Numerical Analysis for Polymer Melt Flow in Injection Molding*

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A numerical method using a finite element approach is proposed to analyze the unsteady three-dimensional flow of power-law fluids with moving free surfaces. Based on the fractional step method and Rational Runge-Kutta (RRK) method for mass and momentum equations, this method is a semi-explicit scheme with unconditional numerical stability for pseudoplastic fluids. The transfer equation for the volume fraction of molten polymer is solved to calculate the moving free surface. The energy equation is divided into the transfer and diffusion equations. These equations are solved by a modified characteristic curve method and the RRK method, respectively. The calculation results are obtained by the present method for two box-shaped cavity flows. These are compared with the experimental results using a short-shot injection technique. Experimental and computational findings agree within 5% regarding location of the meltfronts.

Key Words: Numerical Analysis, Non-Newtonian Fluid, Finite Element Method, Free Surface Flow, Heat Transfer, Unsteady Flow

1. Introduction

The kinematic behavior of non-Newtonian fluids such as polymeric fluids which are utilized in injection molding is very different from that of Newtonian fluids such as water and gas. This difference is due to the non-Newtonian viscosity; i.e., the viscosity of the fluid changes with the shear rate. Many studies⁽¹⁾⁻⁽⁴⁾ have been conducted to calculate polymer melt flow with non-Newtonian viscosity. For example, a numerical method was proposed by Hieber and Shen⁽⁴⁾. This method, using the finite element method (FEM), calculates polymer melt flow which was approximated with the Hele-Shaw model. The Hele-Shaw model applies to polymer melt flow in a mold of small gap thickness. This model is frequently used as a practical calculation model for polymer melt flow in injection molding. A power-law model is utilized as the rheological relation in the method by Hieber and Shen. The power-law is shown by $\eta \propto \dot{\gamma}^{n-1}$, where η is the viscosity, $\dot{\gamma}$ is

the shear rate, and n is the power index. This empirical expression is well-known and widely used in engineering work, such as injection molding, to describe non-Newtonian viscosity. A more general method which is not based on the Hele-Shaw model is presented in this study. A numerical method is developed using a finite element approach to analyze the unsteady three-dimensional flow of power-law fluids with free surfaces. Based on the Fractional Step method⁽⁵⁾ and the Rational Runge-Kutta (RRK) method⁽⁶⁾ to calculate the mass and momentum equation, the new method consists of a semi-explicit scheme with unconditional numerical stability for pseudoplastic fluids, with power indices $0 < n < 1$. The transfer equation for the volume fraction of molten polymer in an element is solved to calculate the moving free surface. The energy equation is divided into transfer and diffusion equations. These equations are solved by a modified characteristic curve method⁽⁷⁾ and the RRK method, respectively.

Calculations of moving free surfaces are made by the present method for two box-shaped cavity flows, which represent injection molding. The calculation results are compared with the experiments. In these

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experiments, the meltfront, which is the interface between molten polymer and gas, is measured by a technique of short-shot injection.

Nomenclature

- C_p : specific heat [J/(kg·K)]
 e_{ij} : shear rate tensor [s⁻¹]
 F : volume fraction [-]
 k : thermal conductivity [W/(m·K)]
 n : power index [-]
 n_j : unit normal vector [-]
 P : pressure [Pa]
 T : temperature [K]
 t : time [s]
 Δt : time step [s]
 v_i : velocity vector [m/s]
 η : viscosity [Pa·s]
 η_0 : coefficient of viscosity [Pa·sⁿ]
 ρ : density [kg/m³]
 σ_{ij} : stress tensor [Pa]
 II : the 2nd invariant of shear rate tensor [s⁻¹]

Superscripts

- ^{*m, m+1*}: *m, m+1* time step, respectively
 *: show increment (correction) value
 ~: show prediction value

2. Basic Equation

A polymer melt flow has small Reynolds and high Pechlet numbers because of its properties of high viscosity and low heat conductivity, respectively. Due to this fact, the convective term in the momentum equation can be neglected, whereas that in the energy equation should be taken into account. The basic equations are the following.

