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NUMERICAL SIMULATION OF POLYMER MELT FLOW IN SUDDEN EXPANSIONS

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Abstract. *Sudden expansion is a typical geometry found at the entrance of a mould cavity and is generally known in industrie as gate. Flow simulation of this class of problems poses some difficulties owing to coupling of momentum and energy laws, existence of re-circulation and steep pressure variations. This work focuses on the physical analysis of the laminar and incompressible polymer melt flow inside channels with sudden expansions. The mathematical model comprises the mass, momentum and energy conservation laws. The pressure-velocity coupling is treated on solving a Poisson equation for pressure. The Cross constitutive model is adopted to describe the non-Newtonian behaviour of the flow. The governing equations are discretized using the finite difference method based on central, second order accurate formulas for both convective and diffusive terms. Artificial dissipation terms are added to control the odd-even decoupling problem. The results demonstrate that flow parameters, such as pressure drop and viscosity distribution, are strongly affected by heat transfer features. It has been found that, in such problems, any reliable solution must account for the non-isothermal effects.*

Keywords. *Non-Newtonian flows, numerical analysis, sudden expansions*

1. Introduction

Polymer melt flow is frequently found in many industrial applications such as injection molding processes. The numerical simulation of this class of problems has gained widespread attention in the last years. New mathematical models, realistic rheological descriptions and numerical schemes are ongoing research topics pursuited by the scientific community.

In injection molding, a narrow channel is placed between the feeding channel and the mould cavity, as illustrated at fig. (1). Such contraction is usually known in industry as gate and has, among others, the purpose of heating the melt to best fit the cavity. The heating effect is believed (empirically) to be attained due to high viscous dissipation of polymer melts. In this context, the present work aims at analyzing flow features of polymer melts inside channels with sudden expansions, specially the non-isothermal effects.

The literature in this subject is recent but still scarce, being specially devoted on studying isothermal flows. New numerical methodologies to solve the problem are proposed in Bao (2002) and Missirlis et al. (1998). The former work adopts finite elements whereas the latter uses the finite volume method, both of which within a framework of a generalized Newtonian formulation. Physical analysis of the flow bifurcation phenomenon was discussed by Manica and De Bortoli (2004), Neofytou and Drikakis (2003) and Ternik et al. (2006). The references adopt the generalized Newtonian formulation with an isothermal power-law model to describe the non-Newtonian flow behavior. Pressure drop and vortex length in sudden expansions are flow features studied in Pinho et al. (2003). The authors discuss the effects of the power-law index in isothermal flows. Nitin and Chhabra (2005) present a parametric analysis of non-isothermal power-law fluid flow past a rectangular obstacle. The drag coefficient and Nusselt number are obtained as functions of Reynolds number, power law-index and Peclet number. The solution obtained by the authors corresponds to Reynolds number ranging from 5 to 40, which are typical values for polymeric aqueous solution, but too high for polymer melts.

The present work discusses physical aspects of polymer melt flow in sudden expansions. The analysis assesses the influence of temperature on flow parameters such as pressure drop and viscosity distribution. The numerical scheme is based on the techniques originally conceived to solve Newtonian flows (Zdanski et al., 2004). The capability of the scheme to handle non-Newtonian flows inside plane channels was demonstrated in Zdanski and Vaz Jr. (2006a; 2006b), being its extension to solve sudden expansion flows straightforward. The results obtained show strong dependence of flow parameters with respect to temperature so that any reliable solution, in this class of problems, must account for the non-isothermal effects.

