Use of "Penalty" Finite Elements in Analysis of Polymer Melt Processing

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The finite element method is an approximate numerical analysis approach of great applicability to a wide variety of field problems. This paper describes the formulation of a convenient method for treating fluid-flow problems relevant to analysis of polymer processing operations, and illustrates its use by means of some linear and nonlinear problems in melt extrusion.

INTRODUCTION

Although a good many of the developments in polymer melt processing have been—and will continue to be—largely Edisonian in nature, polymer processing technology is now sufficiently mature that further development will profit considerably by improved analytical means of estimating the effects of processing variables on final-part quality and process economics without resorting to purely empirical experimental searches. The engineer is interested in such effects as the location and minimization of regions of excessive shear deformation and mechanical degradation within the flow field, regions of stagnation at which overlong material residence and thermal degradation might occur, development of molecular orientation along desired directions by employing preplanned velocity gradients, and predictions of power requirements and process efficiency. In a closely related discipline, the polymer rheologist is interested in means whereby the consequences of newly-developed material constitutive models might be assessed. This eventually improves the capability to design the molecular and supermolecular architecture of the polymer so as to manipulate favorably the relationships between material structure, processing, and properties. This latter goal is one of the central themes of materials science and engineering.

Problems of viscous fluid flow, even when the simplifying assumption of incompressibility is applicable, constitute some of the most challenging problems in applied mathematics. They are typically mixed boundary-value problems (velocities or velocity gradients being specified over some portions of the boundary, forces or tractions over other portions), and are often both nonlinear and time-dependent. Certain of these problems can be attacked successfully using closed-form mathematical methods, and these classical problems provide an important basis of understanding in fluid mechanics. In practical problems, however, one commonly encounters boundary conditions which are difficult to describe mathematically, and which in any case are sufficiently complex to render the resulting system of equations intractable. For these situations, the fluid analyst has developed an extensive and powerful array of numerical means of obtaining approximate solutions. These have emphasized the use of finite-difference methods, in which the partial derivatives found in the fluid governing equations are approximated by discrete differences in the field variables, the spatial coordinates, and time. Finite difference methods will certainly continue to be very popular in fluid-flow problems, but they do have certain drawbacks which tend to limit their use in some instances. They tend to require rather extensive reworking for each problem so as to fit the grid and the recursive algorithms to the boundaries, and it is sometimes difficult to fit the complex geometrical boundaries encountered in real processing flow problems. For these reasons and others, a good deal of attention is now being directed to the application of finite element methods to fluid flow problems (1,2). The finite element method counts ease of implementation to new problems and ability to fit extremely irregular geometries among its most attractive features.

The finite element method (3,4) is a computer-oriented numerical approach to field problems in which approximations of the field variables within discrete regions of the solution domain are assumed. These approximations are then used to develop relations between the known and unknown values of the field variables at various nodes which are established within and along the element boundaries. These relations typically take the form of a large system of algebraic equations which may be solved using direct or iterative numerical methods. The method was first used principally by engineers who regarded it as an outgrowth of matrix structural analysis. In recent years, however, the method has been placed on a firm foundation in applied mathematics which has facilitated its extension to a wide variety of field problems beyond structural stress analysis. Its ability to handle many diverse problems in fluid flow in a convenient and economic manner makes it very attractive for analyses of polymer processing operations. This paper will discuss a particularly convenient formulation for this purpose, and illustrate its use in some two-dimensional problems in polymer melt extrusion.

PENALTY FORMULATION FOR VISCOUS IMCOMPRESSIBLE FLUIDS

Fundamental Relations

Although the governing equations for two-dimensional fluid flow may be written in several alternative forms, a useful similarity to finite element solid mechanics formulations is obtained if one adopts an Eulerian measure of velocity as the fundamental unknown. Fluid velocity then becomes analogous to solid displacement, and many aspects of solid mechanics computer analysis may be used directly. This approach is discussed in more detail by Zienkiewicz (5), and will be outlined here only briefly.

