such as injection molding of complex-shaped products.

In experimental study [1-5], some interesting three-dimensional flow structures were observed. The authors measured velocity response in start-up flow of polymer solutions in a planar contraction channel with a laser-Doppler velocimetry and found some transient behaviors of three-dimensional flow profile near the contraction[6]. The mechanism of the flow behavior, however, has not been completely revealed. This fact motivated the authors to perform a three-dimensional numerical simulation.

Numerical simulation of viscoelastic flow is an effective method for understanding three-dimensional viscoelastic flow, and is helpful for analyzing experimental results and for revealing the flow mechanism. Unfortunately, three-dimensional numerical analysis requires great computational resources, and was not carried out easily. However, because of recent progress in computational performance, three-dimensional analysis has been available. For example, contraction flows [7-11], expansion flows [12], and stagnation flows [13] were numerically studied.

In the present study, the viscoelastic flow in two rectangular contraction channels was numerically calculated using the Giesekus model [14] as a constitutive equation and three-dimensional flow patterns such as three-dimensional path lines and the distribution of vortex size were mainly studied. The Giesekus model can describe typical rheological property of polymeric liquids and has been used in many numerical flow analyses [15-22]. The HSMAC (Highly Simplified Marker and Cell) scheme based on the finite difference method was applied for the calculation.

2. Basic Equations

Three-dimensional incompressible viscoelastic flow was considered. The basic equations consist of the equation of continuity (1), the equation of motion (2), and a constitutive equation (3)-(5).

\[ \nabla \cdot \mathbf{v} = 0, \quad (1) \]

\[ \rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) - \nabla \cdot (p \mathbf{I} + \mathbf{T}) = 0, \quad (2) \]

where \( \mathbf{v} \) is the velocity vector, \( \rho \) the fluid density, \( p \) the isotropic pressure, \( \mathbf{r} \) the extra stress tensor, \( \mathbf{I} \) the unit tensor. In the present simulation, the Giesekus model was applied:

\[ \mathbf{T} = \mathbf{T}_s + \mathbf{T}_p, \quad (3) \]

\[ \mathbf{T}_s = \eta_s (\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad (4) \]

\[ \mathbf{T}_p + \lambda \frac{\mathbf{v}}{\eta_p} + \alpha \mathbf{T}_p = \eta_p (\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad (5) \]

where \( \tau_s \) and \( \tau_p \) are solvent and polymer contributions to \( \tau \), respectively. \( \eta_s \) and \( \eta_p \) are solvent and polymer contributions to the zero-shear-rate viscosity, \( \eta_0 = \eta_s + \eta_p \), \( \lambda \) the relaxation time, and \( \alpha \) the mobility factor.
indicates the upper-convected derivative of a tensor, $T$, and is defined by

$$\nabla \cdot \frac{\partial T}{\partial t} + v \cdot \nabla T - \nabla v^T \cdot T - T \cdot \nabla v. \quad (6)$$

The Giesekus model is a constitutive equation based on the dumbbell theory considering anisotropic drag. This model adequately describes rheological behavior of polymeric liquids. Figure 1 shows dimensionless shear viscosity, $\eta/\eta_0$, the dimensionless first normal stress coefficient, $\psi_1/(2\eta_0(1-\epsilon)\lambda)$, versus dimensionless shear rate, $\dot{\gamma}$, and dimensionless uniaxial elongational viscosity, $\eta_E/(3\eta_0)$, versus dimensionless elongational rate, $\dot{e}$, at $\epsilon=0.5$ and $\alpha=0.1$

The basic equations were non-dimensionalized in terms of $v^* = V v^*/v^*$, $\tau^* = (\eta_0 V/H) \tau^*$, $p^* = (\eta_0 V/H) p^*$, $t^* = (H/V) t^*$, $\tau_s^* = (\eta_0 V/H) \tau_s^*$, $\tau_p^* = (\eta_0 V/H) \tau_p^*$, and $\nabla = (1/H) \nabla^*$, where $V$ and $H$ are characteristic velocity and length. In the present analysis, $V$ is the mean velocity at the entrance, and $2H$ is the channel height. The variables with the superscript `*' are non-dimensional. The non-dimensionalized basic equations are as follows:

$$\nabla^* \cdot v^* = 0, \quad (7)$$

$$\frac{\partial v^*}{\partial t^*} + (v^* \cdot \nabla^*) v^* =$$

$$-\frac{1}{Re} \left\{ \nabla^* p^* - \epsilon \nabla^* v^* \right\} \cdot (1-\epsilon) \nabla^* \cdot \tau_p^* \right\}, \quad (8)$$

$$\tau^* = \epsilon \tau_s^* + (1-\epsilon) \tau_p^* \right\}, \quad (9)$$

$$\tau_s^* = \nabla^* v^* + (\nabla^* v^*)^T, \quad (10)$$

$$\tau_p^* + \text{We} (\tau_p^* + \alpha \tau_p^* \cdot \tau_p^*) = \nabla^* v^* + (\nabla^* v^*)^T. \quad (11)$$

Non-dimensional groups in the above equations, that is, the Reynolds number, $Re$ and the Weissenberg number, $We$ are defined by $Re = \rho V H/\eta_0$ and $We = \lambda V/H$. For simplification of the notation, the superscript `*' is omitted hereafter.

