

SIMULATION OF VISCOELASTIC FLUID FLOWS IN EXPANSION GEOMETRY USING FINITE VOLUME APPROACH

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Abstract The simulation results on viscoelastic fluid flows in sudden expansion geometry with different expansion ratios are presented. Oldroyd-B, linear Phan-Thien-Tanner (L-PTT) and Finitely Extensible Nonlinear Elastic (FENE-P) based constitutive equations were applied in two-dimensional Cartesian coordinates. The governing equations in transient and fully developed regions were solved using open source software called OpenFOAM. The flow patterns, including velocity profiles, shear stresses and first normal stress differences in some horizontal and vertical sections are illustrated. In addition, effects of the fluid type, flow dynamics and expansion ratio on the flow and vortex patterns in transient and fully developed regions are presented and discussed. The presented results show that existences of vortices cause the inverse velocity and negative stresses in expansion regions of the channel which increase with increment of expansion ratio and Weissenberg number (We). Furthermore, some dead spaces can be observed at channel expansion regions close to the wall which are also increased. The results also show that at low We numbers all fluids show close behavior while at high We numbers the FENE-P fluid behavior shows high divergence from that of the two other fluids.

Keywords: Expansion flow; Simulation; Finite Volume; OpenFOAM; Viscoelastic Fluids.

INTRODUCTION

Simulation of forming process in order to investigate effects of machinery design and operating conditions on product quality and production costs is an efficient and effective method in polymer processing industries to optimize product quality and cost. Nowadays, evaluation of polymer processing phenomena has an effective role in the production of food, healthy tools and other fields^[1]. The polymer processing industries including extrusion, injection, blow molding and film blowing processes form more than 80 million tons of polymers each year which are more than metallic materials^[2]. During the forming processes, the viscoelastic fluids should flow through many units of different geometries including tubes and channels showing expansion and contraction flows. Therefore, simulation of these flows is very important and has attracted many academic and industrial researchers in all over the world. Due to the viscoelastic nature of fluids and complexity of flow geometry, simulation of such processes could be so tedious and time consuming^[3, 4]. Some researchers have studied the expansion and contraction flow in mold filling process numerically ignoring the surface effects^[5], some others considered this phenomenon in their simulations^[6–10].

Investigation of Newtonian and non-Newtonian fluids and comparison of their behaviors are performed by many researchers^[11–13]. Viscoelastic fluid is one of the most important non-Newtonian fluids which implemented in numerous industrial processes. Due to existence of elasticity effects, prevailing non-Newtonian models are not able to precisely predict viscoelastic phenomena, such as generalized Newtonian models. Consequently, there are several constitutive equations used to represent viscoelastic phenomena. The best-known models are

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Maxwell^[14], UCM and Oldroyd-B^[15], Giesekus^[16], FENE-P-Finitely Extensible Non-linear Elastic-Peterlin^[17], FENE-CR^[18], Phan-Thien-Tanner (PTT)^[19] and DCP^[20]. A rather complete list of models for viscoelastic fluid and some detailed comparisons among them can be found in [21], [22] and [23]. The Maxwell model is one of the viscoelastic models used to evaluation of polymeric solution flows^[24, 25]. Giesekus model is applied to predict behavior of polymeric melting flows^[6] and solution flows^[26, 27]. Furthermore, in several studies, PTT^[11] and L-PTT^[28] were used and in some others FENE models^[29, 30] were used to evaluate polymeric solutions. Some other researchers have simultaneously applied several viscoelastic models to determine flow patterns and other flow characteristics^[1, 31, 32].

OpenFOAM (Open Source Field Operation and Manipulation) is supplied with pre- and post-processing environments. The interface to the pre- and post-processing are themselves OpenFOAM utilities, thereby ensuring consistent data handling across all environments. The overall structure of OpenFOAM is shown in Fig. 1^[33].

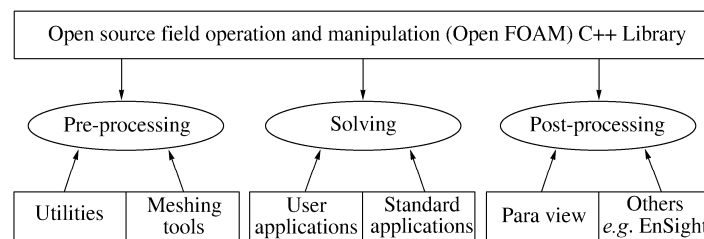


Fig. 1 Overview of OpenFOAM structure^[33]

In this work, we use OpenFOAM software for simulation of expansion channel flows. For establishment of a suitable work and validation of accessed data, we used Oldroyd-B, FENE-P and PTT-Linear three viscoelastic models and works of Azaiez *et al.*, Favero *et al.*, and Quinzani *et al.*^[1, 31, 32], respectively. After validation of evaluated viscoelastic models, velocity, shear rate, and stress normal differences profiles will be studied for three vertical and horizontal sections. After the rheological investigation of flow in the channel for a significant expansion ratio, it has been tried to assess the Weissenberg number and expansion ratio effects in the three definite states on the flow pattern.

THEORETICAL BACKGROUND

Geometry Condition

The geometry considered in this study is a rectangular expansion channel with different expansion ratios and the coordinate system is fixed at the center of the channel entrance as shown in Fig. 2. The upstream and downstream thickness, (M and N) are 0.05 and 0.15 m, respectively. Moreover, the channel length (S) is equal to 0.2 m, and the channel width is considered constant and much bigger than its thickness to satisfy assumption of two dimensional flow conditions everywhere in channel length.

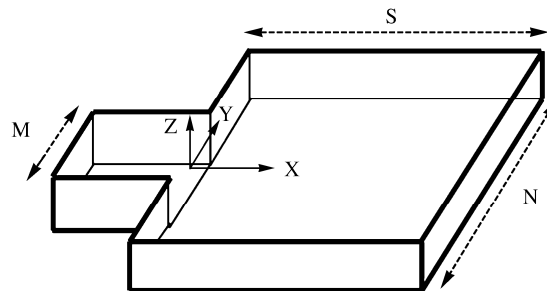


Fig. 2 Expansion rectangular channel

For presentation of the flow characteristics in different regions of flow, three vertical sections A, B and C (Fig. 3) and three horizontal sections A', B' and C' (Fig. 4) are used. The vertical sections are at $X_A = 0.025 S$, $X_B = 0.15 S$, and $X_C = 0.75 S$ in the coordinate system, respectively (see Fig. 3). Sections A, B, and C are, respectively, considered for investigation of upstream, midsection and downstream flows. Figure 4 shows the horizontal sections at $Y_{A'} = 0$, $Y_{B'} = 0.133 N$, and $Y_{C'} = 0.466 N$ parallel to the direction of channel flow. These horizontal sections are considered for evaluation of flow patterns at the symmetric line, an intermediate place and a place close to the channel wall, correspondingly.