Equilibrium of the local stresses $\boldsymbol{\sigma}$ and the body forces $\mathbf{b}$ within the fluid domain may be written in matrix form as

$$\mathbf{L}^T\boldsymbol{\sigma} + \mathbf{b} = 0 \qquad (1)$$

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{bmatrix} \qquad \mathbf{L} = \begin{bmatrix} \partial/\partial x & 0 \\ 0 & \partial/\partial y \\ \partial/\partial y & \partial/\partial x \end{bmatrix}$$

The relation applies equally to solids and fluids. Provision for the convective inertial forces which occur in fluid flow may be obtained by including a d'Alembert term in the body-force vector:

$$\mathbf{b} = \mathbf{b}_o - \rho\mathbf{c} \qquad (2)$$

$$\mathbf{c} = \partial\mathbf{u}/\partial t + (\nabla\cdot\mathbf{u}^T)^T\mathbf{u} \qquad (3)$$

Here $\mathbf{b}_o$ includes the usual body forces (gravitation, etc.), ρ is the fluid density, $\mathbf{u}^T = (u_x, u_y)$ lists the velocity components, and $\nabla^T = (\partial/\partial x, \partial/\partial y)$ is the gradient operator. The $\rho\mathbf{c}$ term may be neglected for steady creeping flows (typical of many flows in polymer melt processing); its inclusion, when necessary, leads to a nonlinear problem with unsymmetric stiffness matrices.

The local strain rates may be written in terms of the velocities as

$$\dot{\boldsymbol{\epsilon}} = \mathbf{L}\,\mathbf{u} \qquad (4)$$

where $\mathbf{L}$ is the same derivative-operator matrix defined in *Eq 1*.

The fluid stresses are related to the strain rates by the material constitutive law. Since the strain rates depend only on the deviatoric components of the stress $\boldsymbol{\sigma}'$, it is convenient to dissociate the stress tensor as

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' + \mathbf{m}\sigma_m \qquad (5)$$

where $\mathbf{m}^T = (1,1,0)$ and $\sigma_m = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$. The mean stress σ_m is the negative of the hydrostatic pressure p. In the case of Newtonian fluids, $\boldsymbol{\sigma}'$ and $\dot{\boldsymbol{\epsilon}}$ are related by

$$\boldsymbol{\sigma}' = \mu\begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}\dot{\boldsymbol{\epsilon}} \equiv \mathbf{D}\,\dot{\boldsymbol{\epsilon}} \qquad (6)$$

where μ is the Newtonian viscosity.

Of course, many constitutive models of polymer melt response beyond that given in *Eq 6* exist, and a principal goal of fluid flow analysis is to provide a means by which these more advanced models can be tested and improved. An often used constitutive model, fairly well suited to many polymer melts, is that of the power-law fluid, in which the Newtonian viscosity is replaced by

$$\mu = \mu_o\left[\frac{\Delta{:}\Delta}{2}\right]^{(n-1)/2} \qquad (7)$$

where

$$\frac{\Delta{:}\Delta}{2} = 2\,[u^2_{x,x} + u^2_{y,y}] + [u_{y,x} + u_{x,y}]^2 \qquad (8)$$

and n is the power-law exponent. Use of this and most other more advanced constitutive laws renders the formulation nonlinear, increasing greatly the difficulty of closed-form solutions and requiring the use of iterative schemes in numerical approaches.

The continuity law may be written:

$$\partial\rho/\partial t = \nabla^T(\rho\mathbf{u}) \qquad (9)$$

which for nearly incompressible fluids simplifies to

$$\nabla^T\mathbf{u} \equiv \dot{\epsilon}_v = 0 \qquad (10)$$

This relation may be viewed as a constraint on the velocities admissable as solutions, and the means of incorporating this constraint constitute one of the principal differences between the various finite element models of fluid flow which have been proposed to date. A very convenient approach is that of the "penalty function" (6), in which the consequences of *not* enforcing incompressibility are "penalized"by writing

$$p = \alpha\,\dot{\epsilon}_v \qquad (11)$$

where α is a large number in comparison with μ. In this context, α is analogous to the bulk modulus of the material.