$$\text{Continuity: } v_{j,j} = 0 \quad (1)$$

$$\text{Momentum Equation: } \rho v_{i,t} - \sigma_{ij,j} = 0 \quad (2)$$

Energy Equation:

$$\rho C_p (T_t + v_j T_{j,j}) = (kT_{j,j})_{,j} + e_{ij} \sigma_{ij} \quad (3)$$

$$\text{Rheology Equation: } \sigma_{ij} = -P \delta_{ij} + 2\eta e_{ij} \quad (4)$$

$$\text{Here, } \eta = \eta_0 \cdot \exp(-cT) \cdot |4II|^{\frac{n-1}{2}} \quad (5)$$

$$e_{ij} = (v_{i,j} + v_{j,i})/2 \quad (6)$$

$$II = -e_{ij}e_{ij}/2 \quad (7)$$

Subscripts with a comma represent partially differentiated terms, and the summation convention for repeated subscripts is used. The power-law model is utilized for the rheological relation for molten polymer. Boundary conditions for flow and temperature are the following.

$$a(\sigma_{ij} + P\delta_{ij}) \cdot n_j + bv_i = 0 \quad (8)$$

- (a) $a=0$; no-slip condition
 (b) $b=0$; slip condition
 (c) $a=0, b=0$; slip between wall and fluid, but friction force depends on the shear rate

$$cT_{j,j} + d \cdot T + e = 0 \quad (9)$$

- (a) $c=0$; constant temperature on the wall
 (b) $d=0$; constant heat flux on the wall
 (c) $c=0, d=0$; heat transfer between wall and fluids is proportional to temperature difference

3. Numerical Method

3.1 Numerical method for mass and momentum equation

The polymer melt flow is incompressible Stokes flow due to high viscosity of molten polymer. The present method is based on the fractional step method⁽⁵⁾ and the RRK method⁽⁶⁾.

- (1) Calculation of prediction value for velocity

$$\tilde{v}_i = v_i^m + \frac{\Delta t}{\rho} \cdot f(P^m, v_i^m, \eta^m) \quad (10)$$

Here, $f = \sigma_{ij,j}$

- (2) Calculation of pressure increment from prediction value for velocity under the condition which satisfies the continuity on the $m+1$ time step

$$P_{,ii}^* = -\frac{\rho}{\Delta t} \tilde{v}_{i,i} \quad (11)$$

- (3) Calculation of correction value for velocity and pressure

$$v_i^{m+1} = \tilde{v}_i - \frac{\Delta t}{\rho} P_{,i}^* \quad (12)$$

$$P^{m+1} = P^m + P^* \quad (13)$$

Equation (10) is solved by the RRK method and is rewritten by it as follows:

$$\tilde{v}_i = v_i^m + \frac{\Delta t}{\rho} \cdot \frac{g_1(g_1, g_3) - g_3(g_1, g_1)}{(g_3, g_3)} \quad (14)$$

Here, $g_1 = f(P^m, v_i^m)$

$$g_2 = f(P^m, v_i^m + c_2 g_1)$$

$$g_3 = b_1 g_1 + b_2 g_2$$

(g, g) shows the inner product. b_1, b_2, c_2 are constants. The RRK method is a semi-explicit scheme with unconditional numerical stability for the linear problem when $b_1 + b_2 = 1$, $b_2 c_2 < -0.5$. Equation (11) is solved by the wavefront method.

3.2 Numerical method for moving free surface

To calculate the moving free surface, which is the interface between molten polymer and gas, the transfer equation for the volume fraction of a molten polymer is solved. The volume fraction is the occupancy rate of a molten polymer in an element. The transfer equation of the volume fraction is represented as follows:

$$F_{,t} + v_j F_{j,j} = 0 \quad (15)$$

Volume fraction is calculated using hypothetical marker particles with no mass. As shown in Fig. 1, an element is divided into several subelements. The volume fraction is calculated by the number of subelements which are filled with marker particles. Marker

particles are transferred by fluid motion. Marker particles are generated from the inner boundary, as shown in Fig. 2, and are deleted when all subelements in an element are filled with them, which shows that the volume fraction in an element is unity. This process is shown in Fig. 3.