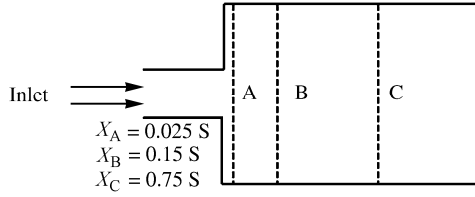


Fig. 3 Sections for evaluation of flow properties in Y direction

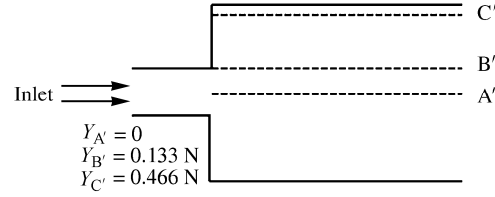


Fig. 4 Sections for evaluation of flow properties in X direction

Mathematical Model

The fluid flow problems concerning viscoelastic fluid flows should combine and solve the constitutive equations of fluids with equations that express conservation of mass, momentum and energy. The governing equations for laminar, isothermal and incompressible flows of viscoelastic fluids including the mass and momentum conservation are presented as Eqs. (1) and (2), respectively:

$$\nabla \cdot (U) = 0 \quad (1)$$

$$\frac{\partial(\rho U)}{\partial(t)} + \nabla \cdot (\rho U U) = -\nabla(P) + \nabla \cdot \tau + \rho g \quad (2)$$

In the above equations ρ , U , P , g , and τ are the fluid density, velocity vector, pressure, gravitational acceleration and the extra stress tensor, respectively.

The fluid constitutive equations which have been used in this work are presented *via* Eqs. (3) to (5)^[21]:

$$\left(1 + \frac{(3)/(1-3/L_K^2) + \lambda_K / \eta_{P_K} \text{tr}(\tau_{P_K})}{L_K^2}\right) \tau_{P_K} + \lambda_K \tau_{P_K} = 2 \frac{1}{(1-3/L_K^2)} \eta_P \quad (\text{FENE-P}) \quad (3)$$

$$\frac{DU}{Dt} - \tau \cdot \nabla U - \nabla U^T \cdot \tau + \frac{1}{\lambda} \left(1 + \frac{\varepsilon \eta_P}{\lambda} \text{tr}(\tau)\right) = \frac{2\lambda D}{\eta_P} \quad (\text{L-PTT}) \quad (4)$$

$$\frac{\partial \tau}{\partial t} + U \cdot \nabla \tau - (\nabla U)^T \cdot \tau - \tau \cdot \nabla U + \frac{1}{\lambda} \tau = 2 \frac{\eta_P}{\lambda} D \quad (\text{Oldroyd-B}) \quad (5)$$

In above equations, λ_k , η_{P_K} and τ_{P_K} are respectively the relaxation time, the viscosity at zero shear rate, and the upper convected derivative applied to the stress tensor.

In Eq. (3), L_k is the length of polymer chain, D is the deformation rate tensor which is defined as:

$$D = \frac{1}{2} (\nabla(U) + [\nabla(U)]^T) \quad (6)$$

In Eq. (4), $\text{tr}(\tau)$ denotes the trace of the stress tensor, ε is the parameter that governs the extensional fluid response and represents the material derivative of the velocity matrix.

The boundary and initial conditions for the above mentioned equations are:

$$\text{At } Y = -N/2 \text{ and } Y = +N/2; U_x = U_y = 0 \quad (7)$$

$$\text{At } Y = 0; \frac{\partial U_x}{\partial y} = \frac{\partial U_y}{\partial y} = 0 \quad (8)$$

$$\text{At } X = 0; U_x = U_0 \quad (9)$$

The values of model parameters for different considered viscoelastic fluids are listed in Table 1.

Table 1. Model parameters for Oldroyd-B, FENE-P, and L-PTT fluids

U_0 (m/s)	λ (s)	ζ	ε	L^2	η_p (Pa·s)	η_s (Pa·s)
0.155	0.03	0.0	0.25	6.0	1.422	0.002

Mesh Dependency Analysis

In all simulations, hexahedral mesh type (see Figs. 5 and 6) has been used in OpenFOAM environment, and analysis of mesh size dependency on simulation results has been done in all sections of flow geometry. Table 2 shows the mesh number at the upstream and downstream of channel in the X and Y directions. Finally, the size of meshes in each section is selected to have no ignorable effects on the simulation results.

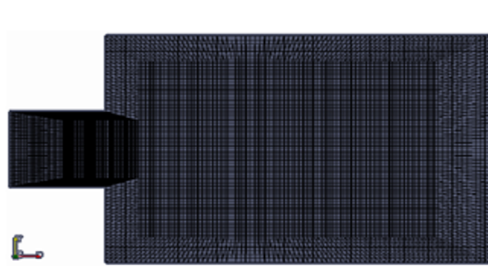


Fig. 5 Computational grid in OpenFOAM software environment

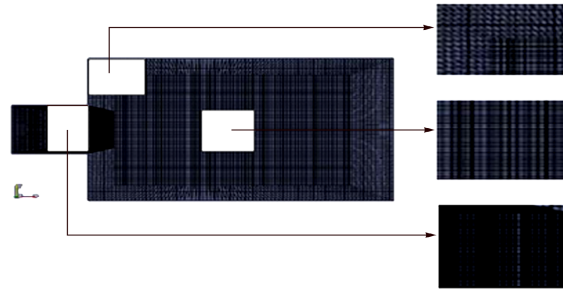


Fig. 6 The zoom of three sections of geometry for more appropriate view

Table 2. Mesh size at upstream and downstream of channel

Upstream		Downstream	
N_y	N_x	N_y	N_x
20	60	80	100

RESULTS AND DISCUSSION

Validation

Due to lack of appropriate experimental or simulation results for expansion flow of viscoelastic fluids, direct validations of the simulation results have not been possible. So, indirect method has been considered for model validation. First, the model and method are used for contraction flow simulation and the results are compared with experimental results presented by Quinzani *et al.* and simulation results presented by Azaiez *et al.* In addition, the expansion flow in steady fully developed regions should be comparable with similar regions in contraction flows. So, simulation results in these regions are compared with experimental results of Quinzani *et al.*, and simulation results of Azaiez *et al.* and Favero *et al.* have been considered for solution validation and comparison of simulation results. Obtained simulation results for velocity profile in three different sections of a contraction flow are compared with the previously mentioned results in Figs. 7(a)–7(c). The presented results are in very good agreement with previously published experimental and simulation results.