Finite-Element Discretization

In the "isoparametric" formulation of the finite element method, one begins by writing an expression for the coordinates within a portion (element) of the solution domain in terms of the coordinates of nodal points which are selected along and within the element boundaries:

$$\mathbf{x} = \mathbf{N}_i\,\mathbf{x}_i \qquad (12)$$

Here $\mathbf{x}^T = (x,y)$ is the position of a point within or on the boundary of the element, $\mathbf{x}_i$ are the $x-y$ coordinates of the element's nodal points, and the "shape functions" $\mathbf{N}_i(x,y)$ are interpolating polynomials chosen to provide the desired variation of $\mathbf{x}$ within the element. Using shape functions which are tabulated in several standard texts (e.g. Refs. (3) and (4)), one may use the transformation of *Eq 12* to map extensive families of linear and curvilinear elements in a simple and convenient manner.

The velocities at arbitrary positions within the element are written in terms of the velocities at the nodes, using the same interpolation shape functions as in *Eq 12*:

$$\mathbf{u}(x,y) = \mathbf{N}_i(x,y)\,\mathbf{u}_i \qquad (13)$$

where here $\mathbf{u}_i$ lists the velocities of the nodal points. The $\mathbf{u}_i$ are of course unknown as yet, and their determination is the first goal of this assumed-velocity form of analysis. *Equation 13* constitutes an approximating assumption as to the variation of the velocity $\mathbf{u}(x,y)$ within the element. As the element size is decreased, this approximation is expected to converge to the correct value. Depending on the order of the interpolating polynomial $\mathbf{N}_i(x,y)$, one may obtain linear, quadratic, or higher order variations of $\mathbf{u}(x,y)$. The higher orders require more computational effort, but are often sufficiently more accurate as to be more efficient than low-order elements.

The fluid strain rates may now be written in terms of the nodal velocities using *Eqs 13* and *4*:

$$\dot{\boldsymbol{\epsilon}} = \mathbf{L}\,\mathbf{u} = \mathbf{L}\,\mathbf{N}_i\,\mathbf{u}_i = \mathbf{B}_i\,\mathbf{u}_i \tag{14}$$

where

$$\mathbf{B}_i = \mathbf{L}\,\mathbf{N}_i = \begin{bmatrix} \mathbf{N}_{i,x} & 0 \\ 0 & \mathbf{N}_{i,y} \\ \mathbf{N}_{i,y} & \mathbf{N}_{i,x} \end{bmatrix} \tag{15}$$

The stresses are then:

$$\boldsymbol{\sigma}' = \mathbf{D}\,\dot{\boldsymbol{\epsilon}} = \mathbf{D}\,\mathbf{B}_i\,\mathbf{u}_i \tag{16}$$

$$p = \alpha\dot{\epsilon}_v = \alpha\,\mathbf{m}^T\,\mathbf{B}_i\,\mathbf{u}_i \tag{17}$$

Equation 17 reveals one of the most attractive features of the penalty function approach: the pressure is computed in terms of the nodal velocities only, whereas other formulations typically introduce additional unknown variables to enforce incompressibility. The penalty formulation is simpler to implement in computer language, and the lower number of unknowns results in significantly shorter run times and costs.

Finally, all of the above relations can be combined in an expression of virtual work:

$$\int_V \delta\dot{\boldsymbol{\epsilon}}^T\boldsymbol{\sigma}\,dV - \int_V \delta\mathbf{u}^t\,\mathbf{b}\,dV - \int_{S_t} \delta\mathbf{u}^T\,\mathbf{t}^*\,dS = 0 \tag{18}$$

where the $\delta\dot{\boldsymbol{\epsilon}}$ and $\delta\mathbf{u}$ represent virtual quantities, V is the element area, and S_t is the portion of the element boundary over which tractions $\mathbf{t}^*$ are prescribed. Substituting the previous expressions for $\dot{\boldsymbol{\epsilon}}$, $\boldsymbol{\sigma}$, and $\mathbf{u}$ into *Eq* 18 and factoring out $\delta\mathbf{u}$ gives eventually

$$\left[\mathbf{K} + \overline{\mathbf{K}} + \overline{\overline{\mathbf{K}}} + \mathbf{M}\frac{d}{dt}\right]\mathbf{u}_i + \mathbf{f}_i = 0 \tag{19}$$

