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Multi-scale filling simulation of micro-injection molding process †

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Abstract

This work proposes a multi-scale simulation method that can simulate filling during the micro-injection molding process. The multi-scale simulation is comprised of two steps. In the first step, the macro-scale flow is analyzed using the conventional method. In the second step, the micro-scale simulation is conducted taking the slip and surface tension into consideration to investigate the filling of micro-cavity. Moreover, a conservative level set method is employed to accurately track the flow front. First, numerical tests have been done for circular micro-channels. The results show that slip and surface tension play important roles in the micro-regime. Second, to verify the multi-scale method, filling of a thin plate with micro-channel patterns has been simulated. The results show that the proposed multi-scale method is promising for micro-injection molding simulations.

Keywords: Micro-injection molding; Multi-scale analysis; Level set method; Slip velocity; Surface tension

1. Introduction

Recently, a lot of polymer-based micro-components are manufactured by the micro-injection molding process thanks to its material efficiency, productivity and cost effectiveness. The first challenge in micro-molding is to fill micro-cavities as designed and intended [1]. In conventional injection molding processes, the flow is controlled by process parameters such as mold temperature, injection speed, holding pressure and cooling time. These parameters are also crucial to micro-injection molding processes. However, polymer melt in micro-cavities may flow differently than in conventional ones. As the system scale becomes smaller, interfacial effects such as the wall slip and surface tension become more pronounced [2].

Nonetheless, it is quite demanding to fully describe characteristics of filling and packing flow as they are. In addition to shear and inertial forces, the flow in a micro-cavity is affected by interactions of various forces such as surface tension on the front and extensional viscous force at an entrance [1]. There have been noticeable advances in numerical simulations of injection molding processes [3]. Several studies have tried mold filling simulations together with experimental visualization in the micro-channels [2]. A filling simulation of a micro-injection molding process is more challenging than that of a conventional injection molding process. A simulation model that simultaneously treats all the micro-cavities on a single molded part will require a huge number of grid nodes. Such an analysis requires a computational time unacceptably long as an engineering simulation. To use the simulation results for product design, process design, tooling and trouble shooting, the run time should be in a reasonable range. Currently, direct modeling of the entire geometry is an infeasible approach. Multi-scale simulation methods that can contiguously simulate filling of macro- and micro-cavities are proposed and investigated in previous works.

In this work, a multi-scale simulation method has been designed and implemented. The proposed method first simulates the macro-scale flow. Then, it simulates local micro-cavity flow by taking the result of the macro-scale flow as an inlet boundary condition. Moreover, a level set method is employed to accurately track the flow front [4]. In this work, the effects of the surface tension and wall slip velocity are also taken into consideration. Micro-scale flow is simulated using COMSOL 4.0 while macro-scale flow using MOLDFLOW MPI 6.2. Furthermore, to integrate them, an in-house code that can fulfill data transfer is developed.

2. Multi-scale simulation model and method

2.1 Review

The multi-scale simulation methods for micro–injection molding processes have been developed in several previous studies. These methods have not been investigated much despite the industrial importance of this process. Recently, simu-

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lations for high aspect ratio features have been tried. These methods consider important characteristics of micro-scale flow of polymer melts. Distinctive features of those studies are compared in Table 1.

Most studies employ commercialized CAE (computer aided engineering) tools for the macro-scale simulation. Several previous works have analyzed the micro-molding process based on combination of Hele-Shaw and Nav er-Stokes simulations [1-3, 5-7]. Those works tried to alleviate the computational load demanded for full three-dimensional simulations. However, recent cost-down in computational resources including memory and CPU has made the benefit of 2.5D simulation insignificant. As already described in the literatures, three-dimensional simulation in the injection molding process is necessary owing to the limitations in the Hele-Shaw formulation. The mid-plane and dual domain approximations have difficulties in simulating the fountain flow, the inertial effects and the flow imbalance in the branching flow. In simulations of the micro-cavity filling, the fountain flow plays an important role since the out-of-plane velocity is expected to affect the filling flow near the inlet of the micro-cavity. Although the macro-flow can be assumed independent of the micro-flow, the viscosity of the inlet flow into the micro-cavity is determined by the shear rate in the macro-regime.

