An inverse problem by boundary element method

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Abstract

Boundary Element Methods (BEM) have been established as useful and powerful tools in a wide range of engineering applications, e.g. Brebbia *et al.*[1] In this paper, we report a particular three dimensional implementation of a direct boundary integral equation (BIE) formulation and its application to numerical simulations of practical polymer processing operations. In particular, we will focus on the application of the present boundary element technology to simulate an inverse problem in plastics processing by extrusion. The task is to design profile extrusion dies for plastics. The problem is highly non-linear due to material viscoelastic behaviours as well as unknown free surface conditions. As an example, the technique is shown to be effective in obtaining the die profiles corresponding to a square viscoelastic extrudate under different processing conditions. To further illustrate the capability of the method, examples of other non-trivial extrudate profiles and processing conditions are also given.

1 Introduction

Polymer extrusion is an important industrial technology with applications vary from consumer plastics products to rocket motors. The complex phenomenon of extrudate swell has kept die design and development largely an empirical and trial and error procedure[2] with associated high costs. An analytical or numerical solution to the inverse problems, i.e., the design of extrusion dies for a given extrudate profile, is highly desirable in reducing the cost. However, as reviewed by Tran-Cong and Phan-Thien[3], solutions to this problem are rare, partly because the extrudate shape is highly de-

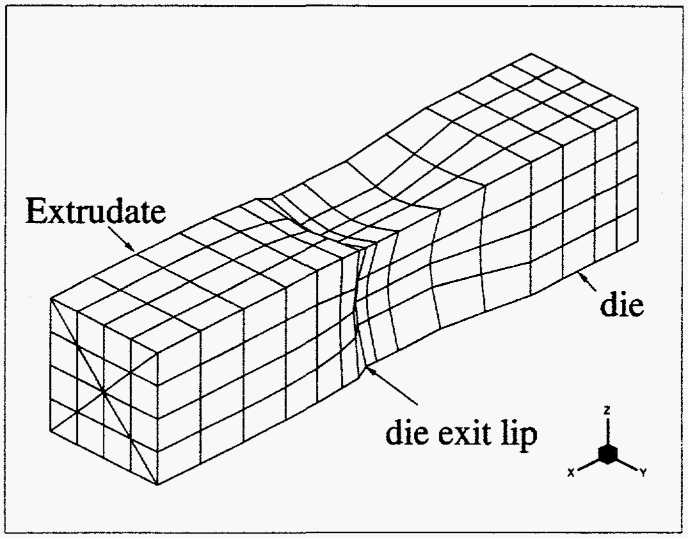

Figure 1: The die and extrudate shape for $Wi = 0.24$. The die consists of three portions. An uniform entry portion, a tapering transional portion and an uniform portion of the die near the exit, which is called the die length l. In this case $l = 1.4$.

pendent on the viscoelasticity of the melt.[4] It appears that the pioneering numerical simulation of die design problem is one based on BEM[5]. The effects of viscoelasticity and relaxation methods on the convergence characteristics of BEM solutions have been discussed previously.[3] In this paper, we review the formulation and the implementation of the present BEM for the inverse die design problem for a viscoelastic fluid of the Oldroyd variety. The die design for a square extrudate is reported, with special emphasis on the effects of die geometry on the convergence characteristics of the method. We also report some results for a more complex profile extrudate.

2 Governing equations

The steady state, isothermal and creeping flow of incompressible viscoelastic fluids is considered. The momentum balance and continuity equations are

$$\nabla \cdot \boldsymbol{\sigma} = 0, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{2}$$

where $\boldsymbol{\sigma}$ is the total stress tensor and $\mathbf{u}$ is the velocity vector.

