A FINITE VOLUME METHOD FOR SIMULATION OF POLYMER MELT FLOW IN CLOSED CHANNELS

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Abstract. *Numerical simulation of polymer injection processes has become increasingly common in mould design. This simulation activity in industry is accomplished mainly by using commercial packages. Due to complexities inherent of this class of problems, most codes attempt to combine realistic rheological descriptions with simplified numerical models. In spite of the apparent success, such approaches are not able to capture important aspects of the polymer melt flow. In the present work a more elaborated mathematical model is used to simulate such problem. The mathematical model comprises the momentum equations and a Poisson equation for pressure, being the flow considered laminar and isothermal. The equations are discretised using the finite volume method based on central, second order accurate formulas for both the convection and diffusion terms. Artificial dissipation terms are added externally in order to control the odd-even de-coupling problem. The simulations presented in this work adopt a power-law based viscosity function to approach the non-Newtonian behaviour of the polymer melt flow. Some physical and numerical aspects are discussed, e.g., the velocity profiles in the entry region and the calibration of artificial viscosity terms. The scheme has shown robust to handle the high non-linearity and coupled character of the problem, and the numerical results were found in agreement with those available in the literature.*

Keywords*: Finite volume, non-Newtonian flow, numerical analysis*

1. Introduction

The development of numerical methods for simulation of polymer melt flow inside channels has gained widespread attention in the last years. The success of these simulations is mainly linked with two distinct features, e.g., realistic rheological descriptions of the polymer melt flow and adoption of an adequate mathematical model. Besides, another important aspect is related to numerical accuracy of the scheme, e.g., the formulae adopted to discretize the derivatives in the governing equations. Indeed, the scheme must have both robustness, to handle the strong non-linearity of the problem, and accuracy for credibility of the results.

In the literature, the landmark work in this subject was Hieber and Shen's (1980) proposition on using the Hele-Shaw approximation to simulate polymer melt flow. This model reduces 3D flows to 2D approximations (plane channels) by assuming that the thickness is much smaller than the channel characteristic length, being the flow properties represented as an average value along the thickness. Such approach is used in commercial packages as C-MOLD and MOLD-FLOW. The fact on using mean properties along the thickness precludes a deeper physical analysis of the flow, being a drawback of the Hele-Shaw formulation. In this context, many works have been elaborated using more realistic formulations to describe the flow and new numerical methods to simulate the problem. Syrjälä (2002) proposes a high order finite element method to simulate the non-Newtonian flow of a power-law fluid in ducts with arbitrary cross-sections. The aim of that work was the prediction of friction factor and the Nusselt number for the fully developed flow regime. Koh et al (2004) have adopted the SIMPLER algorithm (Patankar, 1980) to solve numerically the polymer melt flow inside plane channels. The mathematical model used by the authors is the 2D momentum and energy equations together with three distinct constitutive laws to simulate the non-Newtonian behavior of the polymer. Vaz Jr. and Gaertner (2003) discuss issues about rheological instability that can occur due to viscous heating on polymer melt flow inside channels. The authors adopt the fully developed momentum and energy equations and the numerical solution is attained by a finite volume method. Wei and Luo (2003) adopt the Galerkin finite element method, combined to a temperature-dependent power-law viscosity function, to simulate the problem. The authors were concerned with describing the numerical model and the effect of viscous dissipation on the temperature distributions. The finite difference technique has also been employed to simulate non-Newtonian flows inside channels, such as the works of Manica and De Bortoli (2004) and Zdanski and Vaz Jr. (2005).

The purpose of this paper is to devise a numerical method, based on a finite volume formulation, to simulate the polymer melt flow inside plane channels. The scheme has second order spatial accuracy and uses artificial smoothing terms to control numerical oscillations. The method follows a pseudo-transient march in time, being adopted the explicit Euler method, aiming at the steady-state solution. The mathematical model adopted is the 2D momentum equation in conjunction with a Poisson equation for pressure. In the present analysis the flow is considered isothermal and the power-law model is used to describe the non-Newtonian behavior. Some results featuring both the calibration of artificial viscosity terms and the development of the hydrodynamic boundary layer are reported. The validation of the numerical method is performed by comparing with the analytical solution for the case of a fully developed regime.