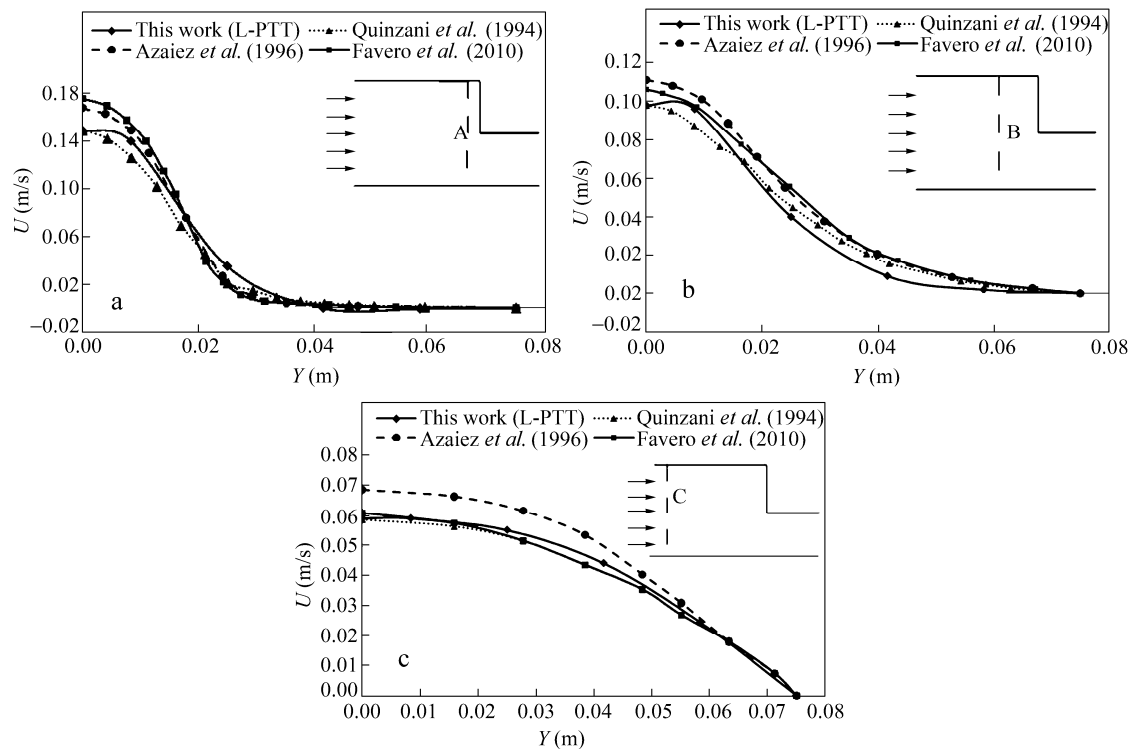


Fig. 7 The velocity profiles along the middle lines of sections A(a), B(b) and C(c), respectively

Velocity Profiles

Simulation results for velocity profiles in expansion flow for Oldroyd-B, FENE-P and PTT Linear (L-PTT) viscoelastic models with an expansion ratio of 3/1 are presented *via* Figs. 8 and 10. Figures 8(a), 8(b), and 8(c) show velocity curves in A, B, C vertical sections, respectively, while Figs. 10(a), 10(b) and 10(c) show those in A', B' and C' horizontal sections, correspondingly.

Figure 8(a) represents the velocity profile in section A, there are three different velocity areas in terms of numerical values. In the first area ($Y < 0.04$ m), the velocity values are positive while in the second area they have negative sign (0.04 m $< Y < 0.06$ m) and in the third region ($Y > 0.06$ m) they have zero values. These regions are related to progressive, vortex and stagnant flow regions, respectively. Appearance of vortex and stagnant regions are due to the sudden flow cross section change, which causes appearance of lateral flow in these regions.

Figure 8(b) illustrates the variation of the velocity in the section B. Comparison of Figs. 8(b) and 8(c) shows that with increasing distance from the expansion point, the negative values of velocity are eliminated and so, vortexes in this region should be eliminated. Nevertheless, the stagnant region can be still observed. This stagnant zone, which is continued to the wall, starts in the separation location of forward and backward (reverse direction) flows. Other noticeable point is the growing of the positive velocity flows. In fact, section B approximately is at the end of the transient region and the start point of the fully developed area, where Figure 8(c) does not show negative and stagnant flow regions and suggests that this region should be in the fully developed area (see Figs. 8a, 8b and 8c). All of the above results can be concluded from Fig. 8 which shows the stream line of flow along the length of channel. The velocity vectors are shown in Fig. 9 in the OpenFOAM software environment.

In order to study in more detail, the velocity profiles are investigated in the three horizontal sections, which are parallel to flow direction. As is illustrated in Figs. 10(a), 10(b), and 10(c), there are sufficient and effective convergences among the results of three investigated viscoelastic models. In Fig. 10(a), the velocity variations have been investigated ($Y = 0$ m) in the central line of the channel. These figures show that with increasing axial

distance from expansion point the flow becomes more stable and changes to fully developed flow at approximately 0.1 m far away from the expansion point. Due to existence of turbulences in section B', the velocity increases. Then, the velocity decreases gradually by the flow pattern development and afterwards it reaches to steady state conditions. In section C' the velocity profiles have some differences with the others which are affected by vortexes. In this section, initially, there is a static region followed by reverse flow region and forward flow area, respectively (Fig. 10c). From the variation of the curves, it is obvious that at a distance of 0.0665 m from the entrance the flow becomes fully-developed and the trend of any curves confirms this claim. Also, it is clearly observed there is good agreement among the three viscoelastic models in all curves.

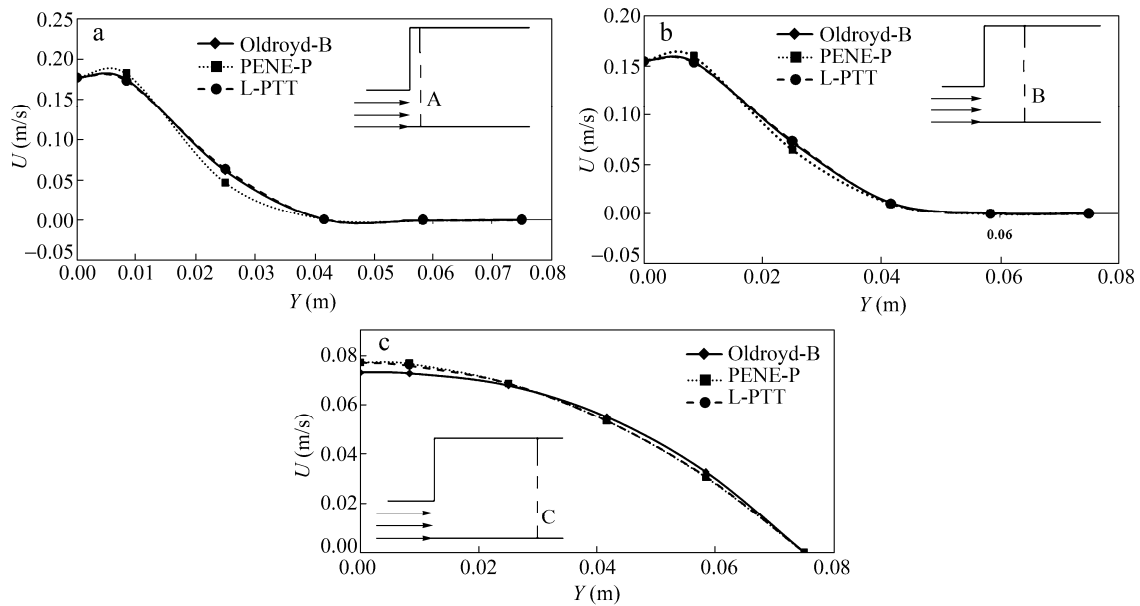


Fig. 8 The velocity profiles along the middle lines of sections A(a), B(b) and C(c), respectively