where

$$\mathbf{K}_{ij} = \int_V \mathbf{B}_i^T\mathbf{D}\,\mathbf{B}_j\,dV \tag{20a}$$

$$\overline{\mathbf{K}}_{ij} = \int_V \rho(\mathbf{N}_i)^T[\nabla\cdot(\mathbf{N}_i\mathbf{u}_i)^T]^T\,\mathbf{N}_j\,dV \tag{20b}$$

$$\overline{\overline{\mathbf{K}}}_{ij} = \int_V (\mathbf{m}^T\mathbf{B}_i)^T\alpha(\mathbf{m}^T\mathbf{B}_j)\,dV \tag{20c}$$

$$\mathbf{M}_{ij} = \int_V (\mathbf{N}_i)^T\rho\,\mathbf{N}_j\,dV \tag{20d}$$

$$\mathbf{f}_i = -\int_V \mathbf{N}_i^T\mathbf{b}_o\,dV - \int_{S_t} \mathbf{N}_i^T\mathbf{t}^*\,dS \tag{20e}$$

Although somewhat complicated in appearance, each of the integrands in *Eqs 20a-e* above is easily computed at any arbitrary point within the element. The integrals themselves are computed numerically, with Gaussian integration used commonly due to its efficiency.

In the case of penalty function formulations, the use of numerical integration also provides a means of improving the accuracy of the analysis. By using a reduced order of integration relative to the number of element degrees of freedom, the assembled **K** matrix tends to singularity. This seemingly undesirable result is in fact necessary to prevent the factor α from dominating the solution and leading to a trivial null solution for the $\mathbf{u}_i$ (6). In the examples to be presented below, a four-point Gaussian integration was used in conjunction with nine-node quadratic elements.

Computer Implementation

In practice, the computations described in the previous section are employed in a computer code which loops through each successive element in turn, developing the submatrices of *Eqs 20a-e*. These submatrices are added to the appropriate positions of global arrays which take cognizance of the nodal numbering scheme for the entire solution domain; these assembled arrays then constitute the coefficient matrix and constant vector of a system of linear algebraic equations. The code must contain provision for accepting or generating the input data, computing and assembling the global arrays, solving the resulting system in an efficient manner, computing such ancillary data as strain rates and stresses in terms of the resulting nodal velocities, and providing a convenient output of the results.

The researcher or educator wishing to use finite element analysis must decide on the sort of code he wishes to obtain or write for this purpose. Several large, production-oriented codes are available (7), but these are often proprietary and not available in their source version. Even when their source language is available, these large codes tend to be difficult to modify due to their complexity. Further, their considerable ability to preprocess and postprocess the data so as to provide, for instance, convenient graphical input-output procedures may sometimes mask errors in numerical approximation which often arise as new element types are being developed.

For the purpose of implementing the fluid analyses described above, the present author has selected the code written by Taylor (8) as a good compromise for research purposes. This code is available to all, is well documented and supported by an excellent textbook, and is relatively easy to use and modify. It also contains most of the important features found in the large proprietary codes: economical active-column storage of the stiffness array, an efficient Gaussian equation solver for either symmetric or unsymmetric arrays, a generalized shape-function approach which facilitates the development of new elements, and a mnemonic macrocontrol language which permits the code to attack a wide variety of linear and nonlinear, and steady or transient, problems. The fluid element developed for this present work was constructed along the lines suggested by Taylor for this code.

APPLICATION TO POLYMER PROCESSING: MELT EXTRUSION

In principle, finite element analysis is ideally suited to the requirements of analytical models outlined earlier. Once the nodal velocities have been computed, *Eq 13-17* permit the velocities, strain rates, shear stresses and pressure to be computed at any point in the flow domain. Force reactions at the boundaries are also obtained easily, and integration of these over the boundary surfaces permits a computation of the total forces which must be supplied by the equipment, and the power needed to operate the process.

