INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS
Int. J. Numer. Meth. Fluids 2008; **57**:139–155
Published online 25 October 2007 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/fld.1630

Penalty formulation for postfilling analysis during injection molding

Sung Yong Kang[1], Sun Kyoung Kim[2] and Woo Il Lee[1,*,†]

[1]*Department of Mechanical and Aerospace Engineering, Seoul National University, Seoul 151-742, Republic of Korea*
[2]*Department of Die and Mold Design, Seoul National University of Technology, Seoul 139-743, Republic of Korea*

SUMMARY

We propose an approximate method that can simulate the packing stage during the injection molding using the penalty parameter method. In order to account for the compressibility effect, an update scheme based on similarity between the slightly compressible and the penalty formulations is proposed. The method allows for solving the entire injection molding process using a single algorithm with the penalty method in spite of the transition from the incompressible regime during the filling stage into the compressible regime for the packing stage. Several test cases have been presented to prove the validity of the method. It has been shown that the accuracy of the proposed method is identical to that of the mixed method.

Received 5 January 2007; Revised 30 August 2007; Accepted 4 September 2007

KEY WORDS: penalty formulation; slightly compressible flow; injection molding; packing stage

1. INTRODUCTION

Injection molding for plastic processing consists of three distinctive stages, namely, the filling, the packing and the cooling stages. In the filling stage, polymer melt is introduced into the mold. Once the mold is completely filled, packing stage ensues during which additional polymer melt is supplied to compensate the shrinkage during cooling. As the melt has to be pressed into the mold with a fixed volume, applied pressure during packing is very high and the flow is inherently

*Correspondence to: Woo Il Lee, Department of Mechanical and Aerospace Engineering, Seoul National University, Seoul 151-742, Republic of Korea.
†E-mail: wilee@snu.ac.kr

Contract/grant sponsor: Ministry of Commerce, Industry and Energy (MOCIE), Republic of Korea
Contract/grant sponsor: Korea Science and Engineering Foundation (KOSEF); contract/grant number: R11-2005-065

compressible. After packing, the mold is cooled down to a preset temperature and the polymer melt is solidified.

Integrated simulation of the injection molding process, involving the filling, packing and cooling stages, is already full fledged. Filling and packing stages in injection molding process have been analyzed based on the generalized Hele–Shaw (GHS) model for relatively thin parts [1]. However, three-dimensional phenomena such as the fountain flow and the flow instability cannot be simulated with such approximated models [2]. In order to consider such out-of-plane phenomena, any model with approximation in thickness direction as in the GHS model should not be employed. Instead, a set of the governing equations which is composed of the conservation of mass, momentum, energy and corresponding constitutive equations should be solved simultaneously considering through-thickness variation of all the variables. Especially, the Navier–Stokes equations with compressibility effect allow simulation of the packing stage during injection molding.

Three-dimensional simulations of the injection molding are gaining more popularity in the design and troubleshooting of the process as the parts are becoming complicated and the products in the design stage are modeled using three-dimensional tools. Nowadays, several commercial computer-aided engineering packages for injection molding simulation provide such capability [3]. However, the computational time is a major bottleneck in the three-dimensional simulation.

It is well known that the penalty method is advantageous in reducing the computational time for analyzing many fluid flow problems [4]. In the injection molding process, even though the filling stage can be handled by incompressible flow assumption, compressibility effect should be included in the analysis of the packing stage. As a result, it has been a common practice to solve different governing equations and hence to employ separate numerical codes for the filling and packing stages. The penalty method basically assumes the flow to be incompressible by choosing a very large value of the penalty parameter. Therefore, the penalty method is not widely employed for simulating the compressible flows such as those encountered during the packing stage of injection molding.

This study is motivated by the apparent similarity between the slightly compressible formulation and the penalty formulation [5]. Hesthaven [6] has provided a mathematical foundation for solving the compressible Navier–Stokes equations using the penalty method. Kellogg and Liu [7] have proposed a mathematical formulation for compressible Stokes problem based on the penalty method. Utilizing these formulations, this work presents and implements a numerical method that handles the filling and packing stages of the injection molding process in the same manner. The proposed method presents a scheme that updates the penalty parameter in accordance with the compression of the fluid (molten thermoplastic resin). In order to demonstrate the feasibility of the proposed scheme, we have analyzed the injection molding process from the filling to the packing for two-dimensional and three-dimensional cases. Validity of the method has been examined through comparisons with the results by the mixed method. We have also shown that the current method can significantly reduce the computation time for the grid systems with a similar number of nodes.

2. GOVERNING EQUATIONS

As previously noted, it is essential to consider the effect of melt compressibility for simulation of the packing stage in injection molding [8]. The equation of mass conservation in the packing

DOI: 10.1002/fld

stage is different from that of incompressible polymer flow encountered during the filling stage. For convenience, isothermal condition is assumed in this study.

2.1. Momentum equation for packing stage

Consider the velocity vector $\mathbf{u}$ and pressure p. For the given time t and density ρ, momentum conservation requires [9]

$$\rho\left[\frac{\partial u_i}{\partial t}+u_k\frac{\partial u_i}{\partial x_k}\right]=-p_{,i}+\frac{\partial \tau_{ij}}{\partial x_j} \tag{1}$$

Body force can be neglected since the injection pressure is usually very high. Here, for a given temperature T, the shear stress tensor τ_{ij} is expressed as

$$\tau_{ij}=2\eta(I_2,T)d_{ij} \tag{2}$$

where the rate-of-deformation tensor d_{ij} and the second invariant of rate-of-deformation tensor I_2 are defined as follows:

$$d_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right) \tag{3}$$

$$I_2=(2d_{ij}d_{ji})^{1/2} \tag{4}$$

The Cross-WLF model for viscosity is adopted to describe the non-Newtonian behavior of polymer melt [10]. For the given temperature T, the corresponding viscosity function $\eta(I_2,T)$ takes the following form [10]:

$$\eta(I_2,T)=\frac{\eta_0(T)}{1+(\eta_0(T)\cdot I_2/\tau)^{1-n}} \tag{5}$$

where $\eta_0=D_1\exp[-A_1(T-D_2)/(A_2+T-D_2)]$ for $T\geqslant D_2$ and $T<D_2$ for $\eta_0=\infty$. Here, D_1, D_2, A_1, A_2 and τ are constant values that should be determined from experimental measurements for a specific polymer. The values of constants for polymethylmethacrylate are listed in Table II.