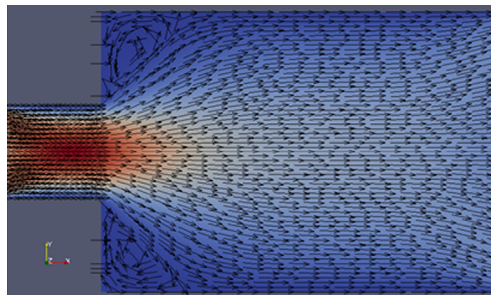


Fig. 9 Velocity vectors in OpenFOAM software environment

For more detail investigation on the velocity in the horizontal sections, the Y -component of the velocity U_y is presented in Figs. 11(a), 11(b) and 11(c). As it can be seen from these figures, the velocity in Y direction at the centerline of channel is approximately equal to zero, because at the centerline of the channel, as it can be anticipated, there is only a velocity in the X direction. In Figs. 11(b) and 11(c) the velocity component U_y in the B' and C' sections is shown. At the beginning of B' section and the section close to channel wall (section C'), there is interaction between the U_y s resulted from vortexes and from the progressive flow at the expansion point. By movement of the flow to downstream, due to vanishing the vortexes and entering to fully developed regime, the velocities U_y are close to zero values. The existence of vortexes can be observed in Fig. 11(c) clearly. Actually, the negative values of velocity represent the existence of vortexes.

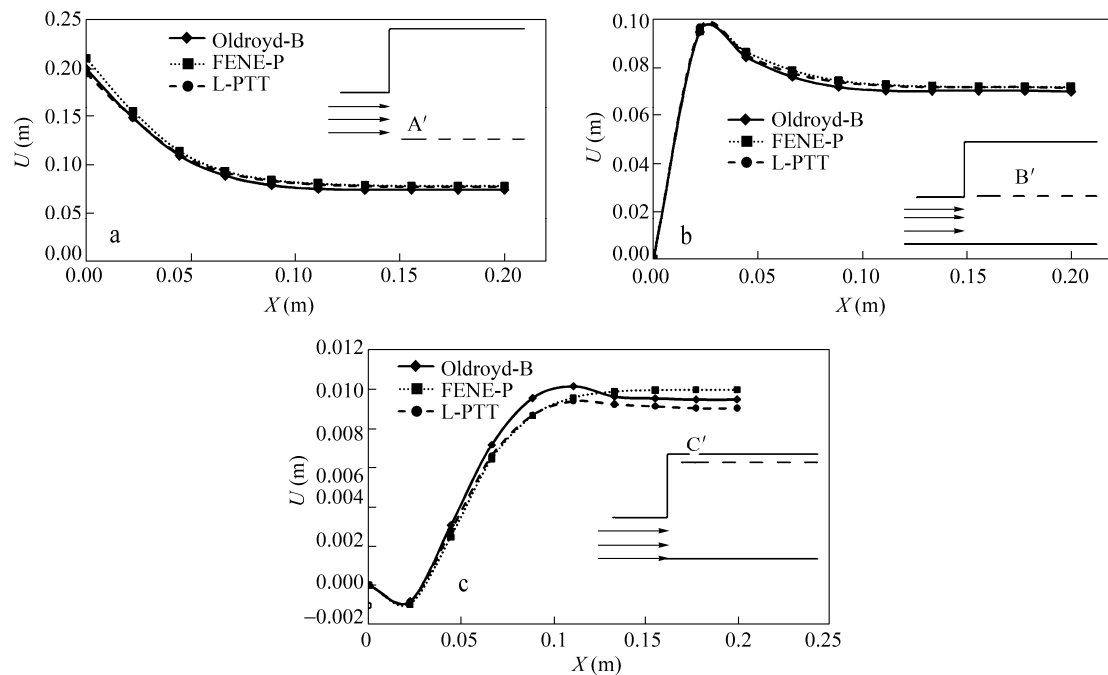


Fig. 10 The velocity profiles along the middle lines of sections A'(a), B'(b) and C'(c), respectively

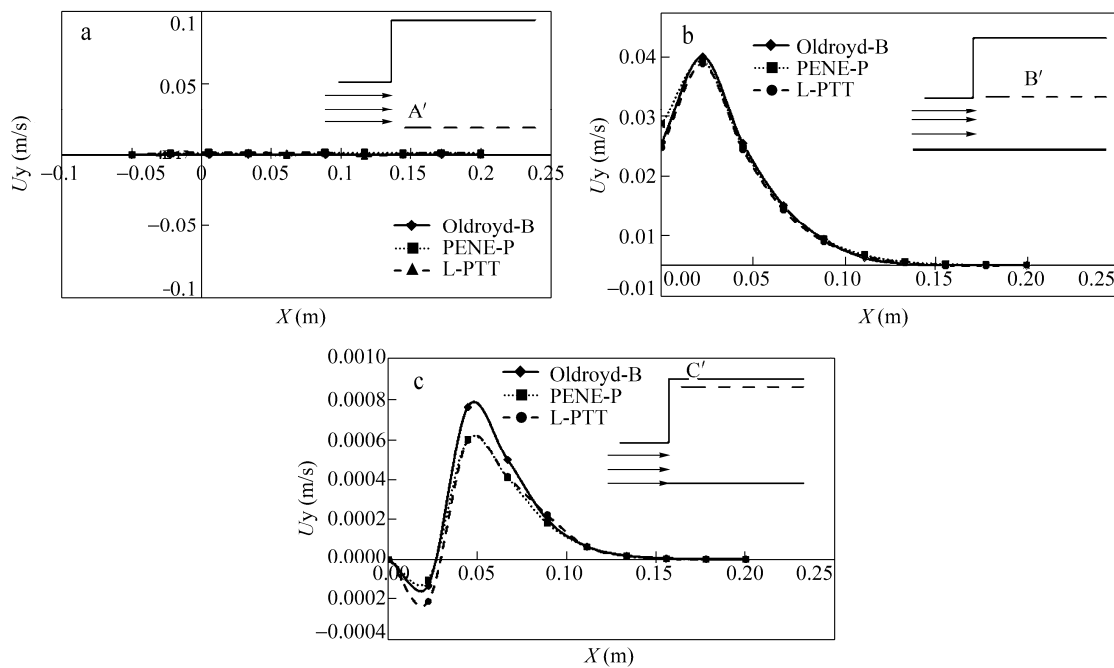


Fig. 11 The profiles of velocity component U_y along the lines of sections A'(a), B'(b) and C'(c), respectively

Shear Stress Profiles

The shear stress profiles are investigated in three vertical and horizontal sections for all fluids. Figures 12(a), 12(b) and 12(c) show shear stress profiles in A, B, and C vertical sections, respectively, and Figs. 13(a), 13(b) and 13(c) show shear stresses profiles in direction of flow in A', B', and C' sections, correspondingly.