3. Numerical Method

The non-dimensionalized basic equations (7)–(11) were rewritten in component of the Cartesian coordinate system, and were discretized for numerical calculation. The equations were discretized in time with the forward difference method and in space with the central difference method. Moreover, the second order upwind difference scheme was applied to the convection terms in Eqs. (8) and (11).

The HSMAC method was used to solve the equations. The computational domain was divided using a staggered grid. The stress, $\tau_p$, and the pressure, $p$, were defined at the center of the grid cell, and the velocity components were defined at the center of the grid face as shown in Fig.2. $(\tau_p)_{ij}$ means the $ij$th component of $\tau_p$. $u$, $v$, and $w$ are the $x$, $y$, and $z$ components of $v$, respectively. The schematic diagram of the rectangular abrupt contraction channel used in the present simulation is shown in Fig.3. The coordinate system is also defined in the figure. The origin is placed at the center of the contraction plane. In the following discussion, the wall perpendicular to the $y$ axis, and that to the $z$ axis are described as bottom wall and side wall, respectively. Step plane denotes the wall in the contraction plane.
In the present study, two channels were considered: they have the same contraction ratio, \( H:h=4:1 \) (\( H=1 \) and \( h=0.25 \)) and are different in channel width, \( W \). One is a 4:1:2 contraction channel (\( H:h:W=4:1:2 \)) and the other is a 4:1:4 contraction channel (\( H:h:W=4:1:4 \)). The former is called channel A and the latter channel B. The channel length of the upstream part, \( L_1 \), is 16\( h \), and that of the downstream part, \( L_2 \), is 64\( h \).

The channel geometry is symmetric, then, the calculation was carried out for a quarter region to save computational costs. The mesh for channel A is shown in Fig.4. The channel is uniformly divided in the \( z \) direction and non-uniformly in both the \( x \) and \( y \) directions; The mesh is finer near the contraction plane than the other region. The mesh for channel B was created in the same manner.

The boundary conditions for the numerical simulation are as follows: a non-slip condition on the channel wall, zero normal velocities and zero tangential velocity gradients on the symmetry plane, a fully developed flow condition on the entrance, and a Neumann condition for all velocity components, \( \partial u/\partial x = 0, \partial v/\partial x = 0, \partial w/\partial x = 0 \), on the exit. Stress components on the entrance were given by solving the constitutive equation numerically.

### 4. Results and Discussion

Firstly, three-dimensional path lines are drawn to show the outline of the flow. Figure 5 shows three-dimensional path lines of the viscoelastic flow in channel A at \( Re=10, We=0.1, \varepsilon=0.5, \) and \( \alpha=0.1 \). Start points for particle tracking in main flow are \( (x, y, z) = (-3, -0.1, 0.1), (-3, -0.5, 0.4), (-3, -0.8, 0.4) \) for left figure and \( (x, y, z) = (-3, -0.1, 0.1), (-3, -0.5, 0.1), (-3, -0.8, 0.1), (-3, -0.8, 0.25), (-3, -0.8, 0.4) \) for right figure.

In the viscoelastic flows in both channel A and B, path lines of the main flow in the upstream channel inclined towards the symmetric plane (\( z=0 \)). The path lines begin to incline gently near the upstream ends of them and leaned notably near the contraction. This phenomena is also recognized from Fig.8. The figure shows the distribution of flow rate in the \( x \) direction. In the figure, broken lines mean the results for Newtonian flows at \( Re=10 \). \( Q \) is total flow rate and \( q_i \) is the flow rate through the region \( i \) which is defined in Fig.9: the cross section of the channel is symmetric, then, the calculation was carried out for a quarter region to save computational costs. The mesh for channel A is shown in Fig.4. The channel is uniformly divided in the \( z \) direction and non-uniformly in both the \( x \) and \( y \) directions; The mesh is finer near the contraction plane than the other region. The mesh for channel B was created in the same manner.

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Fig. 6: Three-dimensional path lines of Newtonian flow in channel A at $Re=10$. Start points for particle tracking in main flow are $(x, y, z) = (-3, -0.1, 0.1), (-3, -0.1, 0.25), (-3, -0.1, 0.4), (-3, -0.5, 0.4), (-3, -0.8, 0.4)$ for left figure and $(x, y, z) = (-3, -0.1, 0.1), (-3, -0.5, 0.1), (-3, -0.8, 0.1), (-3, -0.8, 0.25), (-3, -0.8, 0.4)$ for right figure.

Fig. 7: Three-dimensional paths line of viscoelastic flow in channel B at $Re=10, We=0.1, \varepsilon=0.5$, and $\alpha=0.1$. Start points for particle tracking in main flow are $(x, y, z) = (-3, -0.1, 0.1), (-3, -0.1, 0.5), (-3, -0.1, 0.8), (-3, -0.5, 0.8), (-3, -0.8, 0.8)$ for left figure and $(x, y, z) = (-3, -0.1, 0.1), (-3, -0.5, 0.1), (-3, -0.8, 0.1), (-3, -0.8, 0.5), (-3, -0.8, 0.8)$ for right figure.