A micro-cavity flow should be modeled with the 3D Navier-Stokes equation since the geometry is not considered thin-walled and boundary effects are noticeable. Kim and Turng argued that the surface tension is negligible since the capillary number is quite big [8]. On the contrary, they commented that the wall slip could more significantly affect the filling flow. Park et al. have employed the Brackbill's model to account the capillary effects, which converts the surface force to a volume force considering the phase-boundary curvature [6]. Lin and Young proposed an analytical model that can consider air-trapping in the micro-cavity [10].

2.2 Macro- and micro-scale models

In this work, a multi-scale simulation model is proposed to simulate the flow without the direct modeling of micro-features. The model is comprised of two major parts as shown in Fig. 1. In the first part, a filling simulation is performed for the macro-scale geometry of the given part. The full Navier-Stokes equations are solved here to provide accurate data near the wall to the micro-scale simulation.

It is assumed that the presence of micro-geometries negligibly affects the macro-scale flow. This is a valid approximation as long as the entire volume of the micro-regime is small in comparison with that of the macro regime. In other words, micro-features on the part wall can be ignored in the macro flow analyses. The validity of this assumption is actually disputable. The micro-cavities play as sinks in the flow domain. If the sinking volume increases, this assumption will make the simulated flow front run faster than the real flow front. However, this sinking volume is not easily compensated simply by correcting the thickness because the velocity, the pressure and the fill time should be accurate at the same time. Thus, any thickness compensation is not included in this work.

In the second part, for a specific micro-scale feature on the part, micro-scale flow is simulated. This simulation is done taking the time-varying pressure, temperature and velocity data of the macro-scale flow as the boundary conditions in the inlet region. This work considers both the surface tension and the wall slip for an accurate simulation of the micro-cavity filling. In the micro-scale analysis, effects of the wall slip and the surface tension are expected to affect the fill pattern during the molding and the quality of the fabricated final product. On the contrary, the macro-scale flows, which is with large momentum and driven by high pressure, are not influenced by the wall slip and the surface tension. This multi-scale approach allows in-depth investigation without simultaneously meshing the entire domain with innumerable elements and nodes. Thanks to this multi-scale simulation, accurate as well as detailed local information will be attained on demand.

2.3 Implementation of numerical models

In the implementation of the described analysis, commer-

Table 1. Comparison of the simulation studies for the micro-injection molding process.

Works	Macroscale G.E.	Microscale G.E.	Microscale feature
Yao and Kim, 2002 [2]	Hele-Shaw (2.5D) In-house code	Modified Hele-Shaw (2.5D) In-house code	Slip, Surface tension Size-dependent viscosity
Yu et al., 2004 [3]	Hele-Shaw (1D) In-house code	Navier-Stokes 2D In-house code	None
Kim and Turng, 2006 [8]	Navier-Stokes 3D In-house code	Navier-Stokes 3D In-house code	None
Tofteberg and Andreassen, 2008 [5]	Hele-Shaw (2.5D) MoldFlow	Navier-Stokes 2D Ansys CFX	None
Shen et al., 2008 [9]	Navier-Stokes (3D) MoldFlow	Navier-Stokes (3D) MoldFlow	None
Park et al., 2008 [6]	Hele-Shaw (2.5D) MoldFlow	Navier-Stokes (2D) In-house code	Surface tension
Lin and Young, 2009 [10]	Navier-Stokes 3D MoldFlow	Analytical (1D)	Air-trapping
This work	Navier-Stokes 3D MoldFlow	Navier-Stokes (2D axisymmetric) Comsol, Fluent	Slip, Surface tension

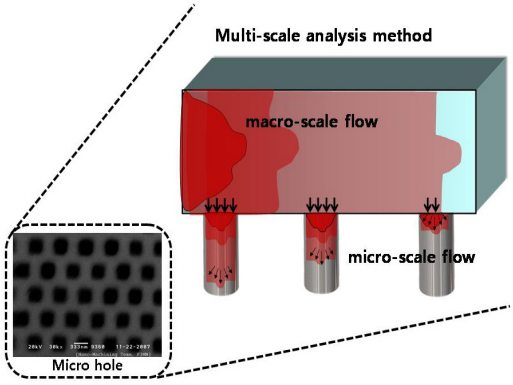


Fig. 1. Interoperation of macro and micro flow simulations in this multi-scale simulations.

cialized CAE tools are selected instead of developing in-house computer codes. Developing an in-house code has some apparent advantages, which are flexibility and freedom in model implementation as well as the computational efficiency. However, a research work with an in-house code does not allow easy reproduction and validation of the work by other researchers. Moreover, recent CAE tools allow convenient interfaces to user codes that facilitate realizing user material models and boundary conditions. This capability has been fully utilized in this work to apply the viscosity, slip and surface tension models.