2.2. Mass conservation equation for packing stage

Conservation of mass can be expressed as [9]

$$\frac{\partial \rho}{\partial t}+(\nabla\cdot\rho\mathbf{u})=0 \tag{6}$$

Expanding the second term in the above equation gives

$$\frac{\partial \rho}{\partial t}+\rho(\nabla\cdot\mathbf{u})+\mathbf{u}\cdot\nabla\rho=0 \tag{7}$$

Density of polymer melt ρ is a function of pressure p and temperature T. The derivatives can be estimated as

$$\frac{\partial \rho}{\partial x_i}=\left(\frac{\partial \rho}{\partial p}\right)_T\frac{\partial p}{\partial x_i}+\left(\frac{\partial \rho}{\partial T}\right)_p\frac{\partial T}{\partial x_i} \tag{8a}$$

DOI: 10.1002/fld

$$\frac{\partial \rho}{\partial t} = \left(\frac{\partial \rho}{\partial p}\right)_T \frac{\partial p}{\partial t} + \left(\frac{\partial \rho}{\partial T}\right)_p \frac{\partial T}{\partial t} \tag{8b}$$

Using the above equalities, the continuity equation can be rewritten as

$$\frac{1}{\rho}\frac{\partial \rho}{\partial p}\left(\frac{\partial p}{\partial t} + \mathbf{u}\cdot\nabla p\right) + \frac{1}{\rho}\frac{\partial \rho}{\partial T}\left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) + \nabla\cdot\mathbf{u} = 0 \tag{9}$$

where κ is the isothermal compressibility ($\equiv (1/\rho)\partial\rho/\partial p$) and β is the coefficient of thermal expansion ($\equiv -(1/\rho)\partial\rho/\partial T$). As a result, the equation of mass conservation can be written as

$$\kappa\left(\frac{\partial p}{\partial t} + \mathbf{u}\cdot\nabla p\right) - \beta\left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) + \nabla\cdot\mathbf{u} = 0 \tag{10}$$

In this analysis, two major assumptions have been made [11]. First, during the packing stage, the flow is assumed to be isothermal since temperature change of the polymer melt in this stage is negligible. Therefore, terms involving temperature change such as $\partial T/\partial t$ and $\mathbf{u}\cdot\nabla T$ can be ignored without inducing significant error. Second, because the mold is volumetrically filled during the packing stage, application of packing pressure tends to pressurize the melt hydrostatically. Even though the pressure itself is very high in the packing stage, pressure gradient is much lower than that in the filling stage. With small value of pressure gradient, the velocity during the packing stage is also small. Therefore, $\mathbf{u}\cdot\nabla p$ is assumed to be negligible during the packing stage.

The above-mentioned assumptions allow the mass conservation equation (Equation (10)) to be expressed in a simpler form as follows:

$$\frac{\partial p}{\partial t} + \frac{1}{\kappa}\nabla\cdot\mathbf{u} = 0 \tag{11}$$

Equation (11) is referred to as the 'slightly compressible' formulation, where κ ranges between 10^{-9} and 10^{-10}/Pa for most liquids. It is noted that the isothermal compressibility κ can be obtained from the equation of state.

2.3. Equation of state for packing stage

The Tait equation [11] is employed to calculate the specific volume of polymer melt v as a function of temperature and pressure. In the present study, the following equation is used to obtain the specific volume [12]:

$$v(T, p) = v_0(T)\left\{1 - C\ln\left(1 + \frac{p}{B(T)}\right)\right\} + v_g(T, p) \tag{12}$$

where $v_0(T) = b_1 + b_2\overline{T}$, $B(T) = b_3\exp[-b_4\overline{T}]$, $v_g(T, p) = b_7\exp[b_8\overline{T} - b_9 p]$ and $\overline{T} = T - b_5$. Values of constants for the above equations are listed in Table III.

3. PENALTY METHOD FOR SLIGHTLY COMPRESSIBLE FLOW

3.1. Mixed and penalty methods for FEM formulation

Many investigators have shown that the finite element method (FEM) can be successfully applied to the problems of compressible or incompressible fluid flow [9]. The FEMs for solving the equations

DOI: 10.1002/fld

associated with polymer processing can be categorized into three groups, depending on the way velocity and pressure are treated [13]. Those three methods are the mixed (velocity–pressure-integrated) method [14–16], the penalty method [17] and the segregated velocity–pressure method [9, 18, 19].

Several numerical studies have been conducted using the three approaches in various fluid flow problems [20–23]. Among these methods, the penalty method is sometimes preferred over the other methods especially for incompressible problems since the computational cost can be saved [4, 9]. Because of decrease in the number of variables appearing in the discretized equations, the penalty method requires less memory and computational time than the mixed method due to the decoupling of velocity and pressure [4].

The finite element formulation and the solution procedure are explained in this section briefly. Rewriting (Equation (1)) in a vector form, we have

$$\rho\frac{\partial \mathbf{u}}{\partial t}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u}=-\nabla p+\nabla(\eta\nabla\mathbf{u}+\eta\nabla^{\mathrm{T}}\mathbf{u}) \tag{13}$$

After applying the weighted residual method to the above momentum equation and the continuity equation, the following expressions are obtained:

$$\int_{\Omega}\rho\frac{\partial \mathbf{u}}{\partial t}\cdot\mathbf{w}\,\mathrm{d}\Omega+\int_{\Omega}\rho(\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{w}\,\mathrm{d}\Omega+\int_{\Omega}(\mu\nabla\mathbf{u}\nabla\mathbf{w}-p(\nabla\cdot\mathbf{w}))\,\mathrm{d}\Omega=\int_{\Gamma}(\sigma\cdot\mathbf{n})\,\mathrm{d}\Gamma \tag{14}$$

$$-\int_{\Omega}(\nabla\cdot\mathbf{u})\cdot\mathbf{q}\,\mathrm{d}\Omega=0 \tag{15}$$

The above weak forms can be discretized by applying the Galerkin method as follows:

$$\mathbf{M}\left(\frac{\mathbf{u}-\mathbf{u}^{p}}{\Delta t}\right)+\mathbf{C}\mathbf{u}+\mathbf{A}\mathbf{u}+\mathbf{Q}\mathbf{p}=\mathbf{B} \tag{16}$$

$$\mathbf{Q}^{\mathrm{T}}\mathbf{u}=0 \tag{17}$$

where $\mathbf{M}, \mathbf{C}, \mathbf{A}, \mathbf{Q}, \mathbf{Q}^{\mathrm{T}}$ and $\mathbf{B}$ are the mass matrix, the convection matrix, the viscous matrix, the pressure matrix, the divergence matrix and the body force matrix, respectively. p and Δt denote the values from the previous time step and the time increment, respectively.