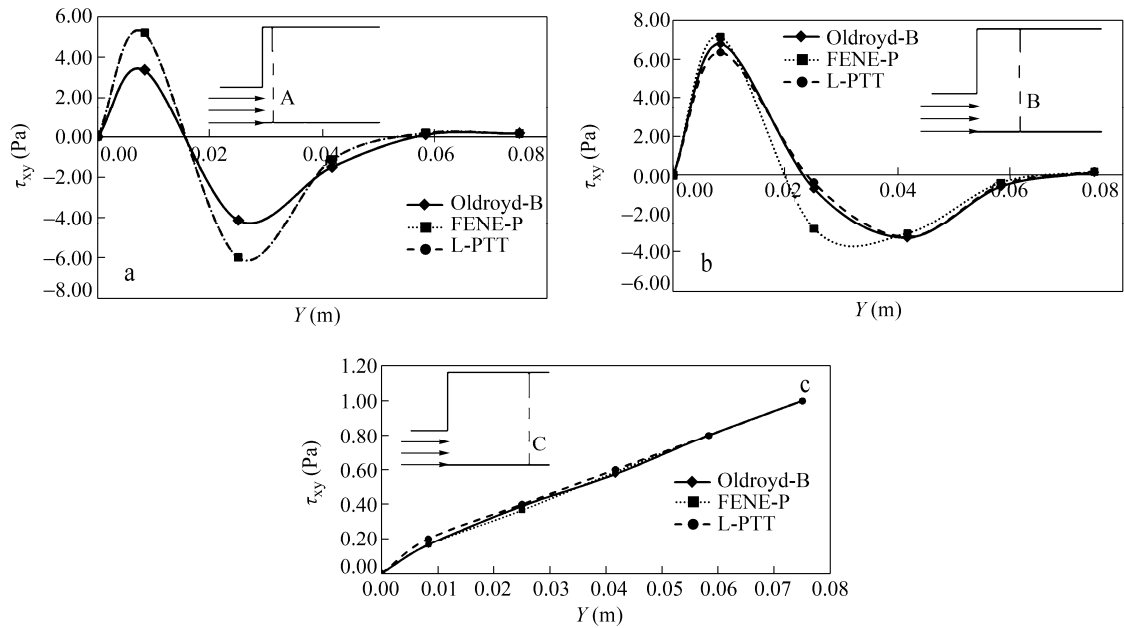


Fig. 12 The shear stress profiles along the middle lines of vertical sections A(a), B(b) and C(c), respectively

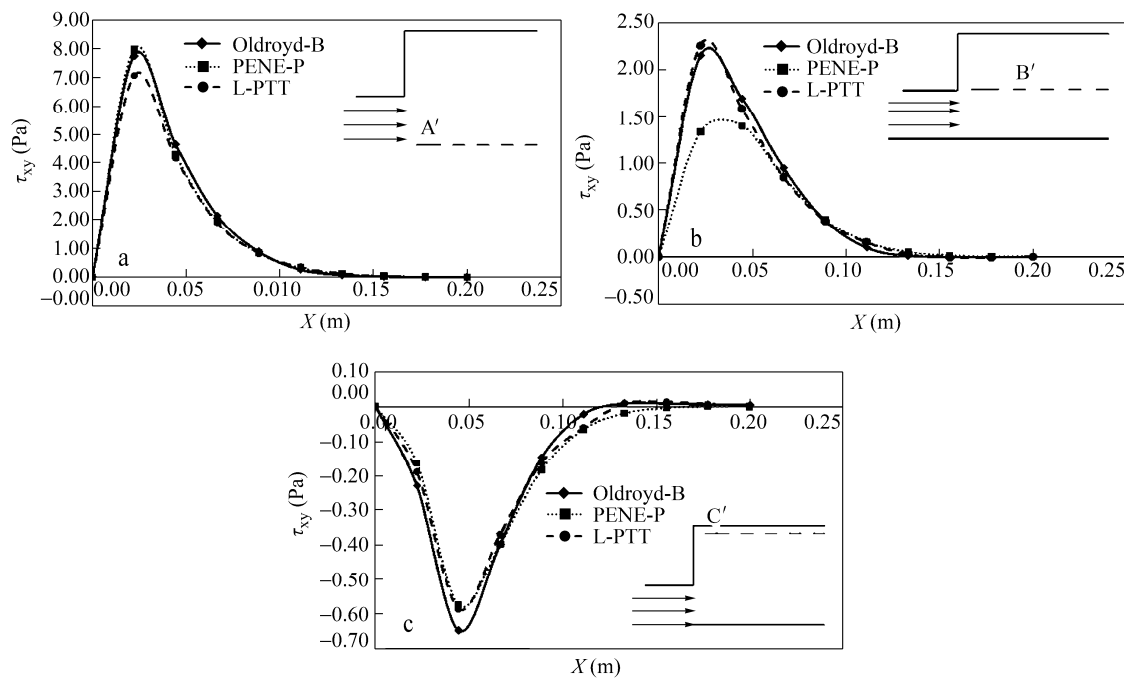


Fig. 13 The shear stress profiles along the middle lines of horizontal sections A'(a), B'(b) and C'(c), respectively

As shown in Fig. 12(a), in section A, shear stress is zero at middle of the channel but increases to its maximum value at a certain distance from channel middle line ($Y = 0.009$ m). Then shear stresses reduce and after a certain distance from channel central line become negative. The maximum shear stress might be related to maximum elongation which also should occur at $Y = 0.0095$ m. At distances more than $Y = 0.0095$ m, the axial velocity rate starts to reduce and at a certain distance from central line the axial rate and stresses become negative which should result in appearance of vortices. Actually, the shear stress will be negative, as soon as the

vortex flows overcome the progressive flows. Then shear stresses present a maximum negative value which is more pronounced for L-PTT and FENE-P fluids. Later, shear stresses increase to zero value, which should be related to stagnant region of flow. Results in Figs. 12(a) and 12(b) show that with increasing distance from entry point the maximum of shear stress increases while the stress related to vortices region decreases, which is more pronounced for L-PTT and FENE-P fluids. In addition, the distance of vortex region from central line in B section is increased in comparison to the distance of vortex region from central line in A section. The vortex effects will be gradually removed in the channel downstream and disappear in the section C. Therefore, the shear stresses have ascending values in this section. Actually, this increasing shear stress shows that the flow should approach to fully-developed in this section (see Fig. 12c). In overview, the channel upstream is simultaneously influenced by these three phenomena: the progressive flows, the reversing flows caused by vortices and the wall effects. Meanwhile, with advancing flow to downstream the vortices effects are gradually being removed and the progressive flow will be the main stream.