2. Theoretical formulation

2.1. Governing equations

The mathematical model for the analysis comprises the 2D momentum equations and a Poisson equation for pressure. The flow is considered two-dimensional, incompressible, laminar and isothermal. The momentum equations, written in conservation law form and for the Cartesian coordinate system, are expressed as

$$\frac{\partial Q}{\partial t}+\frac{\partial E}{\partial x}+\frac{\partial F}{\partial y}=0\ , \tag{1}$$

where Q is the vector of conserved variables,

$$Q=\begin{Bmatrix} ru \\ rv \end{Bmatrix}, \tag{2}$$

u and v are the velocity vector components, and E and F the flux vectors,

$$E=E_e-E_v\,,\ F=F_e-F_v\,, \tag{3}$$

$$E_e=\begin{Bmatrix} ruu+p \\ ruv \end{Bmatrix},\ E_v=\begin{Bmatrix} t_{xx} \\ t_{yx} \end{Bmatrix}, \tag{4}$$

$$F_e=\begin{Bmatrix} ruv \\ rvv+p \end{Bmatrix},\ F_v=\begin{Bmatrix} t_{xy} \\ t_{yy} \end{Bmatrix}, \tag{5}$$

in which subscripts e and v indicate inertia and viscous terms respectively. In the preceding expressions p is the static pressure and r is the specific mass. The formulae for computing the viscous stresses are given by

$$t_{xx}=2h\left(\frac{\partial u}{\partial x}\right),\ t_{yy}=2h\left(\frac{\partial v}{\partial y}\right), \tag{6}$$

$$t_{xy}=t_{yx}=h\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right). \tag{7}$$

The variable h [Eqs.(6) and (7)] is usually known as apparent viscosity, and accounts for the non-Newtonian behavior of the polymer melt flow. In the present research, the power-law model is adopted for computing the apparent viscosity, i.e,

$$h=m\,\dot{g}^{n-1}\,, \tag{8}$$

where m and n are material parameters (for a specific polymer), and $\dot{g}$ is the shear rate,

$$\dot{g}=\sqrt{2\left(\frac{\partial u}{\partial x}\right)^2+\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)^2+2\left(\frac{\partial v}{\partial y}\right)^2}\ . \tag{9}$$

The static pressure, p, which appears in the momentum equations, need also to be determined. For incompressible flows, the pressure is linked to the velocity field, and some pressure-velocity coupling method needs to be employed. The procedure used here follows the same route of Zdanski et al. (2004): (i) derive the x-y-momentum equations with respect to x and y, respectively; (ii) add the two equations resulting from the procedure (ii); and (iii) introduce the continuity equation, i.e, free divergence for the velocity field. The final result is a Poisson equation for pressure

$$\frac{\partial e}{\partial x}+\frac{\partial f}{\partial y}=0\,, \tag{10}$$

being the flux vectors e and f are given by

$$e=e_e+e_p-e_v-e_c\,,\ \ f=f_p+f_e-f_v-f_c\,, \tag{11}$$

$$e_p=\frac{\partial p}{\partial x},\ e_e=\frac{\partial(ruu)}{\partial x}+\frac{\partial(ruv)}{\partial y},\ e_v=\frac{\partial t_{xx}}{\partial x}+\frac{\partial t_{xy}}{\partial y},\ e_c=\frac{1}{\Delta t}(ru), \tag{12}$$

$$f_p=\frac{\partial p}{\partial y},\ f_e=\frac{\partial(ruv)}{\partial x}+\frac{\partial(rvv)}{\partial y},\ f_v=\frac{\partial t_{yx}}{\partial x}+\frac{\partial t_{yy}}{\partial y},\ f_c=\frac{1}{\Delta t}(rv), \tag{13}$$

where Δt represents the time increment.