In the mixed method, the velocity and pressure are simultaneously obtained, whereas in the penalty method the pressure should be estimated by post-processing the velocity. The pressure is coupled with the velocity while updating pressure field does not affect the velocity field in the penalty method. In the mixed method, the solution is obtained by solving the following system of linear equations at each time step:

$$\begin{bmatrix}\mathbf{K} & \mathbf{Q}\\ \mathbf{Q}^{\mathrm{T}} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ \mathbf{p}\end{bmatrix}=\begin{bmatrix}\mathbf{F}\\ \mathbf{0}\end{bmatrix} \tag{18}$$

where $\mathbf{p}$ is the pressure vector at nodal points, $\mathbf{K}$ and $\mathbf{F}$ are given as [9]

$$\mathbf{K}=\mathbf{M}/\Delta t+\mathbf{C}+\mathbf{A} \tag{19}$$

$$\mathbf{F}=\mathbf{M}\mathbf{u}^{p}/\Delta t+\mathbf{B} \tag{20}$$

DOI: 10.1002/fld

The segregated method such as the fractional step method is not treated here since it can be considered an approximation of the mixed method for computational efficiency.

The penalty method approximates the momentum equation by eliminating the pressure from it. It should be noted that the continuity equation is approximately satisfied in the penalty method. Here, pressure is obtained using

$$p+\lambda\nabla\cdot\mathbf{u}=0 \tag{21}$$

where λ is the penalty parameter and $\mathbf{u}$ is the velocity vector.

In the penalty method, the incompressibility constraint is additionally imposed in the momentum equation by introducing the penalty term [4, 17]. Replacing p in Equation (14) with $-\lambda\nabla\cdot\mathbf{u}$ using Equation (21) gives

$$\int_\Omega \rho\frac{\partial\mathbf{u}}{\partial t}\cdot\mathbf{w}\,\mathrm{d}\Omega+\int_\Omega \rho(\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{w}\,\mathrm{d}\Omega+\int_\Omega(\mu\nabla\mathbf{u}\nabla\mathbf{w}+\lambda(\nabla\cdot\mathbf{u})(\nabla\cdot\mathbf{w}))\,\mathrm{d}\Omega=\int_\Gamma(\sigma\cdot\mathbf{n})\,\mathrm{d}\Gamma \tag{22}$$

Applying the Galerkin method, we have the following expression:

$$\mathbf{M}\left(\frac{\mathbf{u}-\mathbf{u}^p}{\Delta t}\right)+\mathbf{C}\mathbf{u}+\mathbf{A}\mathbf{u}+\lambda\mathbf{K}'\mathbf{u}=\mathbf{B} \tag{23}$$

where $\mathbf{K}'$ is the penalty matrix that corresponds to the fourth term on the left-hand side of Equation (22).

The solution for each time step is obtained by solving the following system of linear equations [9]:

$$[\mathbf{K}+\lambda\mathbf{K}'][\mathbf{u}]=[\mathbf{F}] \tag{24}$$

where $\mathbf{K}$ and $\mathbf{F}$ have the same forms as in Equations (19) and (20). The matrix $\mathbf{K}'$ should be integrated with a lower integration order than $\mathbf{K}$ to ensure the convergence of the solution [9]. This results in discontinuity in pressure between elements. It should be emphasized that Equation (24) can be obtained for a Galerkin approximation of the discontinuous pressure fields with the continuous velocity fields [24].

Theoretically, a larger λ forces the mass conservation ($\nabla\cdot\mathbf{u}=0$) satisfied more strictly. However, a larger λ also causes numerical difficulties such as the locking problem in elasticity analysis [9]. On the other hand, a small λ value can induce mass loss. In practice, a couple of tips are found in the literatures. It is known that the penalty parameter should be selected to be two to four orders of magnitude larger than the terms in $\mathbf{K}$ [25]. The magnitude of λ is $O(10^{n/2})$ where n is the number of bits in a word in the computer [26]. Moreover, there is another approach that the penalty parameter should be $(10^7$–$10^8)\mu$ [27]. This work suggests the method of selecting the penalty parameter.

It can be observed that the continuity equation of slightly compressible formulation Equation (11) is analogous to the pressure equation (21) in the penalty formulation. Comparing these two expressions, we can postulate that the compressibility effect during the packing stage can be taken into account by appropriately adjusting the value of the penalty parameter. By doing this, incompressible filling stage and the compressible packing stage can be analyzed using the identical formulation. This study proposes a new penalty method that mimics the slightly compressible formulation by properly controlling the penalty parameter.

DOI: 10.1002/fld

3.2. Penalty formulation for slightly compressible flow

Substituting Equation (14) into Equation (11), we have

$$\frac{\partial \lambda}{\partial t}\nabla\cdot\mathbf{u}-\frac{1}{\kappa}\nabla\cdot\mathbf{u}+\lambda\frac{\partial}{\partial t}\nabla\cdot\mathbf{u}=0 \tag{25}$$

Consider the penalty parameter to be updated every time step as follows:

$$\lambda^{n+1}=\lambda^n+(\Delta\lambda)^n \tag{26}$$

Then, Equation (17) can be discretized to give the increment as

$$(\Delta\lambda)^n=\frac{\Delta t}{\kappa}-\lambda^n\frac{(\nabla\cdot\mathbf{u})^{n+1}-(\nabla\cdot\mathbf{u})^n}{(\nabla\cdot\mathbf{u})^{n+1}} \quad \text{for } n\geqslant 1 \tag{27}$$

The penalty parameter is updated at every time step using the above equation by adding the increment to the old penalty parameter λ^n. In this study, the initial value of the penalty parameter λ^0 is set as 0 for convenience. In this work, the penalty parameter λ is evaluated at the points for reduced integration. As a result, with bilinear quadrilateral elements with reduced integration for $\mathbf{K}'$ (Q_1/Q_0), λ is constant over each element at a given time.

During the filling stage, a large value of penalty parameter is imposed due to the incompressibility of the polymer melt. During the packing stage, however, the penalty parameter should be varied to consider the compressibility effect. The algorithm proposed above allows varying the penalty parameter according to the compressibility. Thus, a single computer code developed based on the penalty method enables seamless analysis of both the filling and the packing stages.

4. NUMERICAL TESTS

4.1. Implementation of the computer code

We have solved verification problems to compare the results of the mixed method and the penalty method during the packing stage. For comparison, we have developed two separate computer codes each using the penalty method and the mixed method to analyze the slightly compressible flow during the packing stage. Fully implicit time integration scheme has been employed. Detailed formulation for both the penalty and the mixed methods can be found elsewhere [9]. The penalty method is equipped with the penalty parameter update scheme as outlined above, which allows simulating the filling and packing in the same framework. After discretization of the governing equations, resulting system of algebraic equations is solved by the frontal method [28].

4.2. Comparison with the mixed method in a two-dimensional case

Consider a rectangular domain of $1\,\mathrm{m}\times 0.1\,\mathrm{m}$ and the structured mesh as shown in Figure 1. All the material properties used for the numerical tests are specified in Tables I–III [29]. Especially, the density and compressibility as functions of pressure are shown in Figure 2. Temperature is kept uniform and packing pressure is assumed to increase at a constant rate.