A two-fluid model is used for calculation of the momentum equation. Location of the free surface is

Fig. 1 Calculation method of the volume fraction

Fig. 2 Two-fluid model

Fig. 3 Process of marker deletion

Fig. 4 Concept of calculation method for the transfer equation

defined as the line where the volume fraction is 0.5. Material properties are calculated using the volume fraction as follows:

$$\begin{aligned}\rho &= \rho_1 F + \rho_2 (1 - F) \\ \eta &= \eta_1 F + \eta_2 (1 - F) \\ k &= k_1 F + k_2 (1 - F) \\ C_p &= C_{p1} F + C_{p2} (1 - F).\end{aligned}\quad (16)$$

Here, $F=1$: region of only molten polymer

$0 < F < 1$: boundary region between molten polymer and gas

$F=0$: region of only gas

3.3 Numerical method for energy equation

The energy equation is divided into the thermal transfer equation and the thermal diffusion equation. These two equations are solved by the modified characteristic curve method and the RRK method, respectively. Temperature is defined as a nodal value of each element, and the temperature distribution is expressed by a combination of nodal values and linear functions in an element. The calculation procedure is shown in Fig. 4.

- (1) A cross point j at the m time step plane with a characteristic curve on a stream line which passes through nodal point i is calculated.
- (2) Temperature T_j^m is interpolated at the cross point j .
- (3) To obtain temperature of the nodal point i at the $m+1$ time step plane, the thermal diffusion equation is solved by the RRK method using temperature T_j^m as an initial value.

Heat transfer from molten polymer in a cavity to the mold is calculated by using two analytical solutions in the direction of shell thickness for the entrance region and the developed flow region.

In the boundary region near the free surface, the interpolation value needed for solving the thermal transfer equation is calculated with a large numerical diffusion by nodal values, because nodal physical quantities and material properties are especially changeable in the boundary region near the free surface. Numerical diffusion for calculation of interpolation values in the boundary region near the free surface is reduced by the next upwinding technique.

This method is compared with the general linear interpolation scheme. Figure 5(a) shows the propagation process of numerical diffusion when interpolation values are calculated by the linear function in an element. Figure 5(b) shows calculation results obtained by the present upwinding technique. The interpolation calculation by this technique substitutes an upstream nodal value with an interpolation value when the volume fraction at cross point A is above 0.5. If the volume fraction at cross point A is less than

(a) Propagation process of numerical diffusion

(b) Present method for one-dimensional linear element

Fig. 5 Concept of present interpolation method

Fig. 6 Concept of present interpolation method for triangular element

0.5, the nodal value for the previous time step is used as the interpolation value. In this case, the temperature profile at $t = \Delta t$ is the same as that at $t = 2\Delta t$. Figure 6 shows the present method for a triangular element. In this case, the upstream nodal point is determined by the volume fraction F of molten polymer at the nodal point. When the nodal point 1 is an upstream nodal point, the interpolation value at point A is calculated by the next equation using the volume fraction at the nodal point and the area coordinates.

$$F_A = F_1 \xi_1 + \frac{F_2 + F_3}{2} (1 - \xi_1) \quad (17)$$

3.4 Space discretization

The Galerkin finite element method using linear elements is used for spatial discretization. A triangular element is used for a quasi three-dimensional calculation in a mold of small gap thickness, where velocity, viscosity, and temperature are linear functions and pressure is constant in an element. A rectangular prism is used for a three-dimensional calculation using the mixed FEM. Integration in an element is analytically solved by area coordinates for the quasi three-dimensional calculation and is numerically solved by Gauss-Legendre integration for the three-

dimensional calculation.