For a macro-scale analysis of injection molding process, several systems are commercially available in the market. For example, Moldflow and Moldex3D, which currently prevail in the market, are fully-fledged in terms of functionality and capability in analyzing the conventional injection molding processes. These systems provide user-friendly interfaces and savvy post-processing capabilities for macro-scale flow analysis. MoldFlow AMI is selected for the macro-scale simulation considering its prominence in that field and wide availability as presented in Table 1. However, it has limited capability in simulating micro-scale flows. Thus, a general purpose CFD (computational fluid dynamics) tool is selected for the analysis of micro-scale flows instead of tools specialized for polymer processes.

In a molding simulation, advancing the flow front is quite an issue. The volume of fluid (VOF) method and the level set method (LSM) have been widely adopted for a variety of applications including boiling, casting, diverse molding processes and broken column flows since they can be easily incorporated with a fixed grid system [11-13]. Each method has its own strength. The LSM is better at curvature representation while the VOF method is stronger in conservation. For simulation of slip and surface tension, the surface curvature is more important [14]. Therefore, this work employs an LSM that is modified to have improved characteristics in conservation [15].

A multi-physics simulation computer software, Comsol, which has a built-in capability of the level set method, is selected for the micro-scale flow analysis [16].

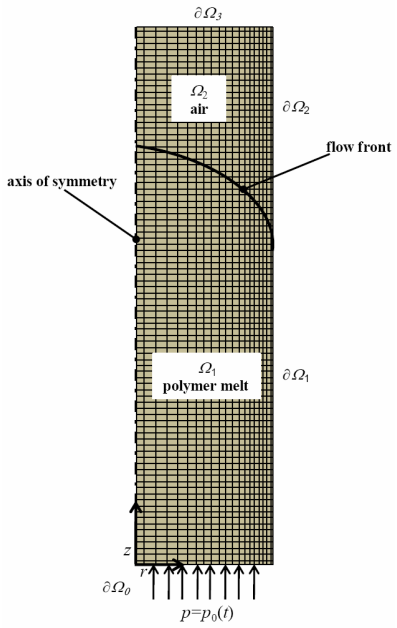


Fig. 2. Computational model and boundary conditions for micro-scale flow.

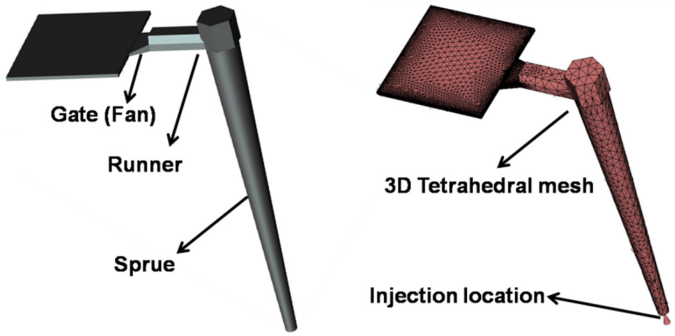
2.4 Interfacing of macro- and micro-models

In order to conduct the multi-scale simulation, MoldFlow and Comsol should be interoperable in a systematic fashion. To perform the data transfer from MoldFlow to Comsol, interfacing capabilities of each package such as export functionality, scripting and user-defined functions are utilized. As aforementioned, the micro-scale simulation requires the time-varying pressure, temperature and velocity data of the macro-scale flow.

The micro-cavity in this study is a circular hole with diameter, D, and depth, $3D$. Over the inlet boundary, pressure, temperature and velocity are assumed constant since the spatial variation will be very limited in that narrow region. Thus, only temporal variations are considered on the boundary, which is the actual interface to the macro-flow.