2. Theoretical formulation

2.1. Governig equations

The fully coupled Navier-Stokes and energy equations, within a framework of generalized Newtonian formulation, is the mathematical model adopted, i.e.

$$\frac{\partial(\rho u_i)}{\partial t}+\frac{\partial(\rho u_j u_i)}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\eta\left(T,\dot{\gamma}\right)\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)\right], \tag{1}$$

$$\frac{\partial(\rho c_p T)}{\partial t}+\frac{\partial(\rho c_p u_i T)}{\partial x_i}=\frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right)+\eta\left(T,\dot{\gamma}\right)\dot{\gamma}^2 , \tag{2}$$

where η is the apparent viscosity, which is function of the temperature and equivalent shear rate ($\dot{\gamma}$). All the symbols appearing in the preceding equations are completely standardized in literature. The simulations performed in this work are for a commercial polymer Polyacetal POM-M90-44, whose non-Newtonian behavior is accounted for the Cross constitutive model as

$$\eta\left(T,\dot{\gamma}\right)=\frac{\eta_0}{1.0+\left[\lambda(T)\dot{\gamma}\right]^{1.0-n(T)}} , \tag{3}$$

in which η_0 is the Newtonian viscosity, n is the power-law index and λ is a material parameter, whose temperature dependence is expressed by the Arrhenius law. For more details about the governing equations and constitutive model the reader is referred to Zdanski and Vaz Jr. (2006a, 2006b). The incompressible flow approach employed to derive the numerical approximation requires use of a pressure-velocity coupling scheme. The method used in this work follows the same route presented in Zdanski et al. (2004), where a Poisson equation for pressure is solved to assure divergence-free velocity field.

2.2. Numerical method

As the emphasis of the present work is the physical analyses of important aspects of polymer melt flow in sudden expansions, only a brief discussion on the numerical method is given. Central finite difference formulae were used to discretize both convection and diffusion terms of the governing equations. The variables are arranged in a co-located mesh, and artificial viscosity terms are added externally to control the odd-even decoupling problem. The method is implicit and follows a pseudo-transient march in time, aiming at achieving the steady state solution. The present methodology was originally proposed to solve Newtonian flows (Zdanski et al., 2004), and has been successfully applied to non-Newtonian flows by Zdanski and Vaz Jr. (2006a, 2006b).

3. Results and discussions

The non-Newtonian flow in sudden expansions, despite the simplicity of the geometry, exhibits some complex fluid flow behavior. The presence of re-circulation regions and steep property variations impose difficulties leading to a demanding computational case. In the practical sense, a flow expansion is typically found at the 'gate' and its physical understanding is important in industrial injection molding processes. Figure (1) represents a typical 'gate' located at the entrance of a mould cavity. The expansion section can be clearly seen and the problem under discussion is of great interest in the practical sense as well as in a scientific ground.

The geometry simulated in the present work is the 1:2 asymmetric expansion, being the channel length 3h and 20h upstream and downstream of the expansion section respectively (h is the channel thickness for the entrance section and is assumed h = 4mm). The geometry, with its main dimensions, is represented at Fig. (2). The computational mesh adopted is non-uniform with points clustering in the regions near the corner and solid walls. A total of 41 x 81 and 151 x 161 grid points are used for mapping the channel regions upstream and downstream of the expansion section respectively. The boundary conditions used in the simulations are the following: no-slip condition for velocity components and prescribed temperature at solid walls; uniform velocity and temperature profile at the entrance and parabolic extrapolation (non-reflexive) at the exit section; for pressure, a linear variation is imposed at the entrance section whereas the parabolic condition is enforced at both solid walls and exit section.

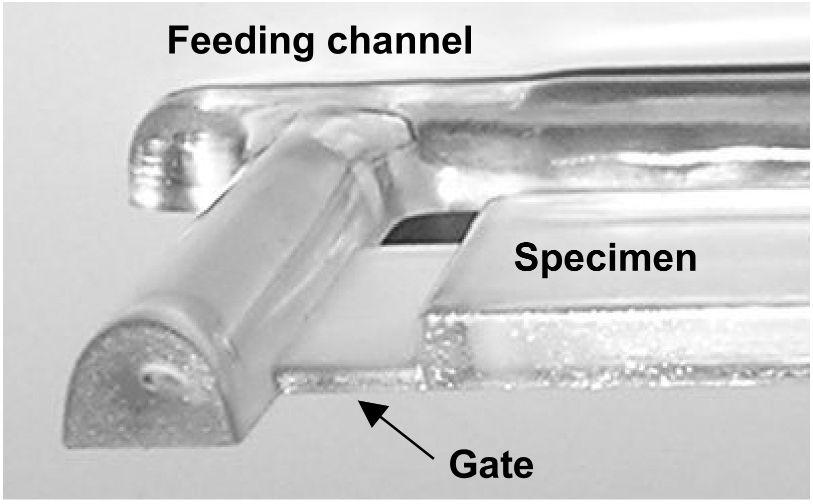

Figure 1. Typical gate as it appears in a mould cavity.