2.2. Numerical method

The equations of the mathematical model are discretized using the finite volume method. The grid arrangement is collocated, being all variables stored at the center of the control volume. Central second order accurate formulas are adopted for discretization of both convection and diffusion terms. Artificial smoothing terms are added to control the numerical oscillations. The pressure-velocity coupling is treated on solving a Poisson equation for pressure [Eq. (10)]. The final algorithm solves the equations in two distinct blocks, i.e., momentum and pressure.

The discrete expressions are obtained by integrating the governing equations in a control volume, as represented in Fig. (1), in which *n*, *s*, *e* and *w* represent the control volume faces and *n-ne*, *n-nw*, *s-se*, *s-sw*, *w-nw*, *w-sw*, *e-ne* and *e-se* are located at the interface of the corresponding volumes. From integration of the momentum equation, [Eq. (1)], one obtains

$$\iiint\frac{\partial Q}{\partial t}\,dxdydt+\iiint\frac{\partial E}{\partial x}\,dtdydx+\iiint\frac{\partial F}{\partial y}\,dtdxdy=0\,, \tag{14}$$

$$Q^{k+1}{}_P=Q^k{}_P-\frac{\Delta t}{\Delta x\Delta y}\left\{\left[E_e^k-E_w^k\right]\Delta y+\left[F_n^k-F_s^k\right]\Delta x\right\} \tag{15}$$

The Euler explicit method was adopted for time, while central formulae were used for space discretization. The flux vectors are composed by the inertia (E_e) and viscous terms (E_v). The final expressions are

$$(E_e)_e=\begin{Bmatrix}(ruu+p)_e\\(rvu)_e\end{Bmatrix},\ (E_v)_e=\begin{Bmatrix}(t_{xx})_e\\(t_{xy})_e\end{Bmatrix}, \tag{16}$$

being the viscous stress given by Eqs. (6) and (7). The variables are stored at the center of the control volumes, but according Eq. (16) for convection terms, their values at the control volume face need to be estimated. The following procedure was adopted, i.e.,