Of course, the finite element method is an approximative rather than exact solution scheme, and one should assess the accuracy and reliability of such an approach before embarking on an extensive series of simulations. In addition to approximation errors, newly-developed codes are likely to contain errors in both logic and coding. The melt extruder, in which molten polymer is dragged toward a die by the relative motion of the extruder barrel relative to the screw, is a process of actual interest which is also well suited for illustrating the reliability of the finite element approach. The flow channel is of a sufficiently simple shape to permit theortical solutions for comparison purposes, but the flow is of a general mixed-boundary value nature so that the general applicability of the method may be assessed.

As described in several texts (e.g., Refs. (9-10)), the helical flow path may be idealized as a straight, rectangular channel covered by a plate which moves tangentially to the channel as shown in *Fig. 1*. Due to the tangential motion of the top plate, fluid flow is established in both the axial (down-channel) and transverse (cross-channel) directions. In addition, the axial flow is inhibited by the development of pressure by the die. In the case of Newtonian melts, these two flow fields are uncoupled and may be treated separately.

Figure 2 shows the sixteen-element idealization used to simulate a portion of the axial flow field. Normalized dimensions and operating parameters were used during the analysis; in particular, the pressure increase through the length L was set to unity. The fluid viscosity was then set to that value which the theoretical solution predicts would cause the ratio of drag to pressure flow to have the value -2/3. The normalized axial velocity distribution as computed along a constant-x line near the center of the mesh is compared with the theoretical distribution in *Fig. 3*, and it is seen that the numerical prediction is good in spite of the relatively coarse mesh used.

Figure 3 also shows the numerical results obtained when a non-Newtonian fluid with power-law exponent $n = 0.8$ is considered. This solution was obtained by using the Newtonian solution as an initial estimate for the nodal velocities, then conducting a Newton-Raphson iteration to obtain the nonlinear solution. The macro language provided by the Taylor code makes programming for this iterative solution very convenient, and the Newton-Raphson scheme converged in this case in four iterations. In the case of nonlinear fluids, however, the transverse and axial flow fields are coupled, since the velocity gradients in one field influence the viscosity which in turn perturbs the flow field in the other direction. A three-dimensional analysis is needed to model this situation correctly.

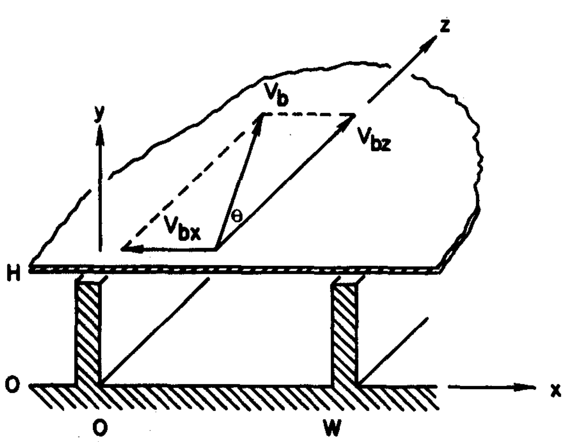

Fig. 1. Straight-channel idealization of single-flight melt extruder.

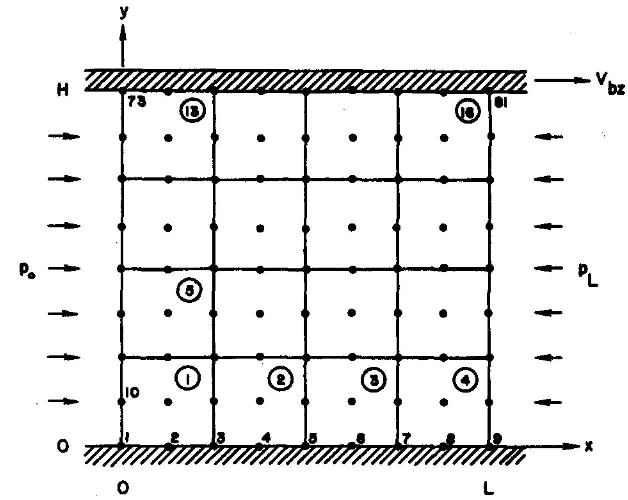

Fig. 2. Finite-element idealization of axial flow. Normalized values: $V_{bz} = p_L = H = L = 1$; $p_o = 0$, $\mu = 0.25$.