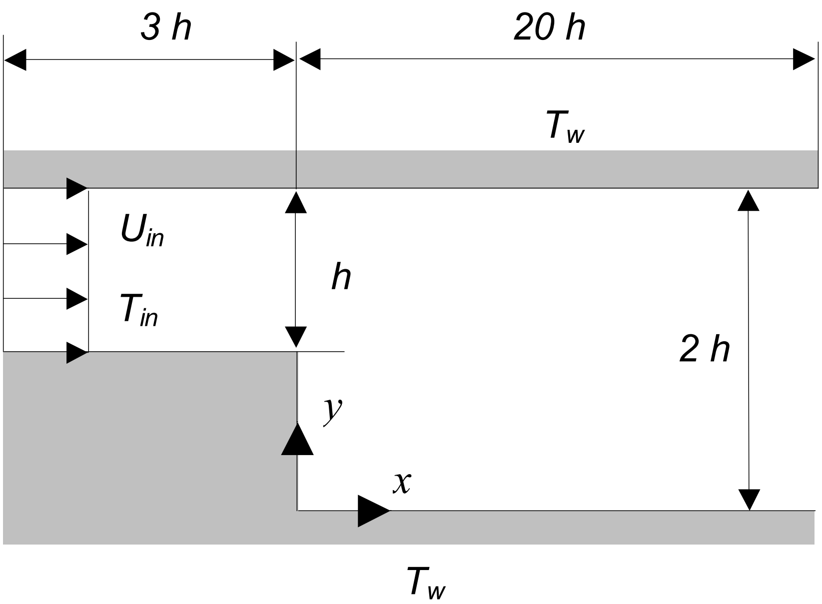

Figure 2. Sudden expansion geometry with its main dimensions.

The aim of the present work is to investigate the influence of temperature on expansion flows. The inlet velocity is assumed constant, u_{in} = 6cm/s, a typical value found in injection molding processes. This velocity renders a Reynolds number around 10^{-4}. The following thermal problems are simulated: (i) both the inlet and wall temperatures are kept at the same value $T_{in} = T_{w,}$ and the role played by viscous heating is assessed; (ii) the wall temperature applied is lower than the inlet value, e.g., T_w = 423.0 and T_{in} = 443.0, and the cooling effect of the channel walls is evaluated.

Results for $T_w = T_{in}$ = 423.0K are presented in fig. (3) – (5). Streamlines at the neighborhood of the step are represented at fig. (3), in which, a small vortex zone appears in the region at the corner. The bubble is extremely confined at the concave corner due to high fluid viscosity of polymer melts. This flow topology is qualitatively in accordance with Bao's results for isothermal flows (Bao, 2003). The re-circulation length measured is approximately x/h = 0.25. It is interesting to mention that the flow topology was very similar for other temperatures, being the differences in the vortex length virtually undetectable.