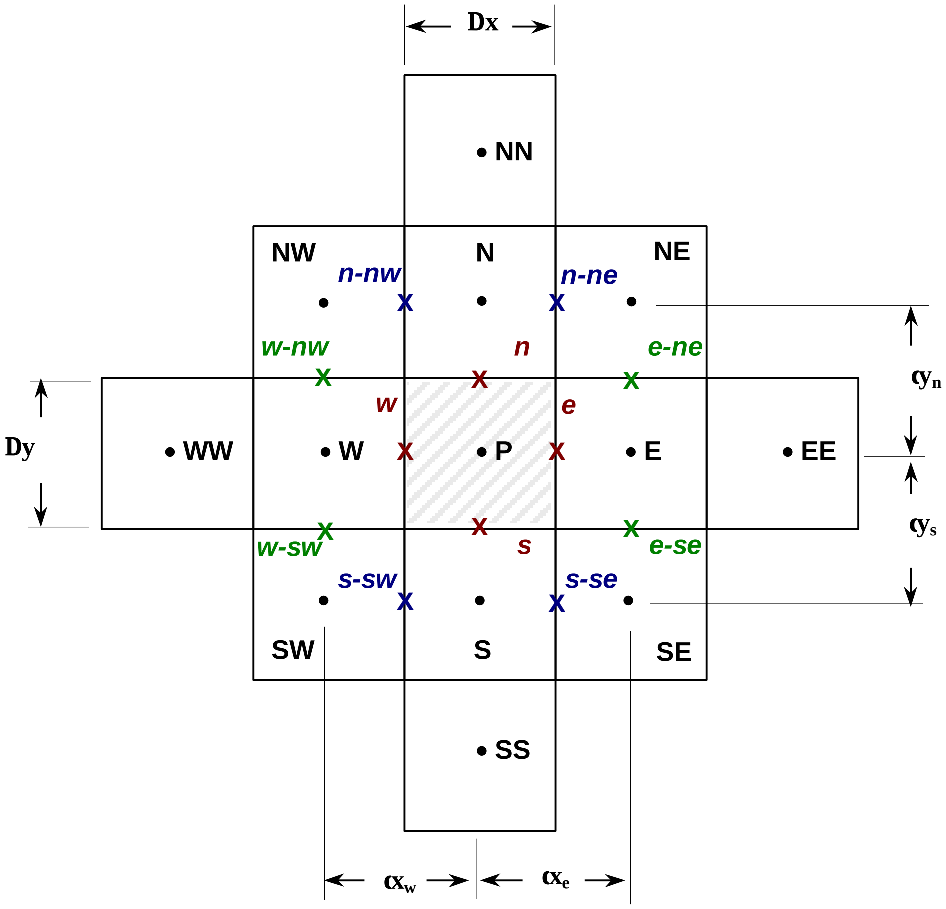

Figure 1. Representation of the main control volume with its neighbors

$$(ruu+p)_e = \frac{(ruu+p)_E + (ruu+p)_P}{2}\,, \tag{17}$$

which corresponds to standard central discretization. The viscous terms are dicretized according to the following

$$(t_{xx})_e = 2\left(\frac{h_E + h_P}{2}\right)\left(\frac{u_E - u_P}{\delta x_e}\right), \tag{18}$$

$$(t_{xy})_e = \left(\frac{h_E + h_P}{2}\right)\left\{\left[\frac{(u_{NE} + u_N)/2 - (u_{SE} + u_S)/2}{\delta y_n + \delta y_s}\right] + \left(\frac{v_E - v_P}{\delta x_e}\right)\right\}. \tag{19}$$

It is well known in literature that use of central dicretization for the convection terms may lead to unrealistic solutions with numerical oscillations (Patankar, 1980). In order to control this problem, artificial dissipation terms are introduced. This procedure was successful to control the problem in the author's previous works dealing with Newtonian (Zdanski et al., 2004 and 2005) and non-Newtonian flows (Zdanski and Vaz Jr., 2005). In the present paper the finite volume discretization is adopted whereas the previous works used finite differences. The artificial smoothing terms are externally added to Eq.(15), and correspond to fourth order derivatives. The final discrete expression is

$$Q_P^{k+1} = Q_P^k - \frac{\Delta t}{\Delta x\,\Delta y}\left\{\left[E_e^k - E_w^k\right]\Delta y + \left[F_n^k - F_s^k\right]\Delta x\right\} - e_e \Delta x^4 D_{x\,P}^k - e_e \Delta y^4 D_{y\,P}^k\,, \tag{20}$$

where k is the time step and

$$D_{x_P} = \frac{\left(Q_{EE} - 4Q_E + 6Q_P - 4Q_W + Q_{WW}\right)}{\Delta x^4} \quad \text{and} \quad D_{y_P} = \frac{\left(Q_{NN} - 4Q_N + 6Q_P - 4Q_S + Q_{SS}\right)}{\Delta y^4}. \tag{21}$$

The coefficient ε_e, appearing in Eq.(20), controls the level of artificial dissipation added. The calibration indicates that ε_e = 3.0 was adequate to both control numerical oscillations and assure convergence of the iterative process. According to Eq. (20), to solve the system of algebraic equations the explicitly point Jacobi method was used.

The Poisson equation for pressure is discretized in a similar fashion, but without adding artificial smoothing terms. The integration of Eq.(10) over a control volume [Fig.(1)] will be as follows,

$$\iint \frac{\partial e}{\partial x} dydx + \iint \frac{\partial f}{\partial y} dxdy = 0\ , \tag{22}$$

being the result expressed by

$$\left[(e)_e - (e)_w\right]\Delta y + \left[(f)_n - (f)_s\right]\Delta x = 0\,. \tag{23}$$