4. Numerical Stability for Mass and Momentum Calculation

The pressure calculation of Eq. (11) is usually stable because it is solved by an implicit method. Consequently, the numerical stability of the present method for mass and momentum equations depends on the calculation of Eq. (14) by the RRK method. The discretized momentum equation is described using eigenvector, coefficient matrix, and eigenvalue as follows:

$$\{v_{a,i}\} = A\{v_a\} = \lambda\{v_a\} \quad (18)$$

When the coordinates are selected, as the force of shear distortion is only applied to fluid which passes through an adjacent node, the coefficient matrix is represented by the next equation.

$$A = A_{a\beta} \cdot \eta_0 |v_a - v_\beta|^{n-1} \quad (19)$$

$A_{a\beta}$ is the result of integration in an element. Equation (19) is integrated for time by the RRK method. The eigenvalue at the $m+1$ time step is calculated using the eigenvalue at the m time step as follows:

$$\{v_a^{m+1}\} = \left[1 + \frac{\Delta \lambda^2 \cdot \Delta t}{b_1 \lambda + b_2 (\lambda + \Delta \lambda) (1 + c_2 \lambda \Delta t)} \right] \{v_a^m\} \quad (20)$$

Here $\Delta \lambda$ is the increment of eigenvalue when it is calculated for the intermediate step between m and $m+1$ time step. This increment is given according to an expansion of Eq. (19) in a Taylor series which neglects everything under the third term.

$$\begin{aligned} (\lambda + \Delta \lambda) \{v_a^{m+1}\} &= (A + \Delta A) \{v_a^m\} \\ &= \left[A + \frac{\partial A}{\partial (v_a - v_\beta)} \cdot |v_a - v_\beta| \right] \cdot \{v_a^m\} \\ &= \left[A_{a\beta} \cdot \eta_0 |v_a - v_\beta|^{n-1} \cdot \left\{ 1 + (n-1) \frac{\Delta v_a - \Delta v_\beta}{|v_a - v_\beta|} \right\} \right] \\ &\quad \times \{v_a^m\} \end{aligned} \quad (21)$$

On the other hand, $|\Delta v_a - \Delta v_\beta|$ in the above equation equals the g_1 vector in Eq. (14).

$$|\Delta v_a - \Delta v_\beta| = c_2 |g_{1a} - g_{1\beta}| \cdot \Delta t = c_2 \lambda |v_a - v_\beta| \cdot \Delta t \quad (22)$$

The next equation is obtained by substituting Eq. (22) into Eq. (21) and rearranging.

$$\Delta \lambda = (n-1) \lambda^2 c_2 \Delta t \quad (23)$$

Here constants b_1, b_2, c_2 are 2, -1, 0.5, respectively, and the next equation is obtained by substituting Eq. (23) for Eq. (20).

$$\{v_a^{m+1}\} = \left[\frac{1+c}{1-c \left\{ \frac{1+c(n-1)}{1-c(n-1)} \right\}} \right] \cdot \{v_a^m\} \quad (24)$$

Here, $C = \lambda \cdot \Delta t / 2$

The stable condition is one where there is no divergence of the eigenvalue on repetition of time integration. So,

$$|v_a^{m+1} / v_a^m| < 1 \quad (25)$$

is obtained. Finally, the next inequality is obtained.

$$\lambda' \equiv \left| \frac{1+c}{1-c \left\{ \frac{1+c(n-1)}{1-c(n-1)} \right\}} \right| < 1 \quad (26)$$

Figure 7 shows Eq. (26) for the region of $C < 0$ because the eigenvalue is usually negative in the case of a diffusion equation. Equation (26) is usually applicable to the region of $0 < n < 1$. Consequently, the present method has an unconditional numerical stability for pseudoplastic fluids.

5. Calculation Results and Discussion

To investigate the applicability of the present method, test calculations in two and three dimensions are made.

5.1 Two-dimensional flow

The present method is applied to the two-dimensional Stokes flow coupled with the energy equation for the rectangular computation domain. In this case, thermal conductivity is assumed to be zero in order to evaluate numerical diffusion of the temperature calculation.

Figure 8 shows calculation results by the present method for two-dimensional flow with a moving free surface and coupled with the energy equation. Inlet velocity is 0.5 m/s. Temperature is set to $T = 271^\circ\text{C}$ at the inlet and initial temperature is 38°C throughout the entire computational domain. Calculation results are plotted as temperature profiles at 0.05 s and 0.2 s. Numerical diffusion near the free surface is small and

Fig. 7 Numerical stability of the present method for power-law fluid

Fig. 8 Calculation results for two-dimensional flow

confined to an element near the free surface.