In this study, the inlet boundary of the micro-cavity is defined as shown in Fig. 2. On the interface, the micro-scale simulation can call for pressure, temperature and velocity at arbitrary position, x, and time, t. Such values at the nodal points, which are exported together with the mesh data from MoldFlow as a text file in the Partran format, will be available. A computer code that can read the file and interpolate p (x, t), T (x, t) and u (x, t) with the values at three nearest nodal points on the interfacial plane has been built. Those values are available at discrete times. The micro-scale simulation can demand values at any time as necessary. For a given position, a function interpolating the discrete values is determined in a linear piece-wise manner.

The velocity is not imposed as the boundary condition of the micro-scale simulation since the hesitation effect will not allow entering the micro-cavity with the existing inertia. Imposing the velocity and the pressure at the same time is not



(a) (b)

Fig. 3. (a) Model for macro-scale simulation; (b) the mesh.

numerically amenable. Employing a complex scheme involving a velocity interface would not aid accurate simulation. On the inlet boundary, only pressure is transferred and imposed. The velocity is only utilized for initial guess of the viscosity, which is strongly dependent on the shear rate.

3. Mathematical formulation

3.1 Governing equations

During the filling phase, the air and the molten polymer are considered incompressible fluids. The mass conservation leads to the following continuity equation without any time derivative term

$$\nabla \cdot \rho u = 0 \tag{1}$$

where u is the velocity vector. The momentum equation neglecting the body force is of the form

$$\rho(\frac{\partial u}{\partial t} + u\nabla \cdot u) = -\nabla p + \nabla \cdot \tau + F_{st} \tag{2}$$

where p is the pressure, F_{st} is the surface tension force that acts at the air/polymer interface. Note that the surface tension is nonzero only for the micro-scale flow. Moreover, τ is the deviatoric stress tensor, which is

$$\tau = 2\eta D\,. \tag{3}$$

Here, η is the viscosity and D is the rate of strain tensor of the form

$$D = \frac{1}{2}(\nabla u + \nabla u^T)\,. \tag{4}$$

The energy equation takes the following form

$$\rho C_p(\frac{\partial T}{\partial t} + u \cdot \nabla T) = \nabla \cdot (k\nabla T) + \eta\dot{\gamma}^2\,. \tag{5}$$

In the above equations, t, u, p, ρ, η, C and k are time, velocity, pressure, temperature, density, viscosity, specific heat and thermal conductivity, respectively. The shear rate $\dot{\gamma}$ is given as

$$\dot{\gamma} = (2D : D^T)^{1/2} \tag{6}$$

3.2 Flow front tracking

Amongst many flow tracking methods, there are two prevailing approaches for flow front tracking in a fixed numerical mesh, which are volume-of-fluid (VOF) methods and level set methods (LSM). LSMs represents the interface by the zero contour of a signed distance function while VOF methods reconstructs the interface based on the volume fraction of a fluid in a cell [13, 14]. For front tracking in the micro-channel, this work employs a modified level set method since the level set method has advantage in surface tension and wall slip calculation thanks to accurate representation of curvature [15]. However, it is known that an LSM is not conservative, which can incur physically incorrect gain and loss of mass. Olsson and Kreiss proposed a conservative LSM that is comprised of advective and intermediate steps [15]. A smooth Heaviside function, $\phi = H_{SM}(\Phi)$, is introduced instead of using the original level set function, Φ. Here, ϕ shows smooth transition from 0 (Φ <0) to 1 (Φ >0). The interface is defined by the 0.5 (Φ =0) iso-contour. The motion of an interface is described by [16]

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \gamma \nabla \cdot \left[\varepsilon \nabla \phi - \phi(1-\phi)\frac{\nabla \phi}{|\nabla \phi|} \right]. \tag{7}$$

The parameter, ε, controls the thickness of transition region and γ stabilizes the level set function, which should be set considering the magnitude of u.

3.3 Viscosity model

In the test of the surface tension and wall slip effect, the dynamic viscosity is assumed to be constant for a Newtonian fluid. The Cross-WLF model for viscosity is used to represent the non-Newtonian behavior of polymer melt. For the given

7temperature T, the corresponding viscosity function $\eta(\dot{\gamma},T)$ takes the following form

$$\eta(\dot{\gamma},T)=\frac{\eta_0(T)}{1+(\eta_0(T)\dot{\gamma}/\tau)^{1-n}} \tag{8}$$

$$\eta_0 = D_1 \exp[\frac{-A_1(T-D_2)}{A_2+(T-D_2)}] \ (T \geq D_2) \tag{9}$$

$$\eta_0 = \infty \ (T < D_2) \tag{10}$$

where γ is the shear rate, A_1, A_2, D_1, D_2 and τ are constant values that should be determined from experimental measurements for a specific polymer. This viscosity model is implemented with a user function in Comsol.