The flux vectors (e) and (f) are defined in Eqs.(11), (12) and (13). The terms (e_e), (e_c) and (e_v) are evaluated at time step k following the procedure described in Eqs.(17), (18) and (19). The flux vector containing the pressure, (e_p), has a rather distinct treatment, i.e.,

$$\left(e_p\right)_e - \left(e_p\right)_w = \left(\frac{p_E^k - p_P^{k+1}}{\delta x_e}\right) - \left(\frac{p_P^{k+1} - p_W^k}{\delta x_w}\right), \tag{24}$$

$$\left(f_p\right)_n - \left(f_p\right)_s = \left(\frac{p_N^k - p_P^{k+1}}{\delta y_n}\right) - \left(\frac{p_P^{k+1} - p_S^k}{\delta y_s}\right). \tag{25}$$

Therefore, the final form of discretized pressure equation is given by

$$p_P^{k+1} = \frac{1}{A_p}\left[\frac{\Delta y}{\delta x_e} p_E^k + \frac{\Delta y}{\delta x_w} p_W^k + \frac{\Delta x}{\delta y_n} p_N^k + \frac{\Delta x}{\delta y_s} p_S^k + \Delta y\, Bx_P^k + \Delta x\, By_P^k\right], \tag{26}$$

where

$$A_p = \frac{1}{\left(\dfrac{\Delta y}{\delta x_e} + \dfrac{\Delta y}{\delta x_w} + \dfrac{\Delta x}{\delta y_n} + \dfrac{\Delta x}{\delta y_s}\right)}, \tag{27}$$

$$\begin{aligned} Bx_P^k = & \left\{\left[\frac{(ruu)_E - (ruu)_P}{\delta x_e}\right] + \left[\frac{(rvu)_{n-ne} - (rvu)_{s-se}}{\delta y_n + \delta y_s}\right]\right\} - \left\{\left[\frac{(ruu)_P - (ruu)_W}{\delta x_w}\right] + \left[\frac{(rvu)_{n-nw} - (rvu)_{s-sw}}{\delta y_n + \delta y_s}\right]\right\} + \\ & - \left\{\left[\frac{(t_{xx})_E - (t_{xx})_P}{\delta x_e}\right] + \left[\frac{\left(t_{xy}\right)_{n-ne} - \left(t_{xy}\right)_{s-se}}{\delta y_n + \delta y_s}\right]\right\} + \left\{\left[\frac{(t_{xx})_P - (t_{xx})_W}{\delta x_w}\right] + \left[\frac{\left(t_{xy}\right)_{n-nw} - \left(t_{xy}\right)_{s-sw}}{\delta y_n + \delta y_s}\right]\right\} + \\ & - \frac{1}{\Delta t}\left[\frac{(ru)_E - (ru)_W}{2}\right] \end{aligned} \quad . \tag{28}$$

The discretization of the viscous stress follows the principles expressed in Eq. (17) and (18). A similar expression can be obtained for By_P^n, contained the terms for y direction. The final algorithm consists in the following steps: (i) guess an initial pressure, velocity and viscosity field; (ii) solve the momentum equations explicitly, Eq. (20); (iii) solve the Poisson equation for pressure, Eq. (26); (iv) update the velocity and pressure field; (v) calculate the new viscosity distribution from Eq. (8); (vi) return to step (ii) and iterate until the convergence be reached.

3. Results and discussions

The flow inside 2D channel was adopted as a reference case for demonstrating the capability of the scheme to handle non-Newtonian flows. The geometry with its main dimensions is represented in Fig.(2). The channel thickness is $h = 15\ mm$, being adopted a uniform mesh size for mapping the computational domain. The uniform inlet velocity is $U_0 = 16\ cm/s$, being applied a parabolic boundary condition at the exit section. For pressure, a linear variation is imposed as boundary condition for both, the channel entrance and exit. In the present simulations, the rheological parameters $m = 18332.63$ and $n = 0.361$ [Eq.(8)] have been obtained from Pedro Bom at al. (2000), and correspond to the Poliacetal POM-M90-44 at temperature 493 K.

