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A CONTROL VOLUME METHOD FOR NON-NEWTONIAN FLOW AND ITS APPLICATION TO POLYMER PROCESSING

X.-L. LUO

CSIRO Division of Mathematics & Statistics
PO Box 218, Lindfield, NSW 2070, AUSTRALIA

ABSTRACT

A numerical algorithm using a control volume discretization is developed for non-Newtonian flow. The integral-type viscoelastic constitutive equation of the KBKZ family is employed for modeling polymer melts with strong viscoelastic properties. An efficient particle and strain history tracking method is incorporated into the control volume context to compute the "fading memory" stress tensor, and the non-Newtonian stress contribution is treated as a source in the control volume. Numerical modeling is carried out for the abrupt circular contraction flow of low density polyethylene (LDPE) melts, which is characterised by a strong corner vortex/recirculation growth as the elasticity in the flow is increased. A comparison of the results with the actual experiments as well as finite element computations shows very good agreement.

1. INTRODUCTION

In recent years some rapid progress has been made in the field of numerical simulation of non-Newtonian flow, mainly due to the use of realistic integral type constitutive models, particularly the KBKZ model (Luo and Tanner, 1986, 1988; Dupont and Crochet, 1988). The KBKZ model with multiple relaxation times provides good fits of shear, elongational and normal stress data for some polymer melts such as low-density and high-density polyethelyne. This model has been shown to work well for various extrusion and entry flows common in polymer processing industry. Generally speaking, integral-type models are more difficult to apply in numerical work than differential models, due to difficulties in doing accurate and efficient particle tracking and strain tensor calculations.

Up to now all the full numerical simulations of integral-type non-Newtonian fluids have used Finite Element Method (FEM). Even relatively efficient FEM algorithms for strain tensor calculation are still very time consuming, often at the expense of limiting mesh size (Luo and Mitsoulis, 1989). The Control Volume Method (CVM) provides a more efficient alternative to FEM in dealing with integral-type non-Newtonian models. The contribution of non-Newtonian stress can be naturally treated as a source term, and the particle and strain history tracking can be made very efficient by the simple grid structure in CVM, at least in the case of simple geometries. The cost of 3D simulation of non-Newtonian flow using CVM is expected to be much less than FEM. In this work we will develop the algorithm for integral-type non-Newtonian fluids in the CVM context, and demonstrate its application to the abrupt circular contraction flow of polymer melts.

2. THE NUMERICAL ALGORITHM

The flow is governed by the conservation equations of mass and momentum. For an incompressible fluid under isothermal, creeping flow conditions ($Re = 0$) we have

$$\nabla \cdot \mathbf{v} = 0 \quad (1)$$

$$\mathbf{0} = -\nabla p + \nabla \cdot \tau \quad (2)$$

where $\mathbf{v}$ is the velocity vector, τ is the extra-stress tensor and p is the scalar pressure. The constitutive equation that relates τ to the deformation history is a KBKZ equation proposed by Papanastasiou et al. (1983) and is written as:

$$\tau(t) = \int_{-\infty}^{t} \left[\sum \frac{a_k}{\lambda_k} e^{-\frac{t-t'}{\lambda_k}}\right] \times \frac{\alpha}{(\alpha-3)+\beta I_{c^{-1}} + (1-\beta) I_c} \mathbf{C}_t^{-1}(t')dt' \quad (3)$$

where λ_k and a_k are the relaxation times and relaxation modulus coefficients at a reference temperature T_0, respectively, α and β are material constants, and I_c, $I_{c^{-1}}$ are the first invariants of the Cauchy-Green tensor $\mathbf{C}_t$ and its inverse $\mathbf{C}_t^{-1}$, the Finger strain tensor.

Because the non-Newtonian stress is dependent on the entire history of deformation rate in the fluids, as indicated by equation (3), a fully coulpled solution strategy is almost impossible to apply, and the velocity and stress have to be solved iteratively, in addition to the coupling of velocity and pressure.