In addition to the above field equations, the constitutive equation of the particular fluid is needed. This work is concerned with viscoelastic fluids with a single relaxation time of the Oldroyd variety where the stress tensor

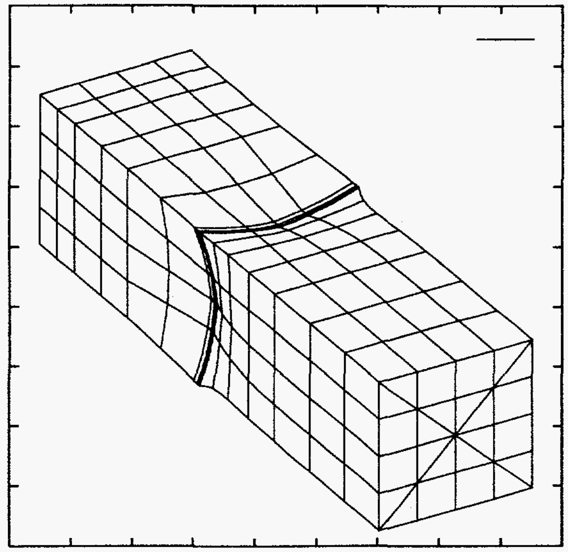

Figure 2: A short die problem. The uniform portion of the die near the exit is called the die length l. In this case $l = 0.14$.

can be written as

$$\boldsymbol{\sigma} = -p\mathbf{1} + 2\eta_s\mathbf{D} + \boldsymbol{\tau}, \tag{3}$$

where p is the hydrostatic pressure which arises due to the incompressibility constraint (2), $\mathbf{1}$ is the unit tensor, η_s is the solvent viscosity, $\mathbf{D}$ is the rate-of-strain tensor, $\boldsymbol{\tau}$ is the extra stress tensor which is governed by constitutive equations of the Maxwell type

$$\lambda\frac{\Delta\boldsymbol{\tau}}{\Delta t} + \mathbf{R} = 0, \tag{4}$$

in which λ is the relaxation time, $\mathbf{R}$ is model dependent, and

$$\frac{\Delta\boldsymbol{\tau}}{\Delta t} \equiv \frac{\partial\boldsymbol{\tau}}{\partial t} + \mathbf{u}\cdot\boldsymbol{\nabla}\boldsymbol{\tau} - \mathbf{L}\boldsymbol{\tau} - \boldsymbol{\tau}\mathbf{L}^T \tag{5}$$

is the upper-convected derivative of the extra stress tensor, where $\mathbf{L}$ is the velocity gradient tensor and $\mathbf{L}^T$ denotes its transpose.

3 Integral equation formulation

In the present method, Eq. (3) in conjunction with Eq. (4) is rewritten as

$$\boldsymbol{\sigma} = -p\mathbf{1} + 2\eta_p\mathbf{D} + \boldsymbol{\varepsilon}, \tag{6}$$

where $2\eta_p\mathbf{D}$ represents a linear part of the stress tensor and $\boldsymbol{\varepsilon}$ the remaining. The linear part can be chosen arbitrarily, but a good choice would be either the solvent stress, or the total Newtonian stress (the extra stress in the limit of slow flow). Then the set of governing equations (1), (2) and (6) is recast in integral form, following Bush and Tanner,[6]

$$\begin{aligned} C_{ij}(\mathbf{x})u_j(\mathbf{x}) &= \int_{\partial\mathbf{D}} u^*_{ij}(\mathbf{x},\mathbf{y})t_j(\mathbf{y})d\Gamma(\mathbf{y}) - \int_{\partial\mathbf{D}} t^*_{ij}(\mathbf{x},\mathbf{y})u_j(\mathbf{y})d\Gamma(\mathbf{y}) \\ &\quad - \int_{\mathbf{D}} \varepsilon_{jk}(\mathbf{y})\frac{\partial u^*_{ij}(\mathbf{x},\mathbf{y})}{\partial x_k}d\Omega(\mathbf{y}), \end{aligned} \tag{7}$$