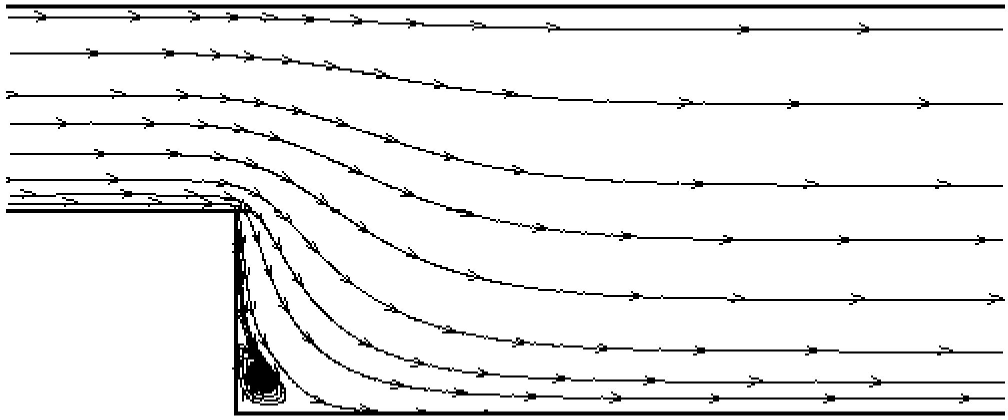

Figure 3. Streamlines at the expansion region for T_{in} = 423.0K.

The temperature field is shown in fig. (4) whereas viscosity distribution is represented in fig. (5). It has been found that viscous heating promotes a maximum temperature rise of 1.0K for the conditions simulated. Otherwise, the higher viscosity zone is attained at the vortex region as well as near the channel center where the shear rate is lower. The region near the channel walls, at the upstream of the expansion section, presents very low viscosities due to local high shear rate values. Besides, from fig. (4) one can realize that there is a core region at the center of the channel unaffected by viscous heating. Obviously, the heat generated near the walls is transported by convection and diffusion mechanisms. As the thermal conductivity of the Polymer is very low (practically a thermal isolator), it takes a very long distance downstream for the channel center to sense the heating effect. This interesting aspect was fully explored by Zdanski and Vaz Jr. (2006a, 2006b) for Polymer melts in plane channels.

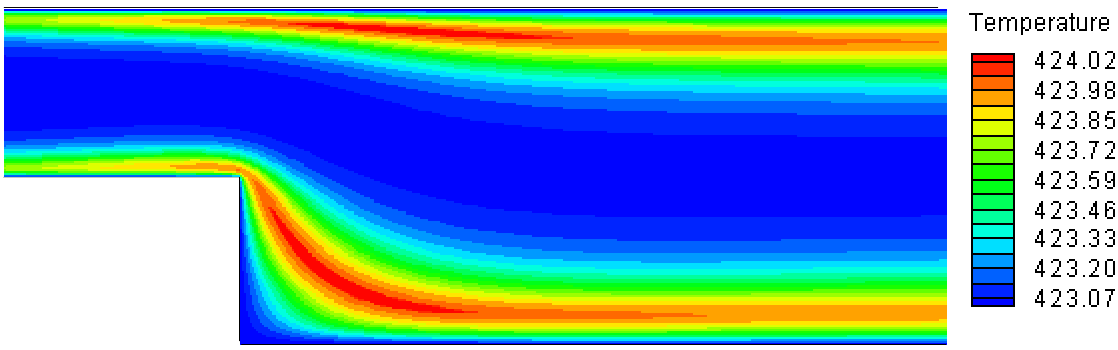

Figure 4. Temperature distribution for T_{in} = 423.0K.

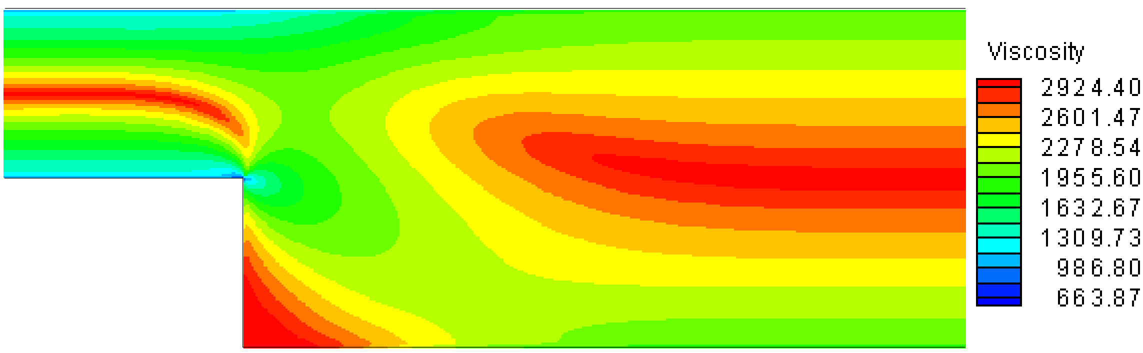

Figure 5. Viscosity distribution for T_{in} = 423.0K.

