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I. K. Berezin^a; A. M. Golubicky^a; A. I. Ponomarchuk^a a Institute of Continuous Media Mechanics, Perm, USSR

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Finite and Boundary Elements for the Simulation of Injection Molding Process

1. K. BEREZIN, A. M. GOLUBICKY and A. I. PONOMARCHUK

Institute of *Continuous Media Mechanics, Perm, USSR*

Problems dealing with computations of pressure and velocity fields in the fluid flow through channels of complete geometry are discussed.

KEY WORDS Fluid flow, complex channel geometry. simulation injection molding.

INTRODUCTION

The advanced technology of polymer processing gives rise to a number of rather essential problems, dealing with computation of pressure and velocity fields and determination of the boundary position (free surface boundaries) in the fluid flow with nontrivial rheological properties through a channel of complex geometry. Numerous mathematical methods which have been proposed to date provide numerical simulation of unsteady viscous flows with a free surface. To model the flows with insignificant medium displacement one employs a Lagrangian approach according to which the computational mesh is moving together with the continuum. The Eulerian interpretation is found to be suitable for the flows without unsteady free boundaries. The mixed Euler-Lagrangian methods are commonly used for problems which require description of the free surface shape. What is specific for the above-mentioned problems is the existence of a computational stage, which involves evaluation of principal variables for the known domain with the specified boundary conditions at a given time step. To this end the present work employs methods of finite and boundary elements.

MATHEMATICAL MODEL

This paper is concerned with the process of viscous flow through a channel with rigid walls, at the specified flow rate or pressure with a free surface of undetermined position, varying with time. It is worth noting that in the present problem the integration domain of the equation of motion is generally unknown and should be subsequently defined. This suggests nonlinearity of the boundary condition problem since the unknown boundaries should be derived from the unknown solution. In this case the solution can be obtained by using the iteration procedure to define the shape of the boundary, starting with some known reference position in space. The entire process is subdivided into a finite number of time steps. Finite element methods (FEM) and boundary element methods (BEM) have been applied to solve the equation of motion and define the velocity field and pressure at the time step under consideration. Then, using the kinematic equation one defines the position of the free surface at the subsequent time increment. **A** new boundary configuration determines a new integration range for the equations of motion. The time stepping is repeated up to the desired time increment. Mathematical treatment of the problem reduces to integration of the motion equations for an incompressible fluid which, upon elimination of the Newtonian part of the stress tensor, are written as:

$$
-\nabla p/\rho + \nu \Delta U = (\partial U/\partial t + U \cdot \nabla U) + \text{div } T' + \rho g; \quad \text{div } U = 0; \quad (1)
$$

where *U* is the velocity, p is the pressure, **p** is the density, *u* is kinematic Newtonian viscosity, g is the acceleration of gravity and T' is the extra-tensor, the form of which depends on the type of rheological law. In the case where tensor T' depends npnlinearly on the shear rate, solution to the system (1) can be obtained by performing iteration separately at each time increment. If $\Gamma = \Gamma_1 \cup \Gamma_2$ are boundaries of the domain, the following boundary conditions are satisfied on it:

$$
x \in \Gamma_1: U = U_b; \qquad x \in \Gamma_2: t = T \cdot n = -(p_0 + \alpha K) \tag{2}
$$

where T is the stress tensor, n is the outward normal, p_0 is the external gas pressure, α is the coefficient of the surface tension and K is the surface curvature. The Equations (1) and **(2)** constitute a boundary-value problem for the domain with defined boundaries. Boundary deformation due to the fluid motion can be represented mathematically through kinematic conditions. By denoting the radiusvector of the material particle at the surface by *r* and assuming that the particle preserves its position within the domain (but is allowed to move at the solid boundary) one obtains the boundary relation $U = dr/dt$ in terms of substantial products, which is a special case of the kinematic condition $dF/dt = 0$, where $F(r) = 0$ specifies the free-surface position in terms of Eulerian variables. This condition doesn't hold at the line at the 3-phase contact due to the existence of singularity, which is ignored in the present work.

FEM SIMULATION

The FEM is one of the possible routes to numerical realization of the above procedure. **In** the present paper the FEM is used to analyze slow isothermal flows of highly-viscous fluid. In this case we consider the whole process of movement according to quasi-stationary statement based on the solution of the series of elliptic problems. As a variational functional we choose

$$
J(U, p) = \int (-pe_{ij}/p + ve_{ij}e_{ij} - g_iU_i) d\Omega - \int t_iU_i d\Gamma_2,
$$
 (3)

where e_{ij} are the component of the strain rate tensor. In the case of a free surface, the second integral is set of zero. Numerical analysis for choosing the FE grid and the approximation degree has shown that the triangular element grid using the linear velocity approximation and the constant pressure magnitude inside the quadrilateral associating two neighboring triangles is a suitable approach.