DOI: 10.1002/fld

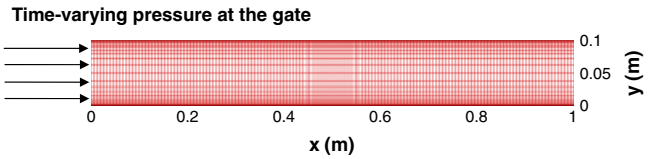

Figure 1. Geometry and mesh for test cases.

Table I. Thermophysical properties of the resin.

β (m/m K)	6.3×10^{-5}
C_p (J/kg K)	2.4×10^{3}
k_{ij} (W/m K)	0.177
ρ (kg/m^3)*	1.007×10^{3}

*A representative ρ-value.

Table II. Constants for the Cross-WLF equation (Equation (5)).

n	0.3894
A_1	40.50
A_2 (K)	51.60
D_1 (Pa s)	1.5168×10^{16}
D_2 (K)	343.15
τ (Pa)	4.0405×10^{4}

Table III. Values of constants required for the Tait equation (Equation (12)).

	For $T>T_g$	For $T\leqslant T_g$
T_g (K)	408.12	408.12
b_1 (m^3/kg)	1.0100×10^{-3}	1.0100×10^{-3}
b_2 (m^3/kg K)	6.4677×10^{-7}	2.0123×10^{-7}
b_3 (Pa)	1.9109×10^{8}	2.9835×10^{8}
b_4 (K^{-1})	4.7537×10^{-3}	2.0032×10^{-3}
b_5 (K)	408.12	408.12
b_6 (K/Pa)	3.8307×10^{-7}	3.8307×10^{-7}
b_7 (m^3/kg)	0.0	0.0
b_8 (K^{-1})	0.0	0.0
b_9 (Pa^{-1})	0.0	0.0
C	0.0894×10^{0}	

Due to the compressibility of polymer melt, mass should be added during the packing stage. The amount of total added mass m_a over the packing time can be obtained by simply integrating the mass flow into the control volume over the packing time as

$$m_a(t)=\int_{t_0}^{t}\dot{m}\,d\tau \tag{28}$$

DOI: 10.1002/fld

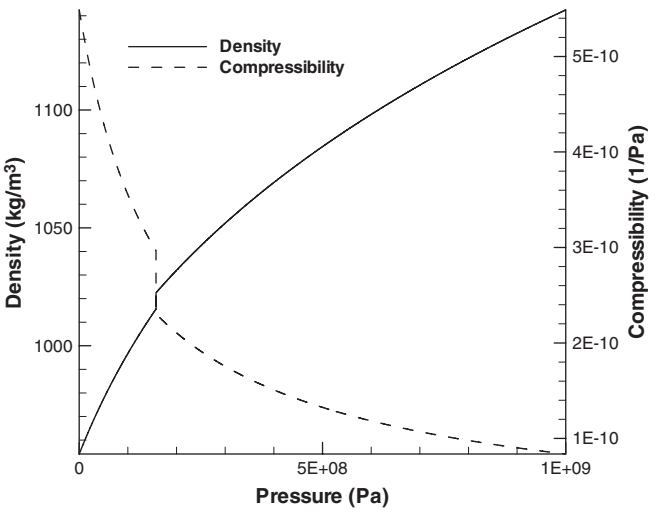

Figure 2. Density and compressibility as functions of pressure.

where t_0 is the initial time of the packing stage. Integrating Equation (6) over the control volume gives

$$\int_{\mathrm{CV}} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u \right) \mathrm{d}V = \int_{\mathrm{CV}} \rho \kappa \frac{\partial p}{\partial t} \mathrm{d}V + \int_{\mathrm{CS}} \rho \mathbf{u} \cdot \mathbf{n} \, \mathrm{d}S = 0 \tag{29}$$

where CV and CS stands for the control volume and surface, respectively. The vector $\mathbf{n}$ is normal to CS. Then, the mass flow rate $\dot{m}$ into CS becomes

$$\dot{m} = -\int_{\mathrm{CV}} \rho \mathbf{u} \cdot \mathbf{n} \, \mathrm{d}S = \int_{\mathrm{CV}} \rho \kappa \frac{\partial p}{\partial t} \mathrm{d}V \tag{30}$$

The same result is obtained using the definition of the isothermal compressibility κ as follows:

$$\dot{m} = \int_{\mathrm{CV}} \frac{\partial \rho}{\partial t} \mathrm{d}V = \int_{\mathrm{CV}} \rho \kappa \frac{\partial p}{\partial t} \mathrm{d}V \tag{31}$$

The horizontal velocity component and the amount of added mass are compared for the slightly compressible and penalty methods. Figure 3(a) and (b) shows the velocity profiles at $t = 5\,\mathrm{s}$ for the pressure increase rate of 10 MPa/s. As can be seen, velocity profiles coincide very well with each other. Figure 4(a) and (b) shows pressure profiles for the same case. The observed discrepancy is negligible in this comparison.

Added masses for both methods are compared in Figure 5(a) and (b). Overall, there is no noticeable difference in the amounts of added mass. In the initial stage of packing, however, the penalty method and the mixed method exhibit slightly different behaviors as shown in the figures. These figures also show that both solutions converge to each other as time progresses despite the presence of initial discrepancy. The reason for the initial discrepancy may be attributed to the inaccuracy in selecting initial value of the penalty parameter.

DOI: 10.1002/fld

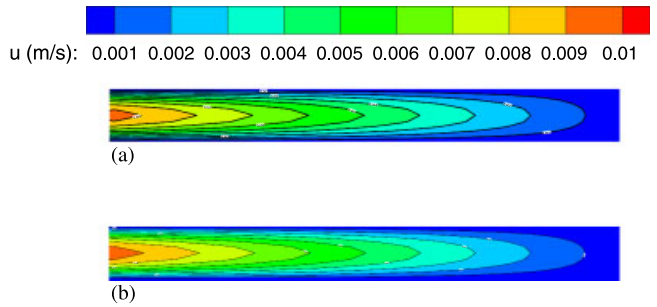

Figure 3. Comparison of the velocity component, u, at $t=5$ s obtained by the mixed (slightly compressible) and penalty methods for gate pressure increase rate of 10 MPa/s: (a) result by the mixed method and (b) result by the penalty method.