The mean pressure drop from inlet to exit channel sections for different inlet temperatures is shown in fig. (6). The temperatures simulated are $T_{in} = T_w = 423.0$, 438.0, 453.0, 468.0 and 483.0. Clearly, the effect of temperature is evinced when an increase of 60K leads to a pressure drop decrease of around 68%. This result demonstrates the great influence of temperature on pressure variations and consequently on power required to pump the polymer inside a mould cavity. A third order polynomial curve fits the data with the determination coefficient R = 0.999 in the temperature range studied.

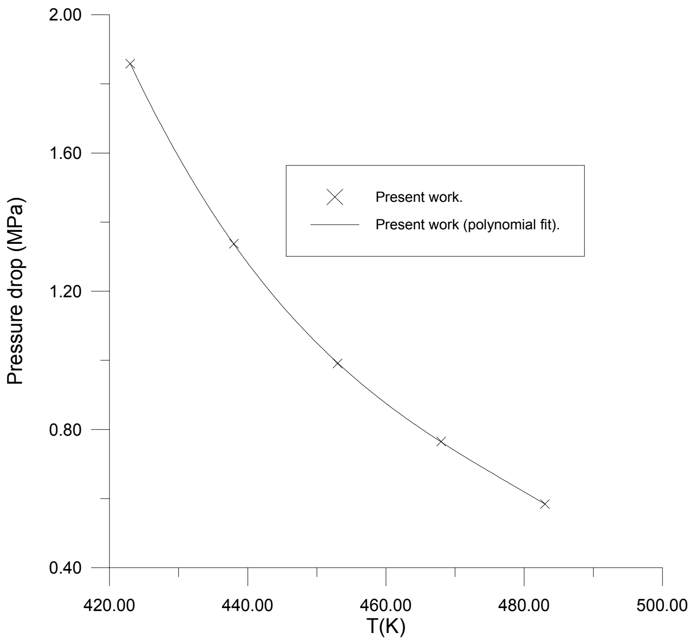

Figure 6. Mean pressure drop from inlet to exit channel sections for $T_{in} = T_w$.

The results presented in figs. (7) to (12) compare the preceding solution ($T_{in} = T_w = 423.0$) with the one obtained by applying higher inlet temperature, e.g., $T_{in} = 443.0$K and $T_w = 423.0$K. Having in mind that, in industrial applications, the mould cavity is always maintained at lower wall temperature due to cooling system, the problem $T_w < T_{in}$ is more realistic than $T_w = T_{in}$. Temperature, velocity and viscosity distributions at selected stations x/h (where x is measured from the expansion section) are plotted in order to evaluate the differences between two solutions. The attention is focused on the neighborhood of the expansion section, e.g., x/h = 0.052; 0.32; 1.76.