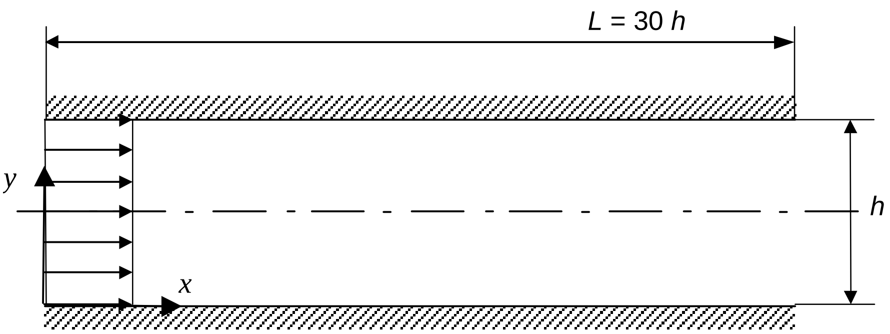

Figure 2. Representation of the geometry with its main dimensions

Firstly, for validation purposes, the velocity and shear rate profiles, at the exit section of the channel, are presented at Figs.(3a) and Figs.(3b). Noticeably, at such channel position the flow regime is fully developed and the analytical solution for the power-law are given by

$$\frac{u(y)}{\bar{u}} = \left(\frac{2n+1}{n+1}\right)\left[1-\left(\frac{2y}{h}\right)^{\frac{n+1}{n}}\right] \qquad \text{and} \qquad \dot{g} = \left|\left[\left(\frac{h}{2m}\right)\frac{\Delta p}{L}\right]^{1/n}\left(\frac{2y}{h}\right)^{1/n}\right|, \tag{29}$$

respectively for velocities and shear rate, where $\bar{u}$ is the average velocity along the cross-section. The agreement between numerical and analytical solutions is quite satisfactory for all cases tested. Figures (3a) and (3b) illustrate the results for meshes *161 x 41*, *161 x 31* and *161 x 21* points (*x* and *y* directions).

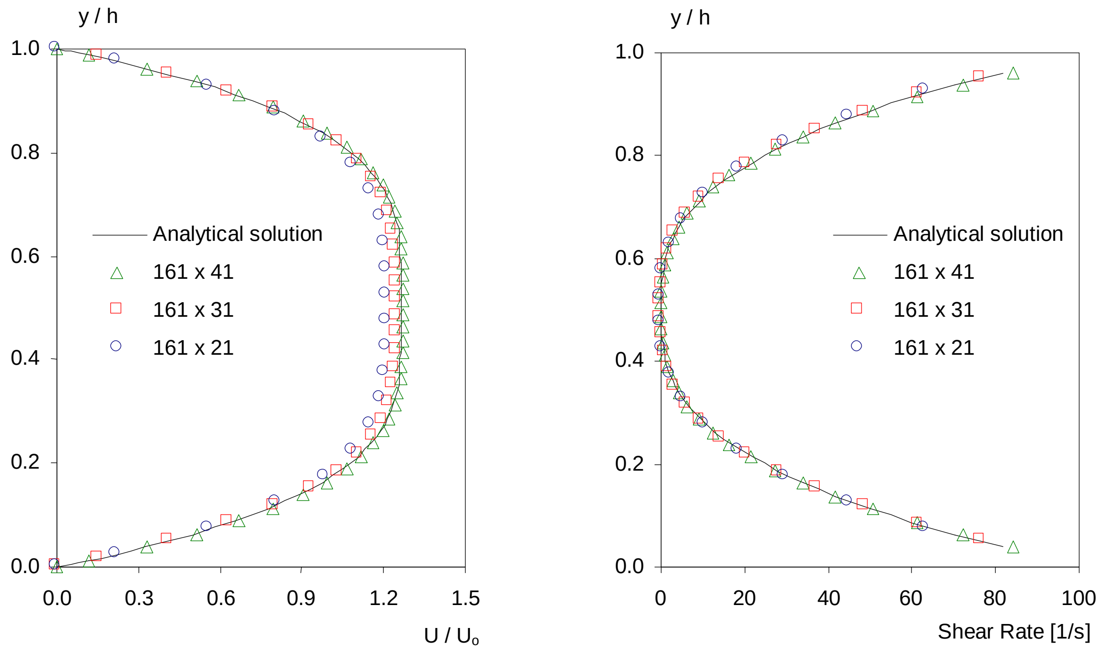

Figure 3. Fully developed velocity and shear rate distributions for the exit channel