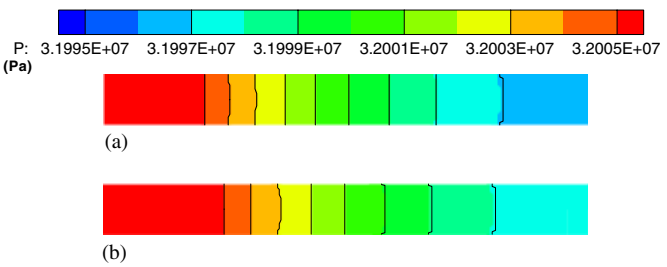

Figure 4. Comparison of the pressure component, p, at $t=5$ s obtained by the mixed (slightly compressible) and penalty methods for gate pressure increase rate of 10 MPa/s: (a) result by the mixed method and (b) result by the penalty method.

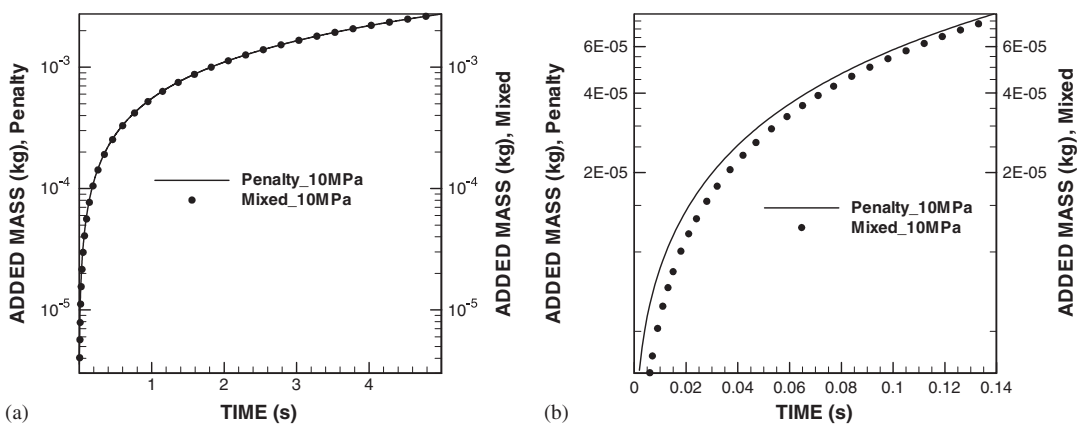

Figure 5. Comparison of the amount of added mass obtained by the mixed (slightly compressible) and penalty methods for gate pressure increase rate of 10 MPa/s: (a) result by the mixed method and (b) result by the penalty method.

DOI: 10.1002/fld

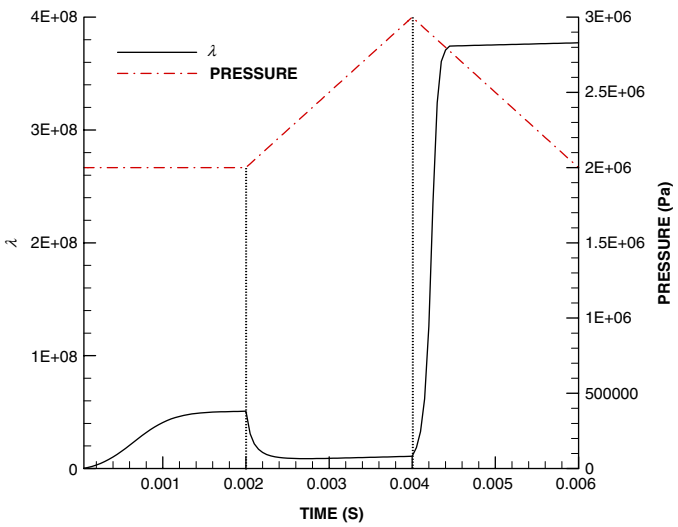

Figure 6. Change of the penalty parameter λ and the gate pressure with time.

4.3. Implication of change in λ

In the proposed scheme, the penalty parameter λ is related to inherent compressibility of the material in the domain. However, the value itself does not bear any strict meaning. On the other hand, its variation $\Delta\lambda$ is greatly affected by the compressibility κ as is evident from Equation (27). Consider a situation where the gate pressure is first linearly increased at $t=0.002$ s. After 0.002 s of increase, pressure is made to decrease at the same rate as shown in Figure 6. This figure shows the change in λ as a function of the gate pressure. Increase of the gate pressure renders the polymer melt compressed and thus λ is significantly decreased at 0.002 s. After that, as the compressibility change becomes smaller, λ increases. When the gate pressure starts to decrease at 0.004 s, λ climbs up to a certain level to reflect the decreased change in compressibility.

4.4. Initial guess of λ

We have tested the proposed algorithm with different initial guesses of the penalty parameter λ. Figure 7(a)–(d) shows the change of λ with the pressure change at the gate. Initially, the pressure is maintained at 0 Pa (gauge). At 0.01 s, pressure goes up at a rate of 500 MPa/s. As shown in Figure 6, before the pressure increase is started, λ goes up at a constant rate of $\Delta t/\kappa$. At the point when the pressure starts to ramp up ($t=0.01$ s), λ value dropped dramatically to accommodate the compressibility change of polymer melt. Figure 7(a)–(d) shows an identical behavior of λ regardless of the initial guess, λ_0. From these results, the proposed method is shown to be insensitive to the selection of initial guess. However, based on Equation (28) and the result shown in Figure 6(d), $\Delta t/\kappa$ is recommended as the initial guess of λ. Figure 8(a)–(d) also demonstrates insensitivity of the results to the initial guess. In this case, pressure is changed in a stepwise manner—pressure is abruptly raised from 20 to 40 MPa at 0.01 s. It is observed that λ abruptly decreases at the point of step increase in the pressure but quickly recovered back to the level before the pressure jump. The imposition of $\Delta t/\kappa$ as the initial guess also works well in this case as can be seen from