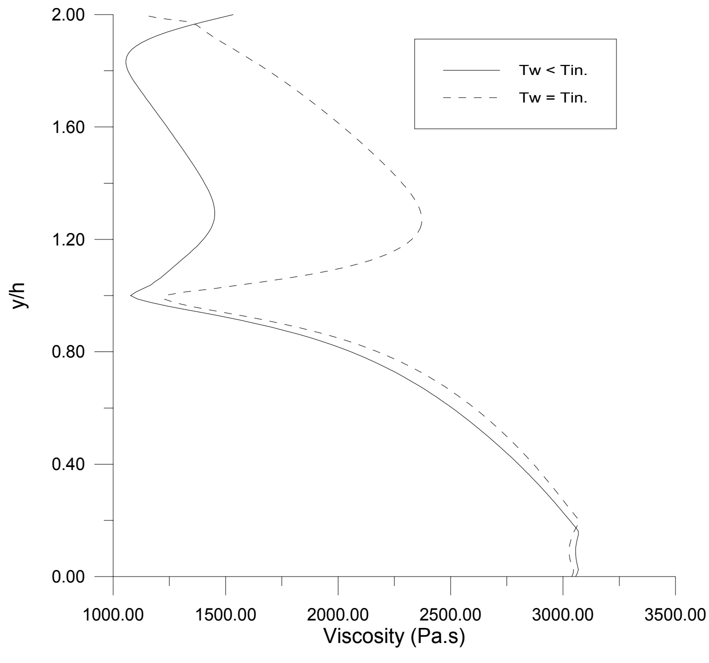

Figure 7. Viscosity distribution from y = 0 (lower wall) to y = 2h (upper wall) for x/h = 0.052.

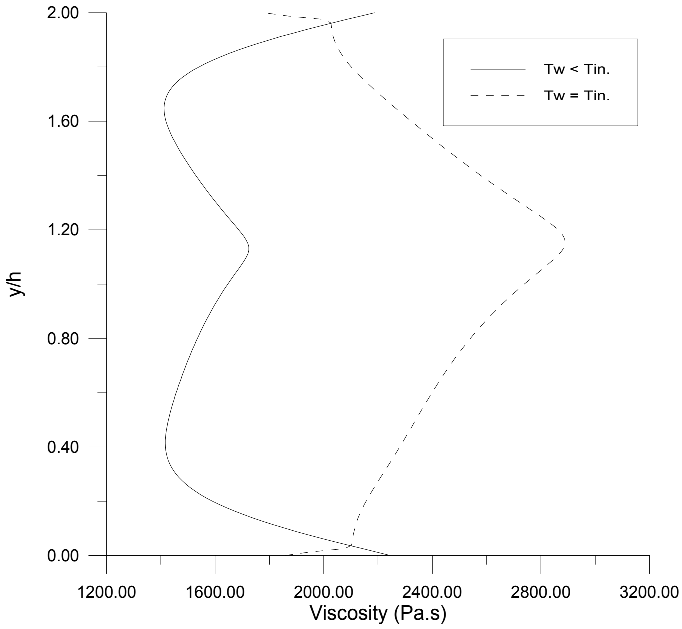

Figure 8. Viscosity distribution from y = 0 (lower wall) to y = 2h (upper wall) for x/h = 1.76.

Figures (7) and (8) present viscosity distribution for the problems analyzed. It can be observed that there are drastic differences in the two solutions. Viscosities are lower all over the cross-stream section for $T_w < T_{in}$, except near the wall where an opposite behavior is identified. Noticeably, the viscosity is strongly affected by polymer temperature. What has happened in the near wall region, where an odd behavior was observed (see fig. (8))? The answer is related to the higher shear rate characteristic of near wall regions, which depends on velocity gradient. Indeed, the problem is strongly coupled because viscous heating grows with both increasing viscosity and shear rate. Otherwise, the viscosity reduces with both increasing temperatures and shear rate thereby rendering lower viscous heating.

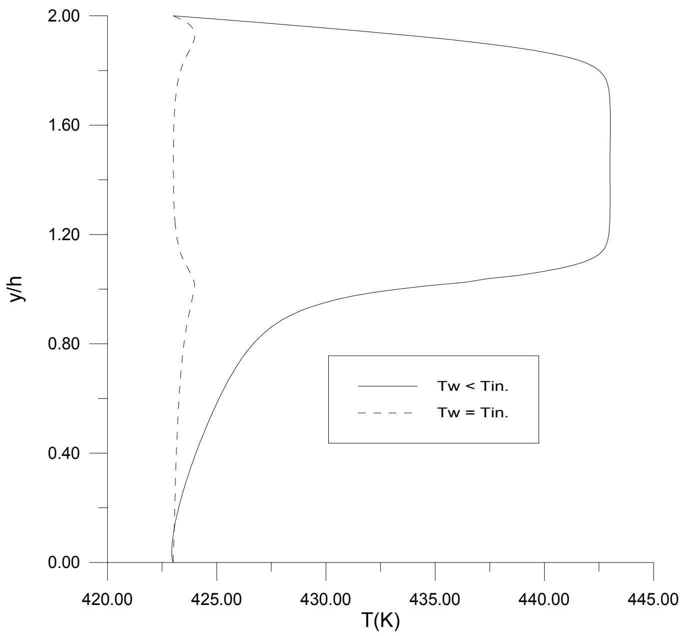

Figure 9. Temperature distribution from y = 0 (lower wall) to y = 2h (upper wall) for x/h = 0.052.