The shear stresses in the three horizontal sections A', B', and C' are respectively presented in Figs. 13(a), 13(b) and 13(c). In Fig. 13(a), the pattern of variations in shear stress is shown in the channel central line. Due to the strong interaction between polymer chains, shear stress initially increases to a maximum value. Furthermore, the shear stress is increased when the flow enters to an expanded environment. After passing the maximum point, shear stress is eventually reduced to proximity zero which is caused by starting polymer solution relaxation. In section B', the negative shear stress values will appear due to reverse flow caused by vortices. Then, the shear stress value increases with decreasing vortices and reaches to a maximum value followed by a descending graph which is similar to the downstream of A' section. In section C', due to existence of vortices, the stresses are mostly negative, just in contrast to sections A' and B', and show a maximum value at a certain distance from the entry point.

First Normal Stress Difference Profiles

Figures 14(a), 14(b) and 14(c) show the first normal stress difference profiles in vertical sections, A, B and C, respectively. Observation of the complete profiles reveals that the greatest differences occur nearby the expansion region, where the highest values of elongation rate and, consequently, of stress should appear. Figure 14(b) shows similar behavior for normal stress difference but, with considerable reduction in difference values. In addition, normal stress difference increases as distance from centerline increases which shows that at this vertical section the flow should approach to a fully developed flow. It should be mentioned that the normal stress difference behavior for Oldroyd-B at this region is somewhat different from that of the two other fluids. The normal stress differences related to cross-section A' are presented in Fig. 15(a). Due to expansion of cross-section, the flow velocity dropped down after entering channel. Therefore, the normal stress differences may be decreased. In fact, the channel expansion is a transient region between the upstream and downstream steady flows. In this region, the velocity gradient trend could be reversed in some points. When the flow progresses in fully-developed region, $\tau_{xx}-\tau_{yy}$ simultaneously approaches to zero in centerline. In section B', the flow pattern is affected by tensions and elongation of the polymer chains. However, due to geometry characteristics, the effects of stresses are negligible rather than those of elongations. Consequently, the normal stress difference is continuously reduced (Fig. 15b). Examination of normal stress differences at regions near entry line suggests that a dead space may exist in section C'. In this region, because of proximity to the channel wall and existence of dead space, the normal stress differences are small. Nevertheless, passing through this region the $\tau_{xx}-\tau_{yy}$ values will increase. Finally these quantities reach to constant values in the fully-developed region (Fig. 15c).

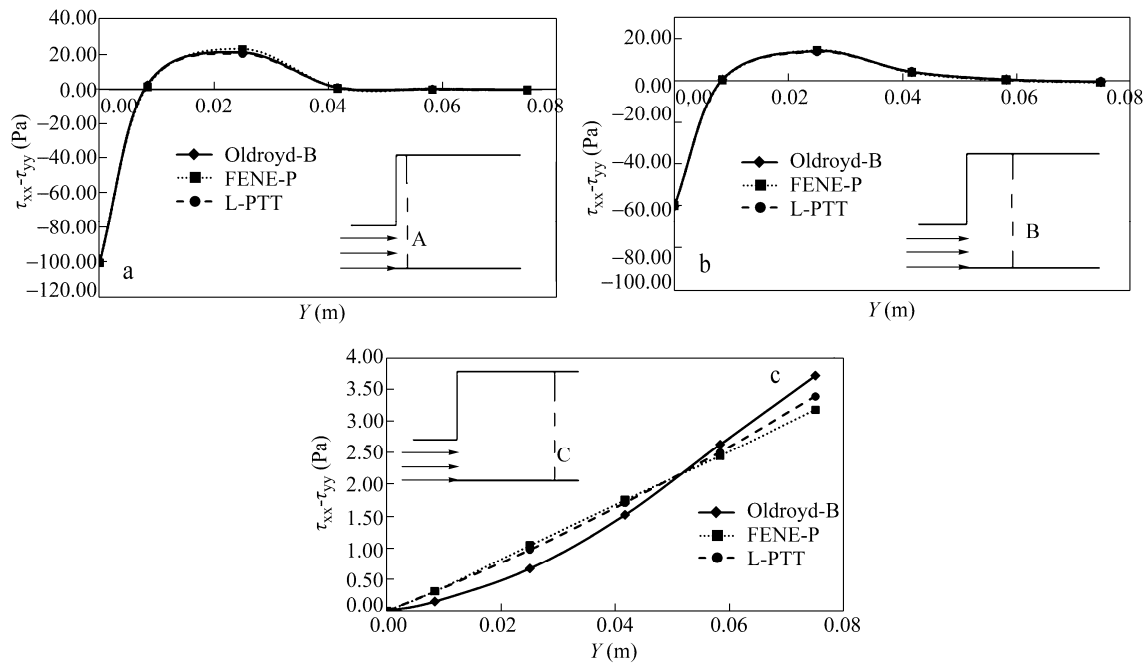


Fig. 14 The first stress normal difference profiles along the middle lines of vertical sections A(a), B(b) and C(c), respectively