where $\mathbf{D}$ is the open domain with connected bounding surface $\partial\mathbf{D}, \mathbf{x}, \mathbf{y} \in \mathbf{D}$, $u_j(\mathbf{y})$ is the j-velocity component at $\mathbf{y}$, $t_j(\mathbf{y})$ is the j-component of boundary traction at $\mathbf{y}$, $\varepsilon_{jk}(\mathbf{y})$ is the jk-component of $\boldsymbol{\varepsilon}$ at $\mathbf{y}$, $u^*_{ij}(\mathbf{x},\mathbf{y})$ is the i-component of velocity field at $\mathbf{x}$ due to a "Stokeslet" in j-direction at $\mathbf{y}$ and $t^*_{ij}(\mathbf{x},\mathbf{y})$ is its associated traction. $C_{ij}(\mathbf{x})$ depends on local geometry, $C_{ij}(\mathbf{x}) = \delta_{ij}$ if $\mathbf{x} \in \mathbf{D}$ and $C_{ij}(\mathbf{x}) = \frac{1}{2}\delta_{ij}$ if $\mathbf{x} \in \partial\mathbf{D}$ and $\partial\mathbf{D}$ is a smooth surface. Details of $u^*_{ij}(\mathbf{x},\mathbf{y})$ and $t^*_{ij}(\mathbf{x},\mathbf{y})$ for three dimensional problems are given elsewhere (e.g., Tran-Cong and Phan-Thien[7]).

4 Boundary Element solution of extrusion problems

The application of equation (7) to solve a number of direct problems is described in detail previously by Tran-Cong and Phan-Thien[7,8] where the corner traction resolution problem has been solved. Here the procedure is briefly recaptured and extended for the inverse problem. Essentially, the problem is solved numerically by decoupling the non-linear effects, which are treated as small perturbations in an otherwise linear solution. In this method, the last integral on the right hand side of Eq. (7), i.e.,

$$\int_{\mathbf{D}} \varepsilon_{jk}(\mathbf{y})\frac{\partial u^*_{ij}(\mathbf{x},\mathbf{y})}{\partial x_k}d\Omega(\mathbf{y}) \tag{8}$$

is considered as a pseudo-body-force in a linear problem. Hence for a given stress field, Eq. (8) is evaluated and Equation (7) is discretised over the boundary $\partial\mathbf{D}$ to yield a system of linear algebraic equation of the form

$$[\mathbf{G}]\{\mathbf{t}\} = [\mathbf{H}]\{\mathbf{u}\} + \{\mathbf{b}\}, \tag{9}$$

where $\{\mathbf{t}\}$, $\{\mathbf{u}\}$, $\{\mathbf{b}\}$ are the global nodal traction, velocity and body force vectors respectively. The unknown boundary tractions $\mathbf{t}$ and velocity $\mathbf{u}$ in Eq. (9) are rearranged and the system is solved by standard Gauss elimination. Equation (7) is then reapplied to evaluate the velocity field in $\mathbf{D}$. The last step in the iterative procedure is to compute the stress field and the whole procedure described above is repeated until a convergence (or the lack of) is obtained. A pseudo-time "marching" technique is employed to obtain the extra stress field. The constitutive Eq. (4) governing the extra stress is written as

$$\mathbf{f} \equiv \frac{\partial \boldsymbol{\tau}}{\partial t} = -\mathbf{u}\cdot\boldsymbol{\nabla}\boldsymbol{\tau} + \mathbf{L}\boldsymbol{\tau} + \boldsymbol{\tau}\mathbf{L}^T - \frac{1}{\lambda}\mathbf{R}, \tag{10}$$

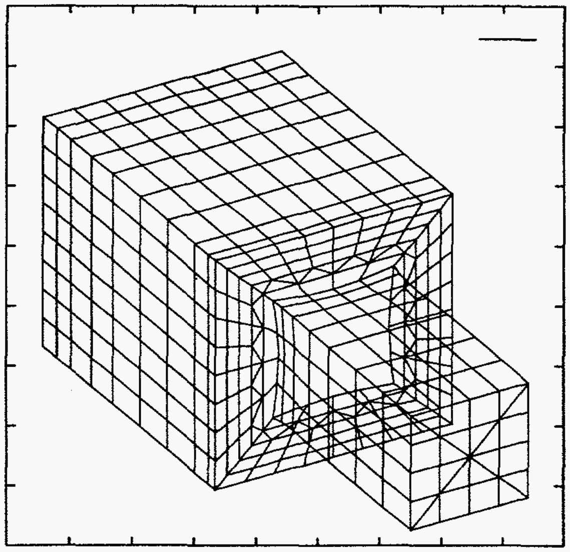

Figure 3: An orifice die with an entrance angle of 180° (Newtonian Fluid)