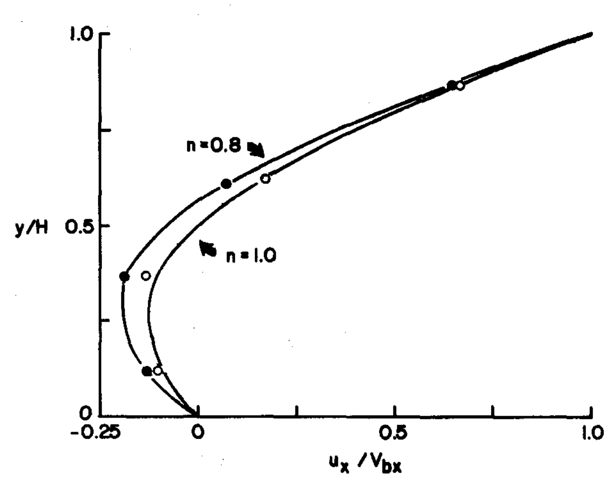

Fig. 3. Variation of axial velocity for Newtonian and power-law fluid along x/L = 0.625. Drawn curve for n = 1 is the theoretical prediction. Circles represent weighted averages of nine nodal velocities.

The variation of pressure along the axial direction is compared with the theoretical linear variation in *Fig. 4*. This figure indicates one of the averaging procedures which often prove useful in these analyses: the pressures are computed initially at the Gaussian integration stations, but some improvement in accuracy may be obtained at times if these values are used to compute an average value within the element.

Figure 5 shows the results obtained using a 6 × 3 element simulation of the transverse flow field. This is a more difficult problem numerically, in spite of the fact that the boundary conditions appear simpler (no prescribed forces). However, the velocities exhibit singularities at the upper corners of the flow field, and a finer mesh is needed to describe these regions accurately. This is also a more difficult problem theoretically: it is usually treated by adopting the lubrication approximation (neglect vertical velocity components) and then viewing the flow as a combined drag and pressure flow similar to the axial flow. The pressure gradient established within the section by the presence of the vertical walls is obtained by insisting that the net flow across any constant-x line must be zero. The velocity arrows drawn in *Fig. 5* are a weighted average of the nine nodal values at each element, and they indicate the circulatory nature of the transverse flow field. The horizontal components of the velocity field agree well with the theoretical prediction, but the coarseness of the mesh in the vertical direction has produced some erroneous values for the y-components of velocity which results in a nonzero net flow across constant-y lines.

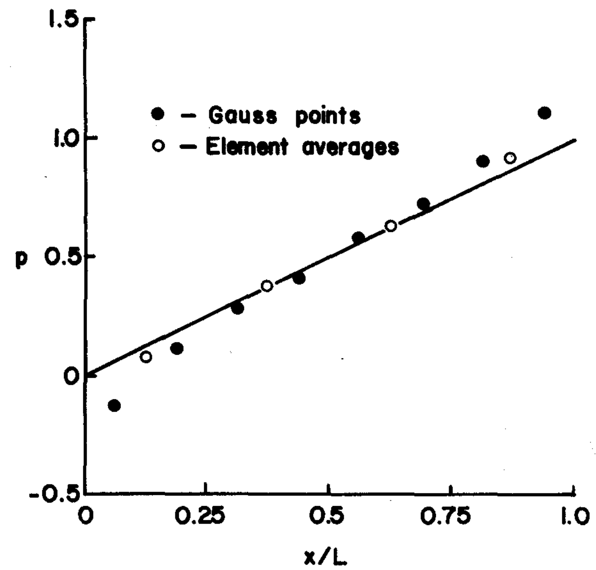

Fig. 4. Comparison of theoretical and computed pressure along axial channel, at y/H = 0.447.

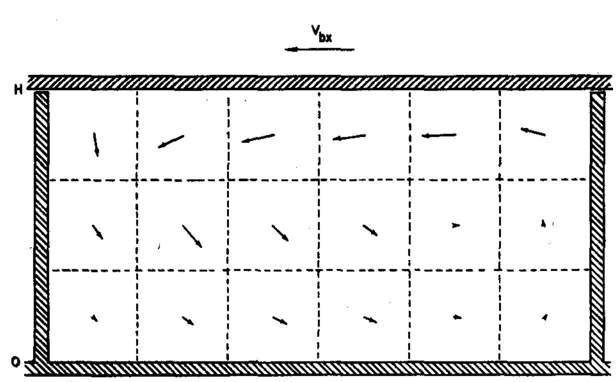

Fig. 5. Representation of computed cross-channel flow field. Drawn arrows are scaled relative to the barrel velocity V_{bx} shown at top.