Figures (9), (10) and (11) show the temperature profiles for cross-stream sections x/h = 0.052; 0.32; 1.76. Noticeably, for $T_w = T_{in}$, the viscous heating effect may be fully appreciated at Fig. (9) where two bumps (y/s ≈ 1.0 and y/s ≈ 1.95) in the curve are identified. Otherwise, for $T_w < T_{in}$, the viscous heating effect is overwhelmed by the strong temperature gradient that exists between the flow core and the channel walls. This observation is in agreement with the work of Koh et al. (2003) for a plane channel. Furthermore, it is interesting to note that temperature distribution plotted in fig. (11) is very similar to the one for plane channels at the entry region (Zdanski and Vaz Jr., 2006a). Therefore, the effect of expansion is very much restricted to its neighborhood. Besides, from viscosity and temperature distributions one can realize that higher temperatures lead to lower viscosities, an observation that obviously agrees with the constitutive law used to model the non-Newtonian behavior of the flow.

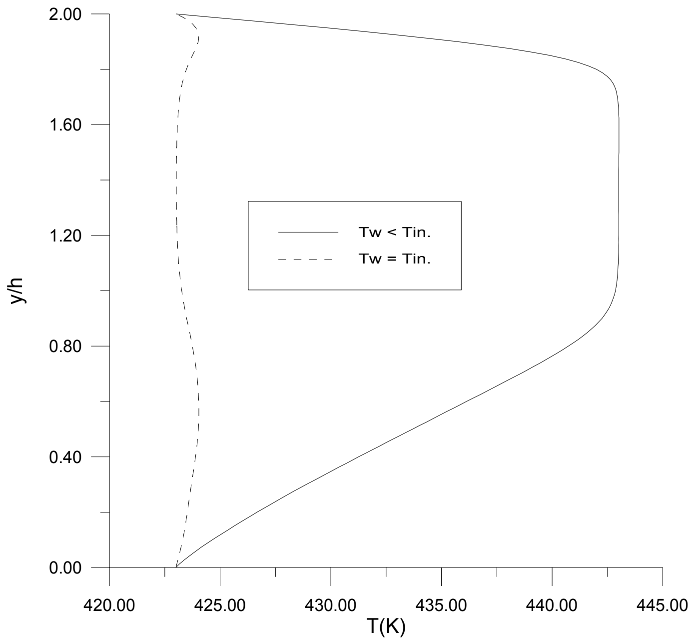

Figure 10. Temperature distribution from y = 0 (lower wall) to y = 2h (upper wall) for x/h = 0.32.