Given an initial guess of the solution, the iterative procedure consists of the following steps:

1. For a given stress field, Eq. (8) is evaluated, and Eq. (9) is assembled and solved for the unknown boundary tractions and velocities;

2. The free surface is computed by a path-line method[7] according to the boundary velocities obtained;

3. The difference in the cross section of the extrudate found in step 2 and the required one is then computed and all the pathlines are translated by the corresponding amount to make the final cross section of the extrudate the required one,[5] and the die profile is modified correspondingly;

4. Eq. (7) is reapplied to compute the velocity field in the domain **D**;

5. The kinematics are kept constant while the stresses are marched using Eq. (10) according to a chosen scheme. In this study a first order Euler scheme is used, i.e.,
$$\boldsymbol{\tau}^{n+1} = \boldsymbol{\tau}^{n} + \Delta t\, \mathbf{f}^{n}, \tag{11}$$
where $\boldsymbol{\tau}^{n+1}$ is the extra stress at step $(n+1)$, $\boldsymbol{\tau}^{n}$, $\mathbf{f}^{n}$ is the extra stress and its partial time derivative given by Eq. (10) at step n, Δt is the pseudo-time step. n is increased until little change is observed (in this study, $\Delta t = 0.01\lambda$, where λ is the relaxation time of the fluid, and the

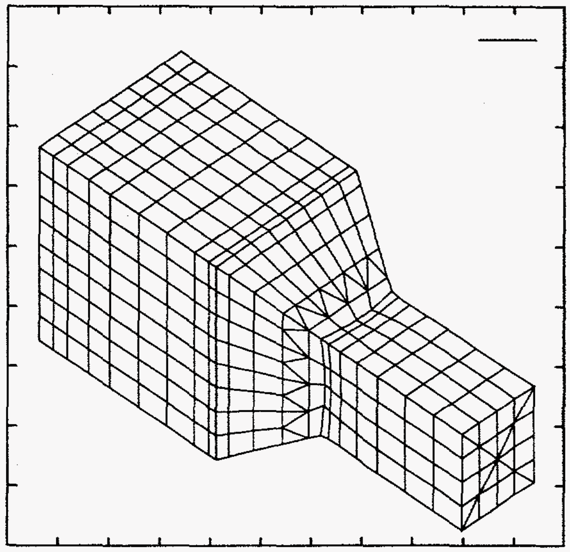

Figure 4: An orifice die with an entrance angle of 53^o (Newtonian fluid)

tolerance for the extra stresses is 10^{-5}). Other higher-order Runge-Kutta schemes, including some fully implicit schemes have been used,[9] yielding essentially the same results, but with larger time steps.

A global convergence measure (CM) in the kinematics is defined by

$$CM = \frac{\{\sum_1^N \sum_{i=1}^3 (u_i^n - u_i^{n-1})^2\}^{\frac{1}{2}}}{\{\sum_1^N \sum_{i=1}^3 (u_i^n)^2\}^{\frac{1}{2}}}, \tag{12}$$

where u_i is the i-velocity component at a node, N is the total number of nodes, n is the iteration number. The computation is stopped when the convergence measure is less than 10^{-4}. The above technique gives a solution to the problem with a given set of parameters and boundary conditions (viscosity, elasticity, processing speed ...). In order to obtain a solution for arbitrary set of parameters, it is necessary to have a reasonably close guess to avoid divergence. For example, to investigate the viscoelastic effect, which is the case in this paper, the Weissenberg number (Wi, defined in a later section) is increased at small discrete steps such that the Newtonian solution can be used as the first guess for a solution corresponding to the smallest Wi. Subsequent solutions use the previous solution corresponding to the previously smaller Wi as the first guess at the beginning of the iterative cycle.