3.4 Local wall slip velocity model

In the micro-injection molding process, the melts are subject to very large shear stresses that can exceed the critical stress. This critical stress is about 0.1MPa for many polymer melts [17, 18]. In this high stress regime, the slip velocity increases with the shear stress. This slip mechanics has been attributed to unravelling of the bulk chains and the chains attached to the wall. In order to consider the slip effect, for simplicity, the local slip velocity is modeled neglecting dependence on pressure and temperature by the following expression [19]

$$u_s = \frac{a}{1+(\sigma_c/\sigma_w)^N}\sigma_w{}^m \tag{11}$$

where σ_w is the wall shear stress, σ_c is the critical wall stress for slip, m is a power-law index, and a is a scalar coefficient. Moreover, N is a large exponent, which is 10 in this work. When the wall stress exceeds the critical value, wall slip will commence. The slip velocity is imposed on $\partial\Omega_1$ only along z-direction in the r-z coordinate shown in Fig. 2

$$u = u_s k \quad on \quad \partial\Omega_1 \tag{12}$$

where k is the unit vector in the z-direction. The slip velocity is calculated using a user function in Comsol.

3.5 Surface tension

In order to account for capillary effects, it is crucial to include surface tension in the model. The surface tension term (a force vector) in Eq. (2), F_{st}, is given by

$$F_{st} = \nabla \cdot S \tag{13}$$

where S is a tensor of the form

$$S = \sigma(I - nn^T)\delta \tag{14}$$

Here, I is the identity matrix, n is interface normal, σ equals the surface tension coeffient (N/m) and δ equals a Dirac delta function that is nonzero only at the fluid interface [20].

It should be noted that the contact angle intrinsic to the fluid does not play any role in this analysis since the flow is not a capillary flow but a pressure-driven viscous flow. That is, the angle between the surface and the flow front is determined by the flow front tracking algorithm not by the static or dynamic contact angle posed determined by the surface energy equilibrium at the phase boundary. With this model, involving the capillary force always impedes the filling flow regardless of wetting or non-wetting nature of the polymer melt. This is justified by the assumption that the flow front will freeze before the capillary force dominates and the curvature is reversed.

Table 2. Polymer melt properties in this work (generic crystalline polypropylene).

Specific heat	2380 J/kg
Thermal conductivity	0.23 W/mK
Glass transition temperature	384 K
Melt density	721.558 kg/
Solid density	904.62 kg/

4. Results and discussions

4.1 Material properties and process setup for the simulation

The polymer melt in this study is a generic crystalline polypropylene whose major properties are presented in Table 2. In addition, the viscosity is modeled with the cross-WLF model, which is widely used for shear-thinning fluid with temperature dependent zero-shear viscosity. The constants for this viscosity model are given in Table 3. Moreover, the constants of the wall slip model for polypropylene are specified in Table 4. As this work is focused on filling simulation, post-filling activities such as packing and cooling are not investigated. Table 5 shows parameters used in filling control, which are the mold temperature and the injection velocity.

4.2 Numerical results of macro scale part

The macro-scale filling simulation is conducted ignoring the presence of micro-features on the part. The part is a rectangular thin plate whose dimension is 30mm by 30mm in plane and 1mm in thickness as shown in Fig. 3(a). Fig. 3(b) shows the part meshed with 4-node tetrahedral elements in Mold-Flow. With the computational model shown above, the macro-scale simulation has been fulfilled. A result that exhibits short shots occurring around locations B and C is obtained as shown in Fig. 4. Short shots take place when the polymer melt cannot fill the entire cavity because of insufficiency in the injection pressure or fluidity. The mold temperature was set as 393K. It was observed that as of 0.0298s the flow front could not proceed further. Pressure at the injection location was set 15MPa