DOI: 10.1002/fld

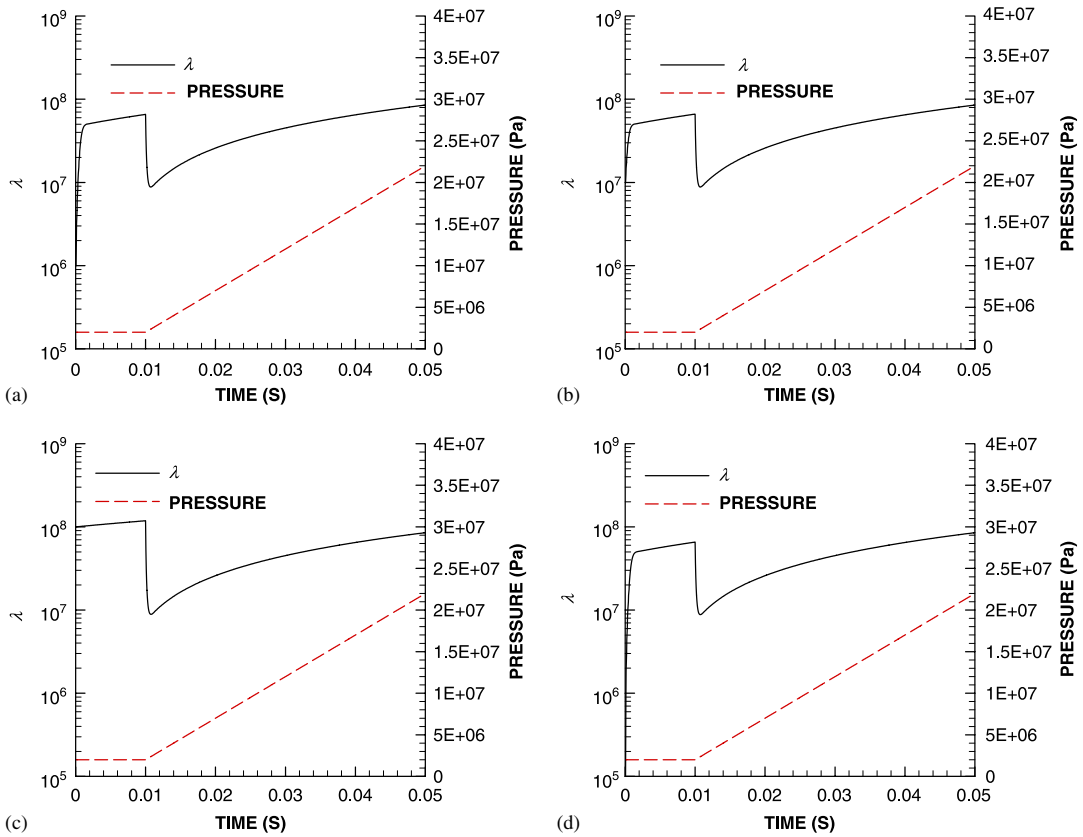

Figure 7. Change of λ when the gate pressure is ramped up at a rate of 500 MPa/s from 0.01 s for different initial values of the penalty parameter: (a) $\lambda_0 = 1.E6$; (b) $\lambda_0 = 1.E7$; (c) $\lambda_0 = 1.E8$; and (d) $\lambda_0 = \Delta t/\kappa$.

Figure 8(d). It is found that λ spontaneously varies along with the inherent compressibility even with rough initial guess.

4.5. Seamless simulation

We have built up a computer code that can seamlessly simulate from mold filling to packing. To realize the free-surface flow, the volume of fluid method with fixed grid system is employed [30]. Further details of the filling simulation are not delineated here. Figure 9(a)–(d) shows the flow front and u for the corresponding filling phases. During the filling process, the inlet velocity is set constant until the entire domain is filled. Figure 9(a) and (b) shows the results when the filling is 50 and 97% completed. Because of the constant inlet flow rate they show a similar pattern near the flow front. After the cavity is completely filled, the magnitude of the velocity over the domain dramatically decreases as shown in Figure 9(c). During the postfilling phase, the magnitude is very small as shown in Figure 9(d).

DOI: 10.1002/fld

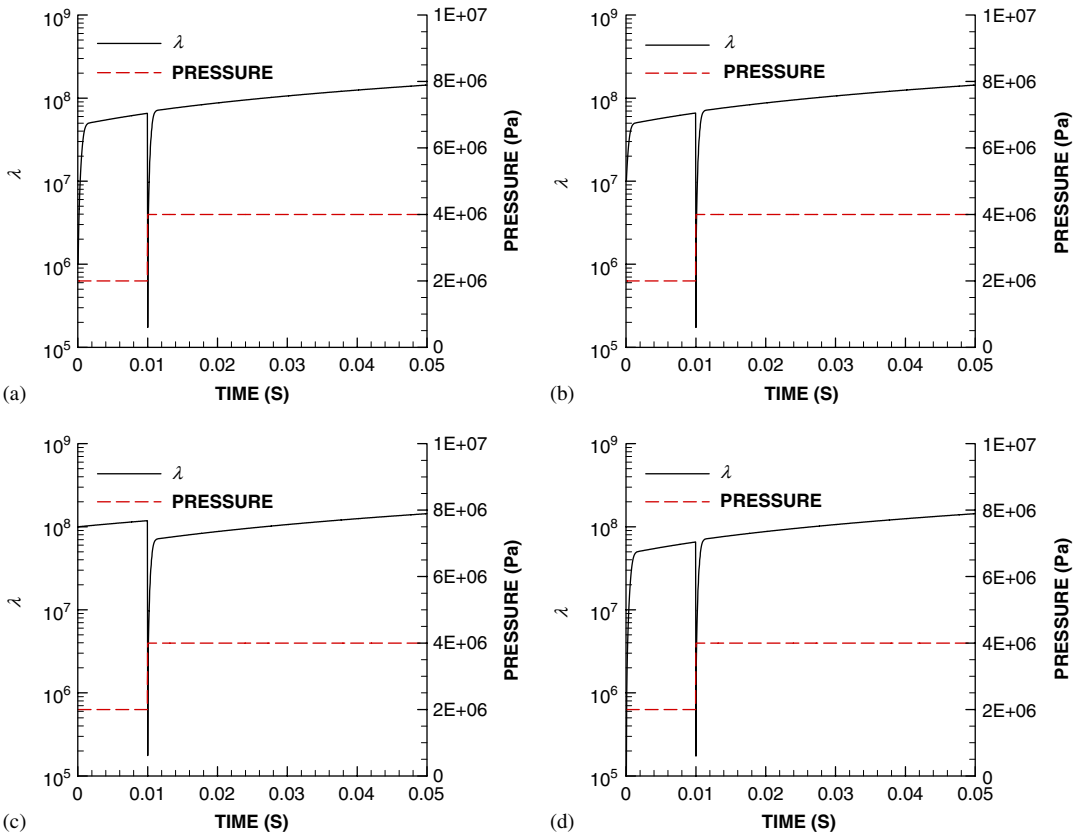

Figure 8. Change of λ when the gate pressure is stepped up from 20 to 40 MPa at 0.01 s for different initial values of the penalty parameter: (a) $\lambda_0 = 1.0 \times 10^6$; (b) $\lambda_0 = 1.0 \times 10^7$; (c) $\lambda_0 = 1.0 \times 10^8$; and (d) $\lambda_0 = \Delta t / \kappa$.

4.6. Application to three-dimensional case

We have conducted a three-dimensional packing analysis with the proposed method. Figure 10 shows the packing pressure history for the three-dimensional test case. Results are presented at 20 s after packing. The velocity in the x-direction and pressure are shown in Figure 11(a) and (b), respectively. Arrows in Figure 11(a) show the region where the packing pressure is applied. Other boundaries are all impermeable walls. Because the lower part of the inlet face is pressurized, asymmetry in pressure profile is observed in Figure 11(b). As can be seen, the proposed algorithm works fine for this three-dimensional problem.