5 Numerical results for a square viscoelastic extrudate

5.1 Definition of a design problem

We now consider an illustrative problem of designing a die to produce a square extrudate. Owing to symmetry, only one eighth of the flow domain need be discretised. Then the discretised mesh contains a total of 156 nodes and 38 boundary elements (8-node quadratic quadrilaterals and 6-node quadratic trilaterals). The total die length is 5 and the extrudate length is 4. Figure 1 shows an isometric view of a final mesh. The experience with Newtonian profile extrusion[5] suggests that a "taper" design is more appropriate. In this approach, the entry profile is chosen such that the best possible approximation to the velocity boundary condition can be found. The entire length of the die is obtained by blending the entry section with the required exit section. Thus only the transitional and the exit lip region are changing in the design process. The customary no slip boundary conditions at the wall and the traction free extrudate surface are assumed in all cases. The choice of Newtonian inlet velocity profile is justified *a posteriori*[8] when fully developed flow is observed at some distance downstream of the inlet. At the downstream section of the discretized flow domain, the plug flow condition is specified, i.e., zero traction in the flow direction and zero radial velocity components.

5.2 A model viscoelatic material

The method discussed above is implemented and tested for a square extrudate profile using a model viscoelastic material. In the following discussion, the characteristic length, a, is half the side of the die entry cross section; the characteristic speed, U, is the centreline (maximum) speed at the inlet; the characteristic time, λ, is the constant relaxation time; η_0 is the zero shear rate viscosity; η_m is the polymer contributed viscosity. For the MPTT model, $\mathbf{R}$ (in Eq. (4)) is given by[10,11,12]

$$\mathbf{R} = g\boldsymbol{\tau} + \lambda\xi(\mathbf{D}\boldsymbol{\tau} + \boldsymbol{\tau}\mathbf{D}^T) - 2\eta_m(\dot{\gamma})\mathbf{D}, \tag{13}$$

where

$$g = \left[1 + \epsilon\frac{\lambda}{\eta_0}\mathrm{tr}(\boldsymbol{\tau})\right], \quad \dot{\gamma} = \sqrt{2\mathrm{tr}(\mathbf{D}^2)}, \quad \eta_m(\dot{\gamma}) = \eta_0\frac{1 + \xi(2-\xi)\lambda^2\dot{\gamma}^2}{(1 + \Gamma^2\dot{\gamma}^2)^{\frac{1-n}{2}}},$$

in which ϵ, ξ, n are dimensionless parameters and Γ is a time constant. The dimensionless variables are given by

$$t' = \frac{t}{\lambda}, \quad \mathbf{x}' = \frac{\mathbf{x}}{\mathbf{a}}, \quad \mathbf{u}' = \frac{\mathbf{u}}{\mathbf{U}}, \quad \boldsymbol{\tau}' = \frac{\boldsymbol{\tau}}{\eta_0\frac{U}{a}}, \quad \eta' = \frac{\eta_m}{\eta_0 + \eta_s},$$

where t is time, $\mathbf{x}$ is the position vector, $\mathbf{u}$ is the velocity vector, $\boldsymbol{\tau}$ is the extra stress tensor and η is the viscosity.

In this study, $\xi = 0$ and $n = 1$ were chosen. Then the constitutive Eq. (4) is given in dimensionless form by (dropping the primes)

$$\frac{\partial\boldsymbol{\tau}}{\partial t} = (2\eta\mathbf{D} - g\boldsymbol{\tau}) - Wi(\mathbf{u}\cdot\boldsymbol{\nabla}\boldsymbol{\tau} - \mathbf{L}\boldsymbol{\tau} - \boldsymbol{\tau}\mathbf{L}^T), \tag{14}$$

Table 1: Die shape relative to a square extrudate as a function of Wi: MPTT fluid ($\epsilon = 0.01$; $\xi = 0$; $n = 1$; $\lambda = 1$). χ_f is percentage reduction in the size of the die relative to the required extrudate at the middle of the flat face; χ_c is the corresponding value at the corner.

Wi	0	0.05	0.10	0.15	0.2	0.22	0.24	0.245
Wi_w	0	0.11	0.22	0.34	0.45	0.495	0.539	0.551
$\chi_f(\%)$	-18.4	- 19.3	-21.0	-23.8	-27.6	-29.5	-30.4	-30.6
$\chi_c(\%)$	+2.6	+1.9	+0.8	-1.3	-6.1	-7.6	-10.8	-11.7

where $g = 1 + \epsilon\, Wi\, \mathrm{tr}(\boldsymbol{\tau})$, and $Wi = \lambda U/a$ is the Weissenberg number.