Rheological behavior of a fluid was described by the power law with the yield strength. Problems of a viscous fluid spreading under various boundary conditions have been solved as test cases. The magnitude of fluid volume varied no more than 0.1 per cent from the initial value. Figure 3 shows one set of calculated results. Figure 1 shows the forming of a Newtonian fluid jet, while Figure 2 shows power law fluid jet with the yield strength. The different characters of fold formation on a free surface are seen. In the problems under consideration we used a Lagrangian grid for the FEM. This grid cannot be used to calculate flows with large forming. For such cases we have developed a numerical procedure that proved successful in modeling the flow in channels with complex geometrical form.

FIGURE 1 Formation of Newtonian fluid jet.

FIGURE 2 Power low fluid jet.

FIGURE 3 Typical viscous fluid spreading.

BEM SIMULATION

In order to calculate Newtonian fluid flows with a free surface the BEM is highly efficient. The equations for Stokes flow provide adequate accuracy as well as the initial linearization when it is necessary to solve Navier-Stokes full equations using the BEM. Approximating the term $\partial U_i/\partial t$ using implicit scheme finite differences, we may write (1) in components of the Cartesian system.

$$
-\beta^2 U_i + T_{ik,k} = -\beta^2 U'_i - (T'_{ik} - U_i U_k), \qquad k = Q_i, \qquad \text{div } U = 0, \quad (4)
$$

where $\beta^2 = 1/\Delta t$, Δt is the discretization-time step, T_{ik} is the Newtonian part of stress tensor, T'_{ik} is the non-Newtonian addition to the full stress tensor, and U'_i is the field on the previous time step. The original system **(4)** is reduced to the integral relation with boundary values defined while solving the boundary integral equation

$$
c_{ij}U_j(\xi) + \oint t_{ij}^*U_j d\Gamma = \oint U_{ij}^*t_j d\Gamma + \int U_{ij}^*Q_j d\Omega, \qquad (5)
$$

where U_{ij}^* , t_{ij}^* is the fundamental solution, ξ is the fixed point at Γ and the coefficient c_{ij} is equal to $1/2\delta_{ij}$ in case of a locally smooth surface in the neighborhood of ξ . The solution *(5)* is carried out by applying the quadrature technique to the system of isoparametric BE and inner cells with linear approximation of the values of field variables. The simplest case of quasi-stationary approximation of slow Newtonian flows $\beta = 0$, $Q_i = 0$ lacks the integral over Ω , so that the total problem is formulated in terms of boundary values. The elementary character of the fundamental solution allows us to estimate all necessary boundary integrals analytically. Consideration of the unsteady state $(\beta \neq 0)$ introduces considerable complication into the fundamental solution, leading to numerical integration over both Γ and Ω . In contrast, to the previous case there appears a source term, which at small values of linearity has the form $Q_i = \beta^2 U'_i$.

It should be emphasized, however, that in the sense of $\partial U_i/\partial t$ approximation. U_i assumes the value derived from Eulerian (stationary) mesh. Lagrangian mesh, fixed to the nodes during the fluid motion, is preferable for problems with free boundaries. Such meshes automatically allow for the convective term of the source $Q_i = \beta^2 U'_i - U_{i,k} U_k = \beta^2 U''_i$

The last special case involved nonlinear quasi-stationary equations of motion with the source term in the form of divergence of symmetrical tensor $T_{ij} - U_i U_j$

FIGURE 4 Newtonian fluid filling a channel of complex geometry.

FIGURE 5 Bubble displacement in inclined channel.

FIGURE 6 Capillary splitting of the free jet.

 $= T_{ij}^{\prime\prime}$, which can be used to tranform the integral over the solution domain and to express it directly in terms of T''_{ij} . The obtained nonlinear integral equation is solved by use of the prime iteration technique, the convergence of which is ensured by an insignificant nonlinear contribution.

The computational algorithms for the above-mentioned cases have been carefully

verified to demonstrate monotonic convergence during transition to a more refined mesh. Special attention has been paid to simulation of the (usually multistage) filling processes observed in the channels of technological equipment. To this end several algorithms have been developed to follow the advance of the fluid front, and plugging of residual gas. Figure **4** shows the stages of consequent filling of a channel of complex geometry with a Newtonian fluid.

Within the framework of the boundary element method one can take into account the effect of capillary forces. This is illustrated by a model problem of a gas bubble displacement from an inclined channel, presented in Figure *5.* It is readily seen that the initially flat liquid-gas interface is gradually dropping under the external pressure loading and then rising to allow for the gas bubble displacement along the upper wall of the channel until it completely escapes. Here, along with internal gas pressure, one more factor has been taken into account: the value of dynamic wetting angle, which in this case is equal to 135°. This factor has a qualitative effect on the total process; hence, at the angular value of **45"** displacement doesn't occur, and the bubble is stabilized at the lower part of the channel. Figure 6 shows the process of capillary splitting of the free jet, which represents the development of initial sinusoidal disturbance of the free surface. According to the well-known Rayleigh criterion, the splitting takes place at $\lambda/2\pi r > 1$, which is in agreement with calculations, carried out for values of 0.8 and 1.2 for the left side of the inequality.