2.1 SIMPLE for Non-Newtonian Fluids

The SIMPLE family of algorithms was first introduced by Patankar and Spalding (1972) and is described in detail by Patankar (1980). It has been widely used in both lamilar and turbulence viscous flow computations. For integral-type non-Newtonian fluids, however, the SIMPLE method as it is cannot resolve the non-linear coupling between velocity and stress. In FEM the non-Newtonian contribution from integral stress equation is often treated as a body force. A natural extension of this idea is to put non-Newtonian stress in the source term for the control volume. Let us split the extra stress tensor τ into two parts:

$$\tau = (\tau - 2\mu\mathbf{D}) + 2\mu\mathbf{D} \quad (4)$$

where $\mathbf{D}$ is the rate of deformation tensor and μ is the viscocity. The first part contains the net non-Newtonian contribution and will be put into the source term, and the second part is simply the familiar viscous stress. Denoting the net non-Newtonian contribution as $\mathbf{T}$, The r-component of equation (2) for axisymmetric flow can be written as

$$\mu[\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u}{\partial r}) + \frac{1}{r}\frac{\partial}{\partial z}(r\frac{\partial u}{\partial z}) - \frac{u}{r^2}] =$$

$$\frac{\partial p}{\partial r} - \frac{1}{r}[\frac{\partial}{\partial r}(rT_{rr}) + \frac{\partial}{\partial z}(rT_{rz}) - T_{\theta\theta}] \quad (5)$$

Similar form can be written for the z-component. Using the staggered grid (Patankar, 1980) for velocity components, integration of equation (5) over the U-cell control volume $2\pi r^c dr dz$ gives the following discretized form

$$a_C u_C = a_E u_E + a_W u_W + a_N u_N + a_S u_S + SN$$

$$a_E = \frac{\mu r^e dz}{\delta r_E} \qquad a_W = \frac{\mu r^w dz}{\delta r_W}$$

$$a_N = \frac{\mu r^c dr}{\delta r_N} \qquad a_S = \frac{\mu r^c dr}{\delta r_S}$$

$$a_C = a_E + a_W + a_N + a_S + \frac{\mu dr dz}{r^c}$$

$$b = -r^c(p^e - p^w)dz$$

$$SN = (r^e T_{rr}^e - r^w T_{rr}^w)dz + r^c(T_{rz}^n - T_{rz}^s)dr - T_{\theta\theta}^c dr dz$$

where the superscripts e, w, w, n stand for east (+r), west (-r), south (-z) and north (+z) faces of the U-cell, and subscripts E, W, N, S indicate the neighbouring velocity nodes, and both c and C stand for the centre point in the control volume. SN is the source term due to net non-Newtonian stress.

The discretized equation for z-component is similar. The pressure correction equation is derived from continuity, thus having the same form as in a pure viscous flow.

2.2 Strain Tensor Calculation

As in FEM, the following relations are used in finding the strain history of a particle relative to the configuration at the present time t,

$$\frac{D\mathbf{F}(s)}{Ds} = -\mathbf{L}(s)\mathbf{F}_t(s) \quad (6)$$

$$\mathbf{F}_t(s)\mid_{s=0} = \mathbf{I} \quad (7)$$

$$\mathbf{C}_t^{-1}(s) = \mathbf{F}_t(s)^{-1}(\mathbf{F}_t(s)^T)^{-1} \quad (8)$$

where $s = t - t'$ is the residence time of the particle, $\mathbf{L}(s)$ is the velocity gradient, $\mathbf{F}(s)$ is the deformation tensor relative to the present configuration, $\mathbf{C}^{-1}(s)$ is the Finger strain tensor, and $\mathbf{I}$ is the unit tensor.

An improved Euler method, i.e. the predictor-corrector formula is chosen for calculating the components of $\mathbf{F}$

$$F_{rr} = 1 - \frac{ds}{2}(\frac{\partial u}{\partial r} + \frac{\partial u'}{\partial r}) + \frac{ds^2}{2}(\frac{\partial u'}{\partial r}\frac{\partial u}{\partial r} + \frac{\partial u'}{\partial z}\frac{\partial v}{\partial r}) \quad (9)$$

$$F_{rz} = -\frac{ds}{2}(\frac{\partial u}{\partial z} + \frac{\partial u'}{\partial z}) + \frac{ds^2}{2}(\frac{\partial u'}{\partial r}\frac{\partial u}{\partial z} + \frac{\partial u'}{\partial z}\frac{\partial v}{\partial z}) \quad (10)$$