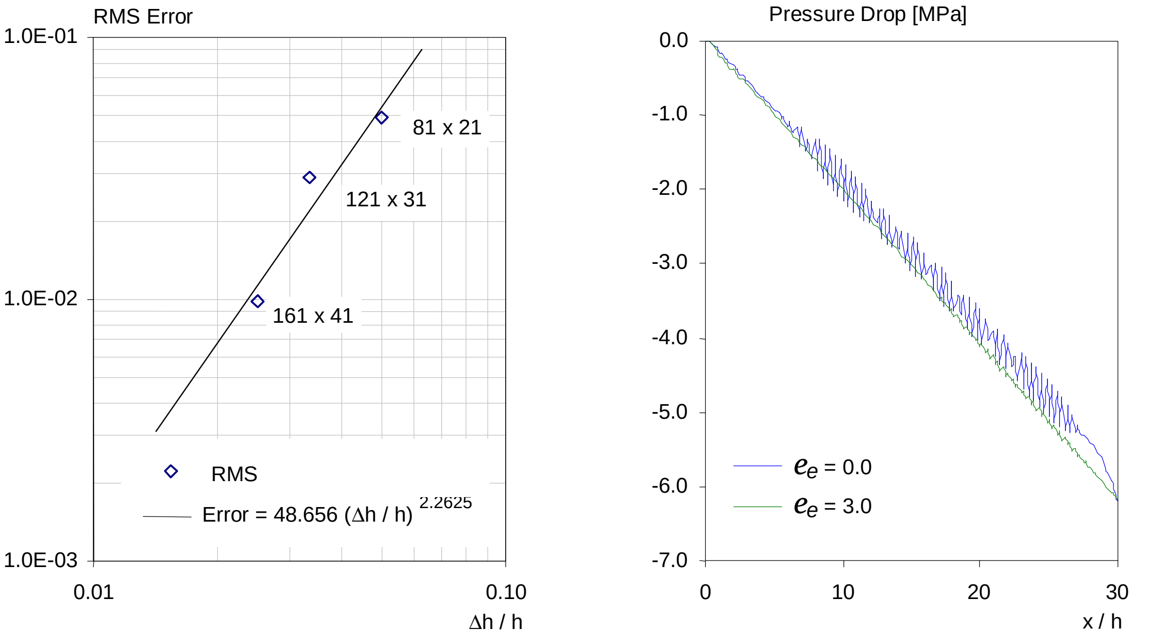

Figure 4. Root Mean Square error and pressure drop along the channel

Figure (4a) illustrates the global convergence of the method. The Root Mean Square (RMS) of the error for three grid resolutions is computed at the channel exit and compares the analytical and numerical solutions for fully developed flow. The pressure distribution at the center of the channel along downstream direction is represented at Fig. (4b). These results clearly illustrate the control of numerical oscillations by artificial viscosity. As expected, the pressure distribution when $e_e = 0$ presents spurious oscillations with high amplitude. Otherwise, the numerical oscillations were almost eliminated when $e_e = 3.0$. Therefore, the odd-even decoupling, a typical problem when using collocated arrangement and central formulae to discretize the convection terms, is adequately controlled by artificial viscosity. In spite of the success on controlling spurious oscillations, some strategy must be employed for avoiding artificial viscosity to compete with physical terms. In the present work, a cut-off value was implemented in the code, i.e., the artificial dissipation terms may not be greater than *1%* of the physical viscous terms when convergence is assured. Thus, the final solution is not contaminated with artificial viscosity, assuring the accuracy of the scheme.