5. CONCLUSION

In this work, an algorithm employing the penalty method for slightly compressible flows has been proposed. An approximate method that can analyze compressible packing stage during injection

DOI: 10.1002/fld

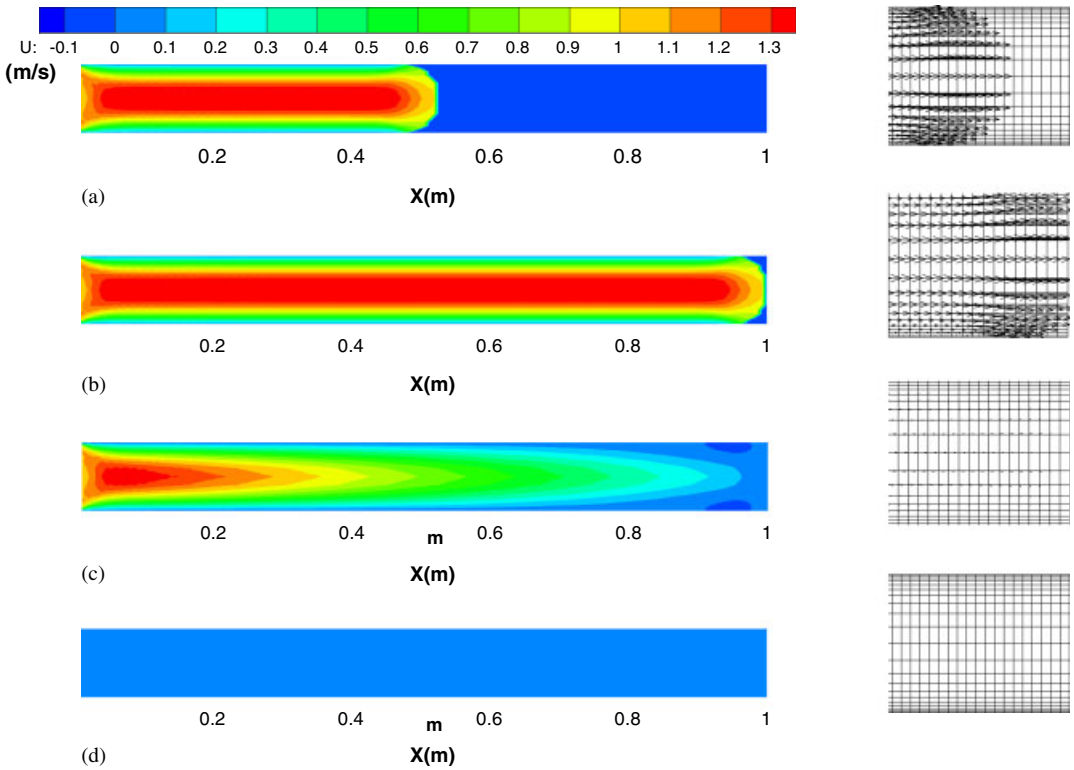

Figure 9. u Contour and velocity vectors during filling of two-dimensional cavity: (a) at 50% filling, 1.494 m/s; (b) at 97% filling, $u_{\max} = 1.494$ m/s; (c) at 100% filling, 1.403 m/s; and (d) at 5 s after 100% filling, $u_{\max} = 0.0096$ m/s.

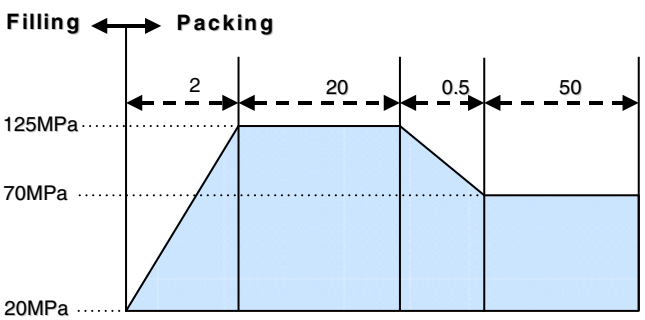

Figure 10. Pressure as a function of time for the three-dimensional test case.

molding is formulated. The method allows solving the entire injection molding process using a single algorithm with the penalty method in spite of the transition from the incompressible regime during the filling stage into compressible regime for the packing stage. We have applied

DOI: 10.1002/fld

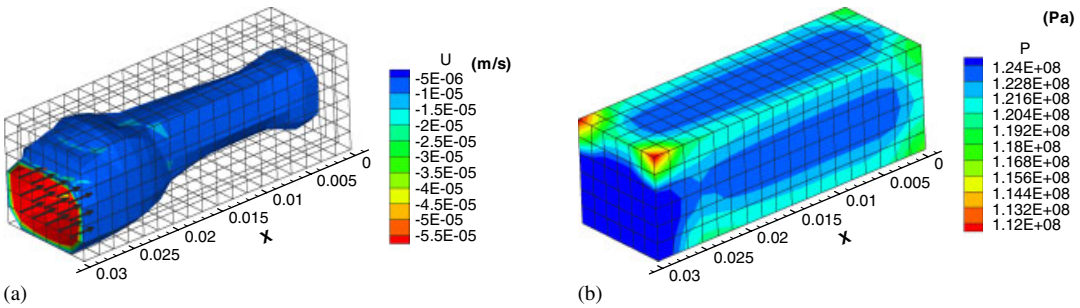

Figure 11. Results for the three-dimensional case at 20 s: (a) u iso-contour surface and (b) pressure contour.

the proposed method to the simulations of the packing stage with different configurations. It has been shown that the accuracy of the proposed method is identical to the mixed method.