$$F_{zr} = -\frac{ds}{2}(\frac{\partial v}{\partial r} + \frac{\partial v'}{\partial r}) + \frac{ds^2}{2}(\frac{\partial v'}{\partial r}\frac{\partial u}{\partial r} + \frac{\partial v'}{\partial z}\frac{\partial v}{\partial r}) \quad (11)$$

$$F_{zz} = 1 - \frac{ds}{2}(\frac{\partial v}{\partial z} + \frac{\partial v'}{\partial z}) + \frac{ds^2}{2}(\frac{\partial v'}{\partial r}\frac{\partial u}{\partial z} + \frac{\partial v'}{\partial z}\frac{\partial v}{\partial z}) \quad (12)$$

$$F_{\theta\theta} = 1 - ds\frac{u}{r} + \frac{ds^2}{2}(\frac{u}{r})^2 \quad (13)$$

where the primes indicate the values at time t'. For incompressible fluids, the determinate $|\mathbf{F}| = 1$, and one can prove the above numerical scheme gives $|\mathbf{F}| = 1 + O(ds^3)$.

3. ABRUPT CONTRACTION FLOW

The abrupt circular contraction flow experiments of White and Kondo (1978) were done with low-density-polyethylene (LDPE) melt under isothermal conditions. The material parameters in the KBKZ model to fit the shear, elongational and normal stress behaviour of LDPE melt are those ued in previous FEM computations (Dupont and Crochet, 1988, Luo and Mitsoulis, 1989). Referring to Fig.1, let L_0, L_{res} be the lengths of the downstream and upstream tubes, respectively, and let D_0 be the diameter of the downstream tube. $\frac{D_{res}}{D_0} = 5.75$ in the experiments. For our calculations we have chosen the ratios $\frac{L_0}{R_0}$ and $\frac{L_{res}}{R_0}$ to be 20 and 12, respectively. For the boundary conditions we assume there is no slip along the walls and impose a fully-developed KBKZ flow profile at the entry and at the exit sections. The relative strain tensor upstream of the entry section is calculated on the basis of the fully developed profile.The computations were performed on the grids shown in Fig.2, which contains 770 control volumes.

The vortex size in the entry flow can be quantified by the opening angle ϕ defined schematically in Fig.1. White and Kondo (1978) measured this opening angle as a function of the dimensionless recoverable shear (or stress ratio) S_R, which is a measure of elasticity level in the flow, and is defined as the ratio of the first normal stress difference N_1 to twice the shear stress τ_w, i.e. $S_R = \frac{N_1}{2\tau_w}$.

The incremental loading of elasticity is applied as part of the iteration strategy. Typically, 1500 iterations (sweeps) were needed for reducing relative change of velocity to less than 10^{-5}, and relative change in pressure to less than 10^{-3}. Despite finer mesh and more iterations, the computing time is still significantly less than FEM computations.

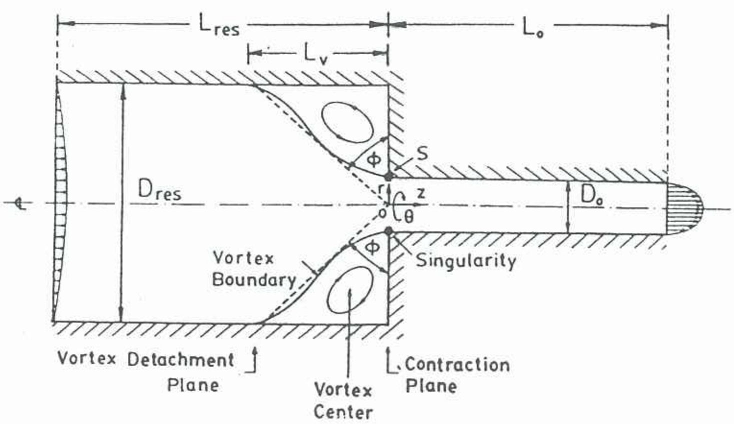

Figure 1. Schematic diagram of the circular abrupt contraction geometry and definition of the vortex opening angle ϕ