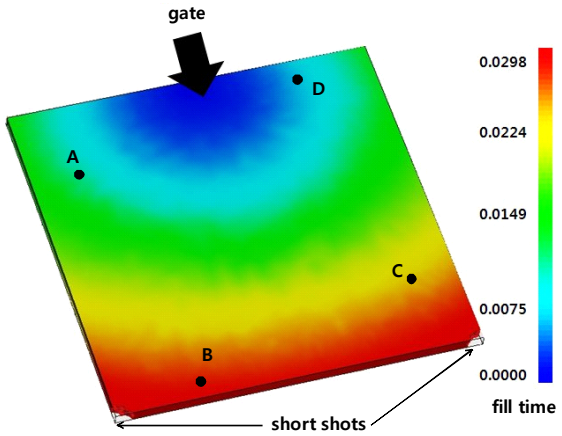


Fig. 4. Fill time of macro-scale simulation and denotation for location of interests.

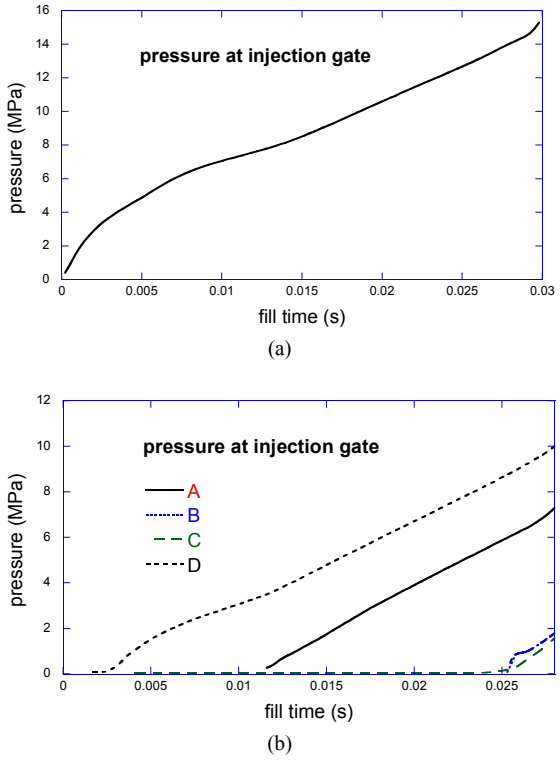


Fig. 5. Pressure history (a) at the injection gate; (b) at locations (A-D) (refer to Fig. 3).

at the end of the filling stage. Pressures at A, B, C and D start to increase at the fill times of 0.011s, 0.025s, 0.026s and 0.003s, respectively. The pressure, temperature and velocity at the four different locations (A-D) were recorded to be used as the boundary condition to the micro-scale simulations. Figure 5(a) shows the pressure history at the injection gate. The pressure histories at the locations A, B, C and D are shown in Fig. 5(b). The pressure, temperature and velocity at the four different locations (A-D) were recorded to be used as the boundary condition to the micro-scale simulations.

4.3 Investigations in micro-scale simulation

The micro-structure in this study is comprised of periodically spaced cylindrical holes on a flat surface. Thus, the flow domain is modeled with axially symmetric cylinder of a uniform diameter in an *r-z* coordinate system. This fairly simple two-dimensional domain is meshed to 1290 elements as shown in Fig. 2, where the boundary conditions are also specified.

In order to scrutinize the effect of the surface tension and the wall slip, the micro-scale filling simulations have been conducted for different channel sizes of 0.1, 0.5, 1, 5, 10, 50 and 100μm. The aspect ratio is maintained at 1:3 for all the channel sizes. The running conditions for all the cases are denoted and specified in Table 6. The simulation has been conducted for the holes with various diameters with and without imposing the slip boundary condition and the surface tension.

In a general two-phase flow, tracking the flow front is not an easy task. The test geometries are as shown in Table 6. The effects of surface tension and boundary slip have been extensively investigated for various diameters of the micro-channels. The results for all the treated cases are presented in Fig. 6. Let us examine the effect of the surface tension first. When larger surface tension is imposed on the interface, the flow front is retarded. Especially for smaller channels, the flow front is noticeably delayed as in A3 of Fig. 6. However, this effect becomes negligible as the diameter becomes larger (compare G1 with G3 in Fig. 6).