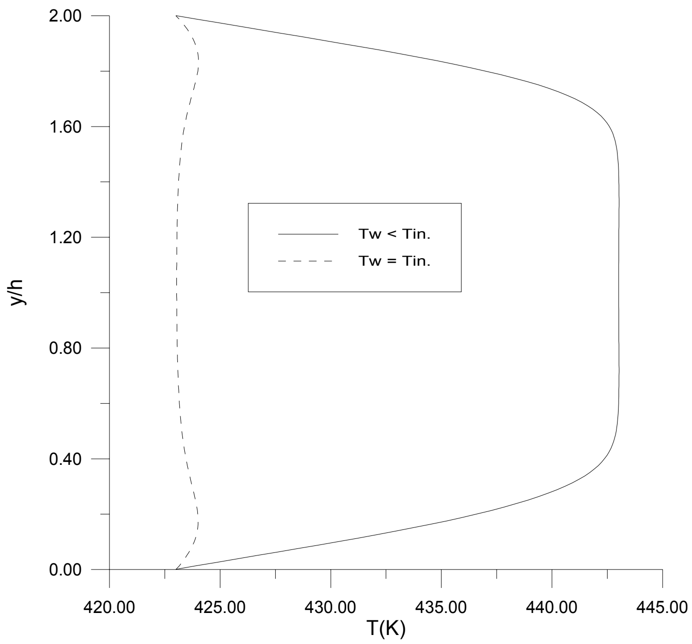

Figure 11. Temperature distribution from y = 0 (lower wall) to y = 2h (upper wall) for x/h = 1.76.

Figure (12) presents the velocity profiles for the cross-stream sections analyzed. The differences between the two thermal problems are remarkably clear. The main conclusion that one can draw from results is as follows: if $T_w = T_{in}$, the velocity gradient near the wall is higher with consequent higher shear rates. Therefore, such behavior may explain the odd variation of viscosities detected near the wall regions shown in figs. (7) and (8), i.e., higher shear rates near walls leads to lower viscosities. The findings may be summarized as follows: in the center of the channel the temperature is more important (shear rate is low) so that high temperature values lead to lower viscosities (see figs (7) and (8)). At the neighborhood of walls, in spite of the higher temperatures for $T_w < T_{in}$, the shear rate is higher for the case $T_w = T_{in}$, overwhelming the effect of temperature and rendering a low viscosity.

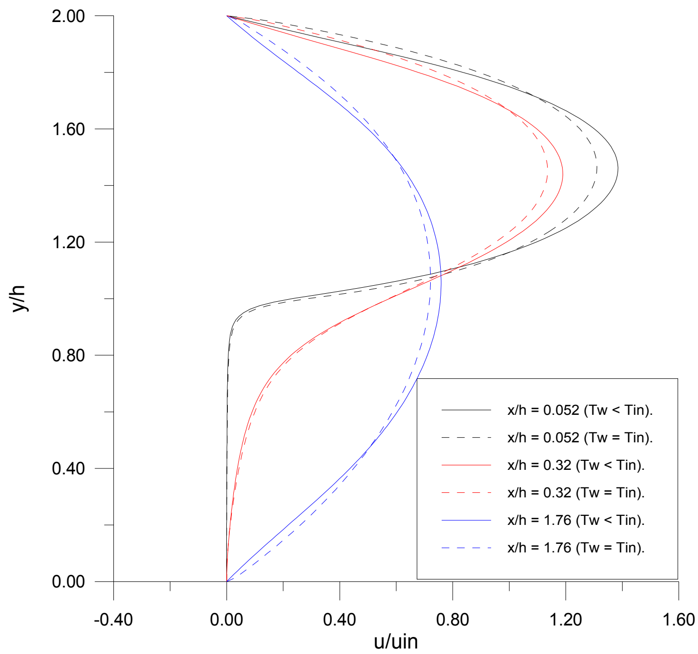

Figure 12. Velocity profiles from y = 0 (lower wall) to y = 2h (upper wall).

4. Conclusions

The Polymer melt flow in sudden expansions is studied numerically. The generalized Newtonian formulation is adopted being the non-Newtonian behavior of the flow described by the Cross constitutive relation. The numerical method was able to handle successfully the strong non-linearity and coupled character of the problem. The results obtained clearly show that, in such problems, any reliable solution must account for the thermal effects. The findings may be summarized as follows: (i) when $T_w = T_{in}$, viscous heating leads to a maximum temperature rise of 1K in the range studied; otherwise, if $T_w < T_{in}$ the steep temperature gradient between mean core and channel walls inhibits viscous heating effects at the expansion section; (ii) pressure drop in the channel is strongly affected by temperature; in the range studied, a temperature rise of 60K leads to a reduction in the mean pressure drop of around 68%; (iii) near the walls, the shear rate dominates the physical scenario thereby eclipsing the temperature effects upon viscosity distribution; this fact basically explains the odd behavior verified at figs. (7) and (8) in the region near the channel walls.

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