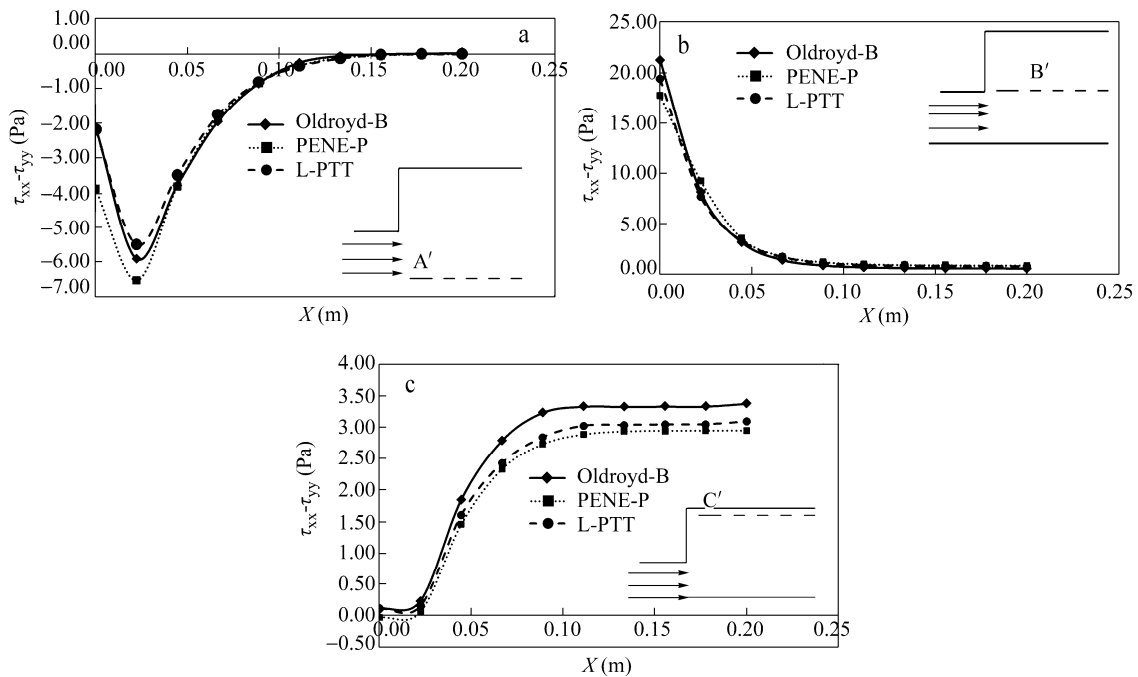


Fig. 15 The first stress normal difference profiles along the middle lines of horizontal sections A'(a), B'(b) and C'(c), respectively

Weissenberg (*We*) Number Effects on Flow Characteristics

Effects of *We* number on flow pattern in vertical and horizontal sections are presented in Fig. 16. As one can see in Fig. 16(a), near the expansion region the velocity profile has not been affected considerably by *We* number while the velocity profiles are affected dramatically by change in *We* number in B and C sections which is more pronounced for FENE-P fluids. Actually in the section C, velocity profiles at high *We* number (*We* = 500) do

not seem still fully developed and show maximum values which are much pronounced for FENE-P fluids. Figures 16(d), 16(e) and 16(f) show velocity profile along the direction of flow in sections A', B', and C', respectively. These figures show that with increment in We number the length of the transient regions increases which is more pronounced for FENE-P fluids. These figures show that at A' and C' sections, profiles of FENE-P fluids show considerable negative values which cannot be seen in profiles of the two other fluids. Actually, these negative values result in production of vortices in these regions of flow.

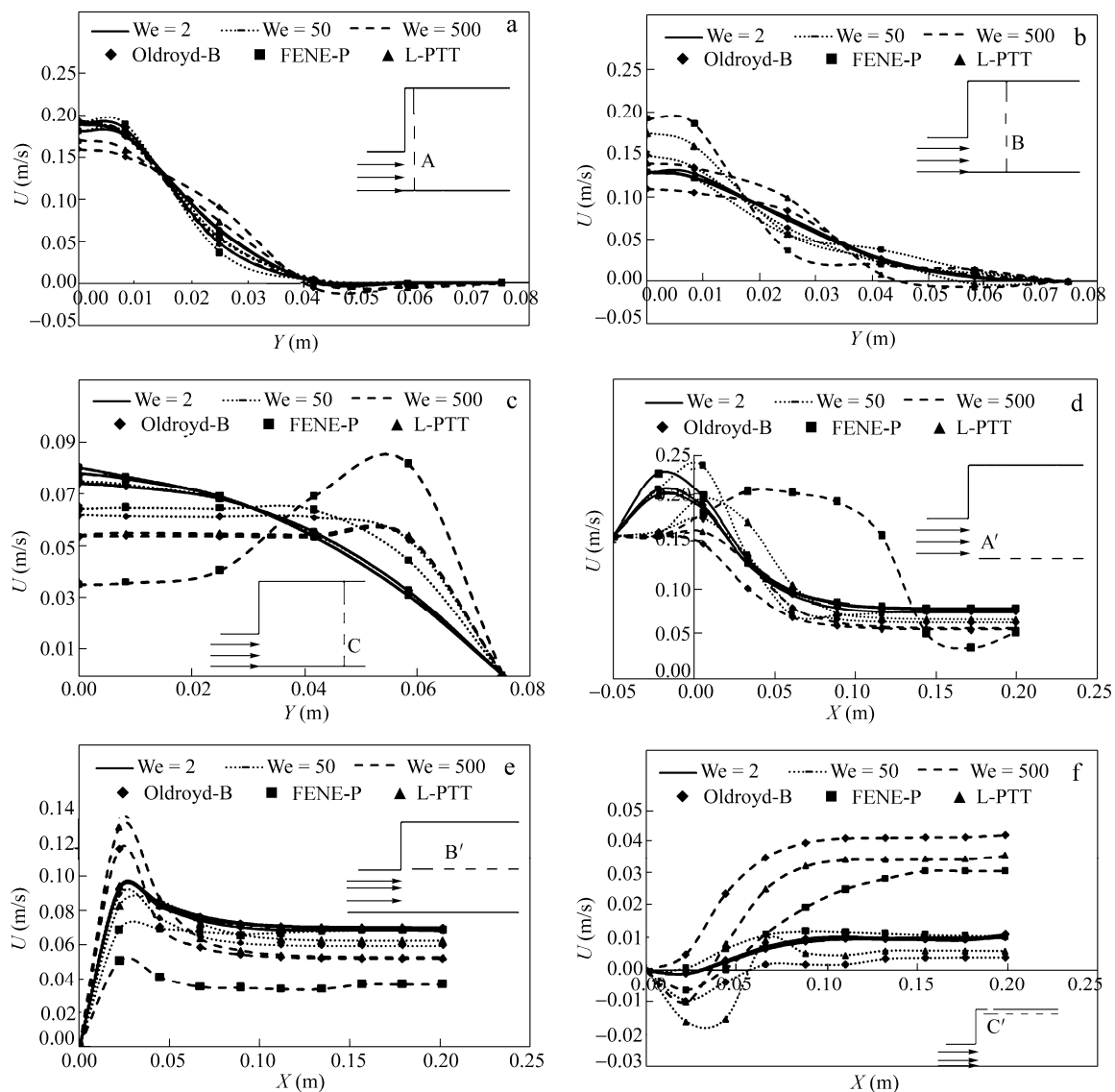


Fig. 16 The velocity profiles along the middle lines of vertical sections A(a), B(b) and C(c) and horizontal sections A'(d), B'(e) and C'(f), respectively

Expansion Ratio Effects on Flow Patterns

Effects of expansion ratio on the vertical and horizontal velocity profiles at $We = 2$ are presented in Fig. 17. Figures 17(a) and 17(b) show that with increasing expansion ratio from 2/1 to 4/1, some vortices appear in A section near the channel center which are almost similar for all fluids in $We = 2$. Figure 17c which represents axial velocity in C section shows that with increasing expansion ratio a maximum value at velocity profile near

centerline appears and the velocity at region near the wall decreases considerably. Figure 17(d) shows that with increasing expansion ratio the centerline axial velocity decreases and the velocity profile becomes more flat for all the fluids. An interesting point in the profile relating to expansion ratio of 4/1 is the existence of a region in which the axial velocity is same for all the fluids.