The pressures along several constant-y lines through the transverse section are plotted in *Fig. 6*. These values are both positive and negative, but they will be added to the pressures developed in the axial direction so as to create all positive values. The drawn line has the slope predicted by the lubrication solution for the pressure gradient, and it is seen that the numerical values agree well. Note the higher pressure near the singularity in the upper left corner. Again, these data are computed by averaging the values of the four Gaussian integration stations within each element.

CONCLUSIONS

The foregoing analysis and illustrative problems indicate that the finite element method can be of considerable utility in providing approximate values for the variables of interest in real polymer melt processing operations. A good many operations exist in which exactly the sort of analysis described above many be used directly. One example might be the circulatory flow in the intermediate stages of the plasticating extruder, in which the flow takes place around a bed of as-yet-unmelted polymer. However, many important processes will require an extention of the numerical method for their proper simulation, and these processes constitute exciting fields of future work. Three such areas might be mentioned briefly: (a) The method can be used advantageously in free-surface flows, such as extrusion through a die and film blowing. This solutions are generally iterative approaches in which the position of the free surface is adjusted until all final velocities are tangential to the surface. Free surface analyses will also profit from incorporation of more advanced viscoelastic fluid constitutive laws, so that proper allowance for normal stresses can be made. (b) The capability for handling temperature dependencies can be improved. A simple step would involve only incorporating a temperature-dependent viscosity in the fluid element, then reading the various element temperatures in as input data. A more substantial development would be to couple the temperature

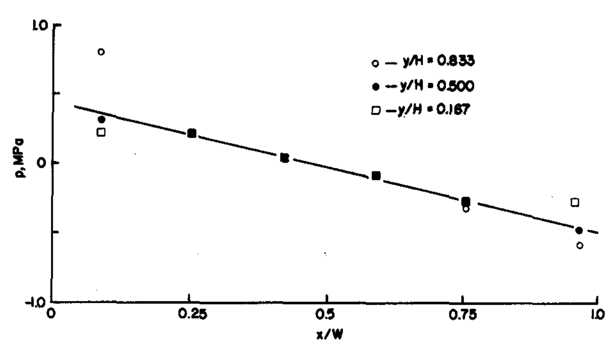

Fig. 6. Computed pressures in transverse flow field, using averaged Gaussian-station values. Drawn line has slope 474 kPa, the theoretical value.

into the formulation as another variable, so as to make proper allowance for shear-generated dissipation and heat transfer. (c) Certain problems, such as the coupling between axial and transverse flow in nonlinear fluid extrusion, will require the use of three-dimensional elements. In all of the above areas and in many others not mentioned, the analyst must choose carefully to make efficient and economical use of this very powerful method.

Finally, the analyst should keep in mind that the application of finite element methods to fluid flow analysis is relatively new, and that several different approaches have appeared in the literature. As mentioned earlier, these various implementations differ most substantially in the manner in which incompressibility is enforced. The penalty method demonstrated in this paper is very convenient in that it requires only minor changes from the isoparametric formulation already widely available for stress analysis, and it does not require the incorporation of additional degrees of freedom. On the other hand, some workers have noted a tendancy for the assembled global stiffness matrix to become ill-conditioned due to the use of the large penalty coefficient, which leads to difficulties in obtaining a numerical solution. The test problems solved in this paper exhibited no such difficulties even when solved using single-precision arithmetic; however, the use of double precision may be prudent in order to help avoid inaccuracies due to ill-conditioning. Given this caveat, the convenience of the penalty formulation would seem to favor its use over such other methods as direct velocity-pressure formulations, Lagrangian multiplier constraints, or stream function formulations. Further discussion of the relative merits of these differing approaches may be found in Refs. (1, 3, and 7).

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