5.2 Three-dimensional flow

The other calculation example is three-dimensional flow in a box-shaped cavity. Inlet velocity is 0.05 m/s at the gate. Boundary condition of pressure is zero at the outlet. Temperature is set to $T = 180^\circ\text{C}$ at the inlet and to $T = 100^\circ\text{C}$ on the mold wall. A plane of symmetry is regarded as the adiabatic wall. Test fluid is a polycarbonate with a power index n of 0.193. Figure 9 (a) shows the calculation model and Fig. 9 (b), (c), and (d) are pressure profile on the surface, velocity profile at $A-A'$ cross section, and location of meltfront at 3 s, respectively. Figures 10(a) and (b) show the surface temperature profile at a plane of symmetry and the temperature profile at $A-A'$ cross section 50 s after complete filling of the computational domain, respectively. These results show good applicability of the present method to three-dimensional polymer melt flow.

Fig. 9 Calculation results for three-dimensional flow 3 seconds after injection

Fig. 10 Temperature profiles 50 seconds after complete filling

5.3 Application for polymer melt flow

To evaluate the method's application to polymer melt flow in injection molding, two calculation results are described next.

Figure 11 shows the geometry of a box-shaped cavity. The gap thickness of the side in this model is thicker than that of the bottom. Consequently, polymer melt flow of the side in this cavity progresses faster than that of the bottom.

Figure 12 shows a calculation model. This calculation model is computed by the quasi three-dimensional calculation using a shell model and is carried

Fig. 11 Geometry of a box-shaped cavity

Fig. 12 Calculation model for box-shaped cavity flow

Fig. 13 Experimental results using short-shot injection technique

out under an isothermal condition because the effect of heat loss to the mold is negligibly small and the increase of temperature by heat generation due to shear is at most 2–3°C. Inlet velocity is 0.31 m/s and the time step is 0.025 s. Polyacetal is used as the molten polymer. Calculation results for the location of the moving free boundary are compared with experimental results using a short-shot injection technique which injects a constant volume of molten polymer into the mold. Experimental results are shown in Fig. 13 for several times. Figure 14 shows calculated and experimental results for the location of the moving free surface. Both results agree within 3% for the distance between the inlet and the free surface, except for the result at 1.75 s.

Figure 15 shows a calculation model for the air conditioner unit case. The geometry of the calculation model is modified by flat planes. Each flat plane in this model has a small gap thickness. So this calculation model is computed by the quasi three-dimensional calculation using the shell model. Inlet velocity is 0.33 m/s and time step is 0.1 s. Polypropylene was used as molten polymer. Figure 16 shows the line of the moving free boundary at each time and the pressure profile at 3 s. The calculation result for the line of the

Fig. 14 Experimental and computational results for the location of meltfront

Fig. 15 Calculation model for air conditioner unit case

Fig. 16 Calculation results

Fig. 17 Experimental and computational results for the location of meltfront

moving free boundary at 3 s is compared with the experimental result using a short-shot injection technique in Fig. 17. Both results agree within 5% for the distance between the inlet and the free surface.

6. Conclusions

A numerical method was developed using a finite element approach to analyze the unsteady three dimensional polymer melts flow in injection molding. Features of the present method include the following.

(1) Based on the fractional step method and the RRK method, this method consists of a semi-explicit scheme with unconditional numerical stability for pseudoplastic fluids, with power indices $0 < n < 1$.

(2) The technique for calculation of the moving free surface is based on a two-fluid model using marker particles and the volume fraction, which is the occupancy rate of molten polymer in an element.

(3) The energy equation is divided into the transfer and diffusion equations. These two equations are solved by a modified characteristic curve method and the RRK method, respectively.

The applicability of the present method was confirmed by the results of test calculations in two and three dimensions. These calculation results were compared with the experiments using a short-shot injection technique. Experimental and computational results agreed within 5% regarding location of the meltfronts.

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