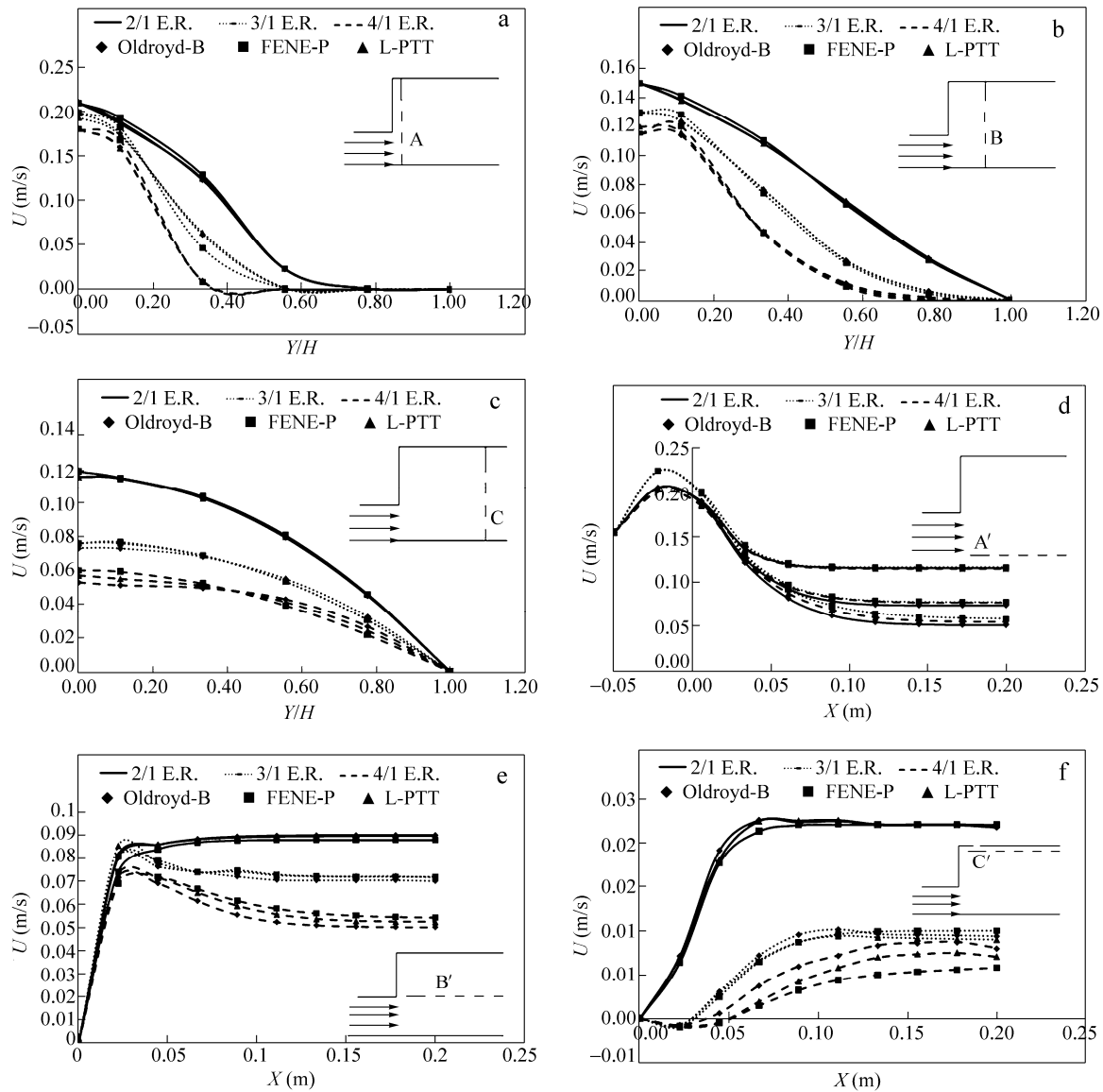


Fig. 17 The velocity profiles in cases of different expansion ratios along the middle lines of vertical sections A(a), B(b) and C(c) and horizontal sections A'(d), B'(e) and C'(f), respectively

Figure 17(d) which represents the axial velocity at the centerline shows that with decreasing the expansion ratio the fluid disturbance at the upstream is more pronounced for all fluids.

Figure 17(e) shows that the fluid type and expansion ratio do not considerably affect flow profile in the B' section near the entrance, but at a distance of 0.03 m from the entry point, an overshoot in flow profile can be seen which increases with expansion ratio. This figure also shows that with increasing in expansion ratio the length of transient flow increases considerably for all studied fluids. Figure 17(f) shows that with increasing expansion ratio from 2/1 to 4/1 the length of transient flow in the C' section increases considerably. This figure

also shows that with increasing expansion ratio some vortexes may appear near the entry point and the length of vortex region increases with increasing expansion ratio. This figure also shows that for the expansion ratio 4/1 the vortexes are more pronounced for FENE-P fluid.

CONCLUSIONS

In this study, expansion and contraction process under isothermal and two dimensional conditions were simulated using OpenFOAM software. Furthermore, in order to validate simulation results, the works of Favero *et al.*, Aziez *et al.* and Quinzani *et al.* have been used. Velocity distribution, shear stress and first normal stress differences profiles were investigated in the various sections. The conclusion could be listed below:

Oldroyd-B model similar to previous models (such as FENE-P and L-PTT) well predicts the flow pattern in the contraction geometry.

In the evaluation of expansion flow, there is a good agreement among the three viscoelastic models. Although, the convergence between Oldroyd-B and L-PTT models is better.

The velocity profile demonstrates zero values in some areas of the channel, that shows the formation of vortexes and reverse flow. Moreover, area by zero or next to the zero value is shown in the edge of channel that represents the dead space in that area (stagnant region).

The flow becomes fully developed and stable after a significant distance from the channel entry which is shown in the velocity and shear rate profile in the horizontal section.

As it is shown from shear rate and first normal stress difference, the maximum of elongations occurs at $Y = 0.095$ m. This area is related to move of polymeric flow from the edge of channel.

After passing of transient area, the negative values of first normal stress differences approach to zero amount.

The vortexes size is increased by increment in the expansion ratio. Also, this trend is repeated in the stagnant region.

The size of vortex and stagnant regions is increased by increment in We number.

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