When the actual surface tension value of PP, 0.073N/m is imposed, the differences has almost vanished. Visible discrepancy is only observed for the 0.1μm channel (compare A2 with A1). As a rough conclusion, the filling delay due to the surface tension is pronounced for smaller channels. This effect is investigated by checking the filled volume. As shown in Fig. 7 (a), for 0.1μm channels, surface tension is very influential. For 0.1μm channel, surface tension does not play practical role in flow advance as is evident from comparison of C1 and C2 in Fig. 7 (b). For 100μm channel, surface tension cannot affect flow front even with unrealistically high value as shown in Fig. 7 (c).

The effect of the slip boundary condition is rather complicated. It is observed that the slip boundary condition deforms the shape of the flow front to a flatter one. The deviation in fill volume is also observed for smaller channels as demonstrated in Figs. 7(d) and (e). The slip boundary condition allows more fill volume in a given fill time by limiting the wall shear friction as can be seen in Fig. 7(e). This effect vanishes when the length scale becomes bigger as shown in Fig. 7(f).

As a conclusion, it is necessary to impose the surface tension and the slip boundary conditions when the characteristic length is in micro-scale. This work recommends that the slip model should be employed for channel diameter less than 10μm while the capillary model is required in submicron regimes.

Table 3. Constants for the Cross-WLF model.

N	0.2849
τ	43215Pa
A_1	16.903
D_1	2.85E+8Pa s
A_2	51.6K
$D2$	343.15K

Table 4. Constants for the wall slip model.

a	1.2
m	3
σ^c	0.12 MPa

Table 5. Constants for macro-scale simulation.

Injection machine	Sumitomo, SE50D
Injection velocity	100mm/s in step 1, 120mm/s in step 2
Melt temperature	393K

Table 6. Cases of micro-scale simulations with the level set method.

Channel diameter	Channel depth	Base model	Surface tension model		Wall slip model
			0.073N/m	1N/m	
0.1μm	0.3μm	A-1	A-2	A-3	A-4
0.5μm	1.5μm	B-1	B-2	B-3	B-4
1μm	3μm	C-1	C-2	C-3	C-4
5μm	15μm	D-1	D-2	D-3	D-4
10μm	30μm	E-1	E-2	E-3	E-4
50μm	150μm	F-1	F-2	F-3	F-4
100μm	300μm	G-1	G-2	G-3	G-4

4.4 Multi-scale simulation with the full model

Based on the elaborations in the previous chapters, the micro-injection molding process will be simulated with minimal assumptions using the multi-scale simulation technique proposed in this study. The pressure variation shown in Fig. 4(b) is imposed as the inlet boundary condition to the micro-scale simulation. Moreover, the cross-WLF viscosity model and The Tait equation of state are fully implemented for an accurate solution. The selected channel diameter is 50μm (case F in Table 6). Both the slip and surface tension boundary conditions are imposed.

The results are presented for two different cases depending on the location of the micro-hole. The location B and C are selected since the fluidity becomes worse in those regions owing to the long travel distance experienced by the polymer melt. Figs. 8(a) and (b) shows the history of phase boundaries, the pressure histories and the filled volumes at locations B and C, respectively. Filling is slower at location C because pressure develops slower than in location B as shown in Fig. 5(b). This is confirmed by the histories of the filled volume shown in Fig. 8(b). Moreover, these results also sustain the necessity of multi-scale simulation since the pressure and filled volume are shown interrelated.

A test result that is obtained with the simulation method integrating all the flow and material models treated in this work is presented. As a conclusion, the proposed method effectively integrates the macro- and micro-simulations for realistic mold filling situations.

5. Conclusions

To simulate filling during the injection molding of parts with micro-geometries, a multi-scale method has been proposed. We have proposed a simple multi-scale simulation method. Through interoperation of two independent CAE systems, one for the conventional macro-flow of polymer, and the other for the local micro-flow, the whole simulation system has been implemented. The proposed method is tested and verified by several test cases. The results show that the slip model is necessary for channel diameter less than 10μm while the capillary model is pronounced in the submicron regime. Moreover, the multi-scale simulations have been done for a realistic situation. The results show that macro-scale and micro-scale simulation can be integrated through the proposed method that can accurately impose the inlet condition of micro-flow from the macro-flow.

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