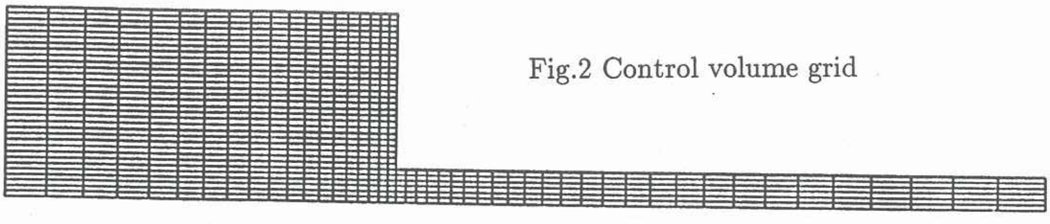

Fig.2 Control volume grid

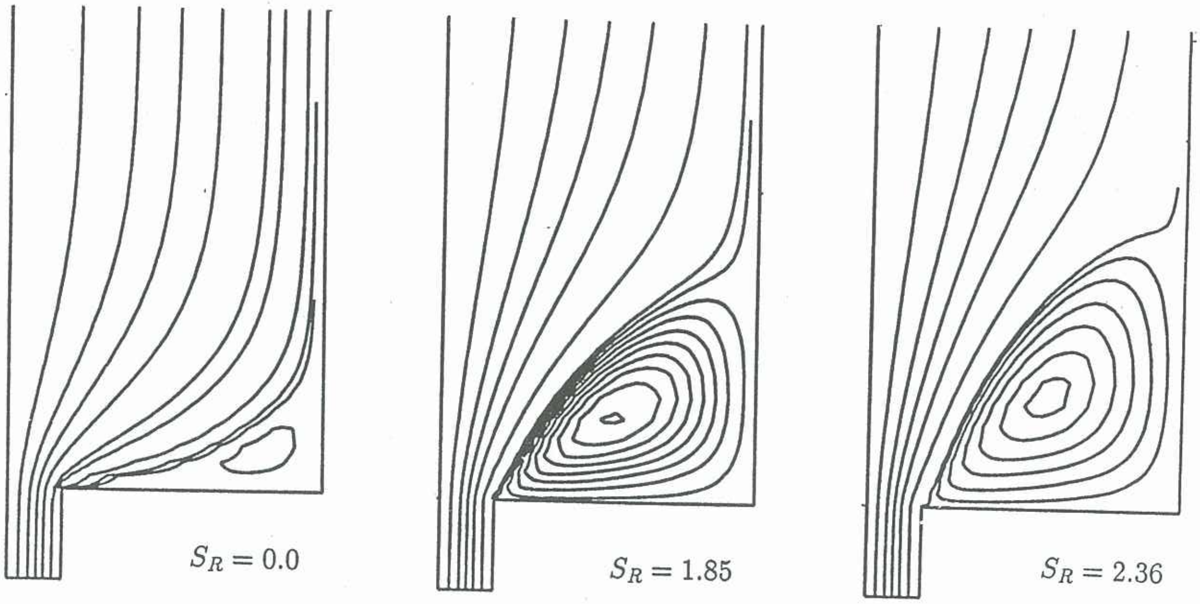

Fig.3 Streamline/vortex patterns at several S_R values.

Fig.3 shows the streamline/vortex patterns at various S_R values. The rapid vortex growth with elasticity number S_R is quite remarkable. Note in Fig.3 $S_R = 0.0$ plot corresponds to pure Newtonian flow. Quantitatively, the predicted opening angles are very close to experimantal measurements, as shown in Table 1. The maximum difference between predicted (CVM) and measured (EXP.) opening angles is only about 2 degrees. Previous FEM results are also shown in Table 1.

	ϕ		
S_R	CVM	EXP.	FEM
1.54	41^o	40^o	39^o
1.85	45^o	46^o	43^o
2.36	50^o	52^o	50^o

Table 1. Opening angles predicted and measured.

4. CONCLUSIONS

This numerical study shows the control volume method is a very attractive alternative to FEM for the modeling of non-Newtonian flow. At least in simple geometries the CVM is much more efficient than FEM in treating integral-type viscoelastic fluids, and the extension to 3D is expected to show even greater advantage of CVM over FEM.

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