5.3 Discussion of results

The only dimensionless parameter to be varied in this study is the Weissenberg number, Wi, defined above. In this study the inlet velocity is kept constant and Wi is increased by increasing the relaxation time λ. However, if the Weissenberg number was based on a wall shear rate at a point far upstream, Wi_w say, as is often the case reported in the literature, the computed wall shear rate $\dot{\gamma}_w = \sqrt{2\mathrm{tr}(\mathbf{D}^2)}$ at the mid-point of a flat face of the die at the inlet shows that $Wi_w \approx 2.25\, Wi$. Both Wi and Wi_w are presented for comparison. Table 1 shows two representative measures of the final die profile for the indicated Wi number. Note that χ's are defined as the percentage difference, in the radial direction, between the die and the extrudate geometry relative to the extrudate geometry (a positive value of χ represents a swelling, and negative value, a shrinkage). Here χ_f is the maximum value of χ measured at the middle of the flat face of the extrudate (always negative at all Weissenberg numbers), and χ_c is the minimum value of χ measured at the corner of the extrudate (which can be positive at low Wi). On a DEC3000 M800, one iteration takes approximately 30 minutes and convergence at $Wi = 0.22$ requires about 40 iterations.

5.4 Further examples

To further demonstrate the capability of the present method, the problem of shortdie and orifice die is also attempted. It is found that short dies severely limit the range of achievable Wi numbers. The limiting Wi number decreases from 0.245 (die length $l = 1.4$, Figure 1) to 0.2 ($l = 0.77$) and 0.01 ($l = 0.14$, Figure 2).

Figures 3 and 4 depict the results of orifice die design for a Newtonian fluid with different entrance angles and a contraction ratio of 2 to 1. It is found that $\chi_f = -6.1\%$, $\chi_c = 1.3\%$ for the entrance angle of 180^o, $\chi_f = -9.6\%$, $\chi_c = -0.2\%$ for the entrance angle of 53^o and $\chi_f = -10.2\%$, $\chi_c =$

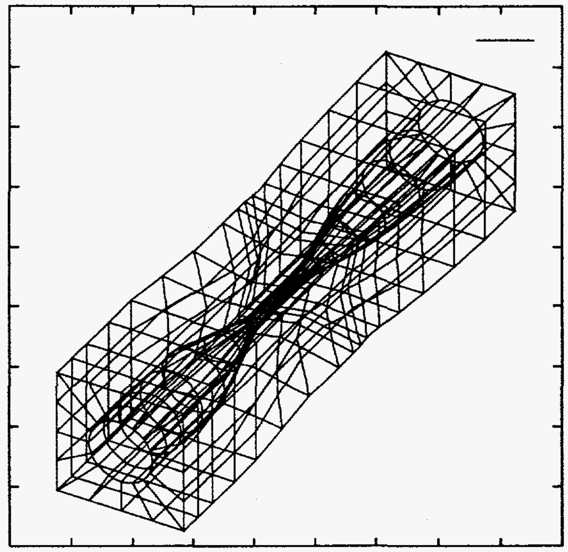

Figure 5: Die design for a complex extrudate profile. The hollow extrudate has an outer square profile and an inner circular profile.

-0.2% for the entrance angle of 40^o.

Finally, Figure 5 depicts a complex hollow Newtonian extrudate with a square outer profile and a circular inner profile. The simulation shows that drastic swelling has occurred. The die core takes an oval shape with swelling varying from -75.8% to -80.8% and the outer die wall experiences swelling of $\chi_f = -28.1\%$ and $\chi_c = -10.1\%$.

6 Concluding remarks

A useful numerical tool based on BEM is developed to simulate plastics extrusion processes. Important trends in the extrudate behaviour are revealed as a result of simulations by BEM. It is demonstrated that die design for complex extrudate shape is achieved by the present technique. Trial and error die cutting process could be significantly minimised. Thus the die design and development cost could be significantly reduced.

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