NOMENCLATURE

A_i (for $i=1,2$)	constants of Cross-WLF model
b_i (for $i=1,2,\ldots,9$)	constants of Tait equation
$B(T)$	intermediate function in the Tait equation ($=b_3\exp[-b_4\overline{T}]$)
C_p	specific heat capacity
CS	control surface
CV	control volume
d_{ij} (for $i,j=1,2,3$)	rate of deformation tensor
D_i (for $i=1,2$)	constants of Cross-WLF model
$\mathbf{F}$	force vector
I_2	second invariant of d_{ij}
k_{ij} (for $i,j=1,2,3$)	thermal conductivity
$\mathbf{K}$	stiffness matrix
$\mathbf{K}'$	penalty matrix
m_a	added mass
$\dot{m}$	mass flow rate
p	pressure
$\mathbf{p}$	pressure vector
$p_{,i}$	derivative of pressure in x_i
$\mathbf{Q}$	pressure gradient matrix
$\mathbf{Q}^{\mathrm{T}}$	divergence matrix
S	surface area
t	time
t_0	initial time of the packing stage
T	temperature
$\overline{T}$	corrected temperature ($=T-b_5$) for the Tait equation
$\mathbf{u}$	velocity vector

DOI: 10.1002/fld

u_i (for $i=1,2,3$)	velocity in the x_i-direction
v	specific volume
$v_0(T)$	intermediate specific volume in the Tait equation ($=b_1+b_2\overline{T}$)
$v_g(T,p)$	intermediate specific volume in the Tait equation ($=b_7\exp[b_8\overline{T}-b_9p]$)
V	volume
x_i (for $i=1,2,3$)	position variable

Greek symbols

β	coefficient of thermal expansion
η	viscosity
η_0	zero shear viscosity
Θ	compression work
κ	isothermal compressibility
λ	penalty parameter
λ^0	initial value of the penalty parameter
λ^n	nth penalty parameter value
λ^{n+1}	$(n+1)$th penalty parameter value
ρ	density
τ	constant of Cross-WLF model
τ_{ij}	deviatoric stress tensor
Φ	viscous dissipation

ACKNOWLEDGEMENTS

This work was supported by a grant from the Center for Advanced Materials Processing (CAMP) of the 21st Century Frontier R&D Program funded by the Ministry of Commerce, Industry and Energy (MOCIE), Republic of Korea. The authors also would like to thank the Korea Science and Engineering Foundation (KOSEF) for financial support through the SRC/ERC Program of MOST/KOSEF (R11-2005-065).

REFERENCES

1. Dantzig JA, Tucker CL. *Modeling in Materials Processing*. Cambridge University Press: Cambridge, 2001.
2. Steinbach J. A generalized temperature-dependent, non-Newtonian Hele-Shaw flow in injection and compression moulding. *Mathematical Methods in the Applied Sciences* 1998; **20**(14):1199–1222.
3. Candal MV, Morales RA. Design of plastic pieces and their molds using CAD/CAE tools. I. *Computer Applications in Engineering Education* 2005; **13**(4):233–239.
4. Reddy JN. On penalty function methods in the finite-element analysis of flow problems. *International Journal for Numerical Methods in Fluids* 1982; **2**(2):151–171.
5. Matthaeus WH, Zank GP. The equations of nearly incompressible fluids. I. Hydrodynamics, turbulence, and waves. *Physics of Fluids A* 1991; **3**(1):69–82.
6. Hesthaven JS, Gottlieb D. A stable penalty method for the compressible Navier–Stokes equations. I. Open boundary condition. *SIAM Journal on Scientific Computing* 1996; **17**(3):579–612.
7. Kellogg RB, Liu BY. A penalized finite-element method for a compressible Stokes system. *SIAM Journal on Numerical Analysis* 1997; **34**(3):1093–1105.
8. Kim IH *et al*. Numerical modeling of injection/compression molding for center-gated disk: Part I. Injection molding with viscoelastic compressible fluid model. *Polymer Engineering and Science* 1999; **39**(10):1930–1942.
9. Reddy JN, Gartling DK. *The Finite Element Method in Heat Transfer and Fluid Dynamics*. CRC Press: Boca Raton, FL, 1994.

DOI: 10.1002/fld

10. Hieber CA, Isayev AI. *Fundamentals in Injection and Compression Molding*. Marcel-Dekker: New York, 1987.
11. Hirschfelder JO, Curtiss CF, Bird RB. *Molecular Theory of Gases and Liquids*. Wiley: New York, 1954.
12. Beiter KA, Ishii K. Incorporating dimensional requirements into material selection and design of injection moulded parts. *Engineering Plastics* 1996; **9**(6):435–456.
13. Tucker CL, Manzione LT, O'Brien KT. *Fundamentals of Computer Modeling for Polymer Processing*, Bernhardt EC (ed.). Hanser Publishers: New York, 1989.
14. Taylor C, Hughes TG. *Finite Element Programming of the Navier–Stokes Equations*. Pineridge Press: Swansea, 1981.
15. Kim SW. A fine grid finite element computation of two-dimensional high Reynolds number flows. *Computers and Fluids* 1988; **16**(4):429–444.
16. Carey GF, Oden JT. *Finite Elements*, *Vol. II*, *A Second Course*, vol. 2. Prentice-Hall: Englewood Cliffs, NJ, 1983.
17. Hughes TJR, Liu WK, Brooks A. Finite element analysis of incompressible viscous flows by the penalty function formulation. *Journal of Computational Physics* 1979; **30**:1–60.
18. Crochet MJ, Davies AR, Walters K. *Numerical Simulation of Non-Newtonian Flow*. Elsevier Science Publishers B.V.: Amsterdam, 1984.
19. Carey GF, Oden JT. *Finite Elements*, *Vol. VI*, *Fluid Mechanics*. Prentice-Hall: Englewood Cliffs, NJ, 1986.
20. Ramaswamy B. Finite element solution for advection and natural convection flows. *Computers and Fluids* 1988; **16**(4):349–388.
21. Mizukami A, Tsuchiya M. A finite element method for the three-dimensional non-steady Navier–Stokes equations. *International Journal for Numerical Methods in Fluids* 1984; **4**:349–357.
22. Kawahara M, Ohmiya K. Finite element analysis of density flow using the velocity correction method. *International Journal for Numerical Methods in Fluids* 1985; **5**:981–993.
23. Hayes RE, Dannelongue HH, Tanguy PA. Numerical simulation of mold filling in reaction injection molding. *Polymer Engineering Science* 1991; **31**(11):842–848.
24. Hughes TJR. *The Finite Element Method*. Prentice-Hall Inc.: Englewood Cliffs, NJ, 1987.
25. Bathe K-J. *Finite Element Procedures in Engineering Analysis*. Prentice-Hall Inc.: Englewood Cliffs, NJ, 1982.
26. Oden JT. *Finite Elements. Fluid Mechanics*. Prentice-Hall Inc.: Englewood Cliffs, NJ, 1986.
27. Zienkiewicz OC, Taylor RL. *The Finite Element Method* (5th edn), vol. 3. Butterworth-Heinemann: Woburn, MA, 2000.
28. Liu JWH. *The Multifrontal Method for Sparse Matrix Solution*: *Theory and Practice*. Department of Computer Science, York University: North York, Ont., Canada, 1990.
29. C-MOLD. *Polymer Properties Test Report*. C-MOLD, Ithaca, NY, 1999.
30. Hirt CW, Nichols BD. Volume of fluid (VOF) methods for the dynamics of free boundaries. *Journal of Computational Physics* 1981; **39**:201–225.

DOI: 10.1002/fld