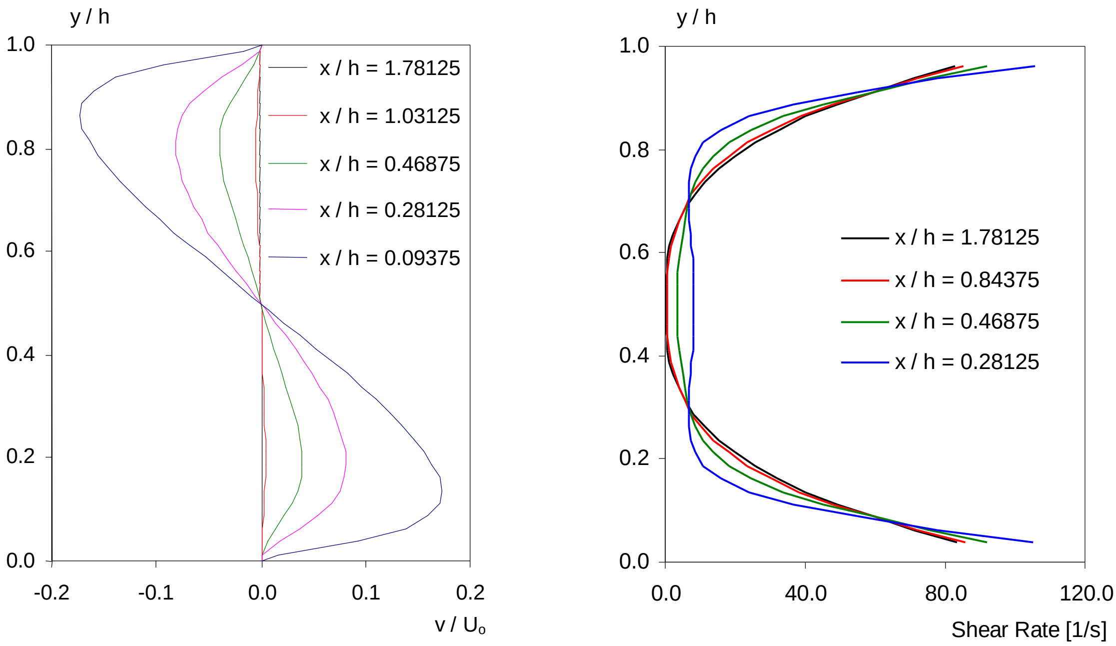

Figure 5. *Y* velocity and shear rate distributions at the entry region

Some aspects featuring the hydrodynamic and thermal boundary layer development for polymer melt flow inside 2D channels were discussed at Zdanski and Vaz Jr. (2005). The emphasis of that work was the analyses of influences of the inlet velocity upon temperature distributions over channel cross-sections and along downstream direction. However, the velocity and shear rate profiles at the entrance region were not discussed in details. Figures (5a) and (5b) present profiles for v (the y velocity component) and $\dot{\gamma}$ at some stations x/h inside the channel. An interesting aspect is related to the magnitude of the y velocity component that may reach a maximum value around *18 %* of U_0 (entrance velocity) at $x/h \cong 0.1$. This behavior is explained by the high growing rate of the hydrodynamic boundary layer thickness due to high viscosity of the polymer. The shear rate at the center of the channel has a non-vanishing value at the entrance region, which may be observed in Fig.(5b). It is interesting to note that this result was already expected because the gradient of velocity components with respect x and y directions are not zero at the entry region.

4. Conclusions

A scheme for numerical simulation of non-Newtonian flows inside channels was presented. The method is based on a finite volume formulation and adopts central second-order accurate formulas to discretize both the convective and diffusive terms. The numerical oscillations are controlled by artificial smoothing terms. The results obtained are very encouraging and demonstrate the potential of the method to handle non-Newtonian flows.

5. Acknowledgements

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7. Responsibility notice

The authors P.S.B. Zdanski, M. Vaz Jr. and M. Schmidt are the only responsible for the printed material included in this paper.