Fig. 8: Distribution of flow rate in $x$ direction: flow in channel B at $Re=10, We=0.1, \varepsilon=0.5$, and $\alpha=0.1$.
channel was equally divided into 8 regions. In the case of viscoelastic flow, flow rate within the region just upstream of the contraction plane decreases near the side wall (region 1), and increases near the symmetric plane (region 8) because the flow inclined towards the symmetric plane. Three-dimensional flow behavior occurs notably near the contraction plane.

Next, the vortex size was investigated using a method similar to a tracer-visualization method: a well-known experiment technique for taking pictures of streamlines. The trajectory of particle which passes through the slit region is projected onto the xy plane, and the projection is drawn (see Fig.10). In the following discussion, the path line at \( z = z_0 \) means the projection of particle path in the region between \( z = z_0 - S/2 \) and \( z = z_0 + S/2 \), where \( S \) is the slit width; \( S \) was 0.01 in the present study.

The results for the viscoelastic flow at \( We = 0.1 \) and the Newtonian flow at \( Re = 10 \) in channel A are shown in Figs.11 and 12, respectively. The results for the viscoelastic flow in channel B are shown in Fig.13. The positions of the slit are near the center plane, \( z = 0.05 \), and near the side wall, \( z = 0.45 \) for channel A and \( z = 0.95 \) for channel B.

In the Newtonian flow (Fig.12), there is not outstanding difference between the results at \( z = 0.05 \) and 0.45 because the flow is two-dimensional over a wide range of the channel width. On the other hand, in the viscoelastic flow in channel A, there is a large vortex region near the wall, while the vortex region near the center plane is small. The trajectory of particle in the vortex region at \( z = 0.45 \) is not closed because the particle does not flow within a parallel plane to the \( xy \) plane at \( z = 0.45 \). In channel B, only a small vortex exists near the side wall, \( z = 0.95 \).

To study the effect of \( We \) on the vortex size, the simulation was carried out under some conditions of \( We \). The upper limit of \( We \) in the present calculation was 0.15 for channel A, and 0.2 for channel B. \( Re \) and \( \varepsilon \), and \( \alpha \) were fixed to 10, 0.5, and 0.1, respectively. The vortex size was evaluated by the dimensionless vortex lengths, \( L_x \) and \( L_y \), defined as shown in Fig.14. When a vortex was not closed in a plane parallel to the \( xy \) plane, the vortex length was determined as a distance between the boundary of the vortex region and the wall; the points where sign of the velocity component in the flow direction changed were searched and the boundary between the vortex region and the main flow was found. Figures 15 and 16 show the distributions of \( L_x \) and \( L_y \) in the \( z \) direction. In both the channels, \( L_x \) and \( L_y \) are small near the center plane \( (z = 0) \) and do not change with increasing \( z \) in most part, and begin to increase near the side wall. The dependence of \( L_x \) and \( L_y \) on \( We \) is outstanding near the side wall; both \( L_x \) and \( L_y \) are larger at larger \( We \). In addition, \( L_x \) and \( L_y \) begin to increase at smaller \( z \) when \( We \) is larger. These results indicate that three-dimensional flow pattern appears more notably at higher Weissenberg number. The effect of wall is drastic when the aspect ratio of channel \((W/H)\) is small, thus both \( L_x \) and \( L_y \) near the side wall in channel A are much larger than those in channel B.

5. Conclusion

In the present study, the three-dimensional viscoelastic flow in two rectangular abrupt contraction channels
Fig.11: Path lines in slit through channel A at (a) $z=0.05$ and (b) $z=0.45$ for viscoelastic flow at $Re=10$, $We=0.1$, $\varepsilon=0.5$, and $\alpha=0.1$.

Fig.12: Path lines in slit through channel A at (a) $z=0.05$ and (b) $z=0.45$ for Newtonian flow at $Re=10$

Fig.13: Path lines in slit through channel B at (a) $z=0.05$ and (b) $z=0.95$ for viscoelastic flow at $Re=10$, $We=0.1$, $\varepsilon=0.5$, and $\alpha=0.1$. 
Fig. 14: Definition of vortex length

Fig. 15: Distributions of vortex length in z direction: flow in channel A at $Re=10$, $\varepsilon=0.5$, and $\alpha=0.1$

Fig. 16: Distributions of vortex length in z direction: flow in channel B at $Re=10$, $\varepsilon=0.5$, and $\alpha=0.1$
was numerically studied using the Giesekus model for a constitutive equation. The numerical prediction showed several interesting three-dimensional flow properties such as the spiral flow. Three-dimensional flow behavior was found more notably at higher Weissenberg number. The vortex size was larger near the wall and the effect of wall was drastic when the aspect ratio of channel was small.

The present analysis mainly focused on flow patterns. Further study should be needed to reveal the mechanism of the three-dimensional contraction flow; e.g., the investigation of the relationship between flow patterns and stress field.

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