

Level Set Method for Fully Thermal-Mechanical Coupled Simulations of Filling in Injection and Micro-Injection Molding Process

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Abstract: In this work we tackle a more theoretical aspect of micro-injection molding, to better understand physics during the process, through numerical simulations of cavity filling. We developed a two phase flow approach by the use of Comsol Multiphysics. In a first step, a Level Set model is applied to several configurations: Newtonian and non-Newtonian fluid (Cross viscosity law), coupled with a thermal equation and a thermal dependence of the viscosity (WLF law). We take into account the unsteady thermal behaviour of the mould while injecting the polymer into the cavity. The viscous thermal dissipation is also integrated in our calculations. Finally, as air –trapping often occurs in the injection molding process, we present some results considering a pseudo-compression law (low Mach number) for the air. To conclude, we show the ability of the Comsol model to simulate polymer filling in micro-features.

Keywords: Injection molding, microstructures, multiphase-flow, level-set, CFD.

1. Introduction

The evolution of technologies since several decades is dominated by the race to miniaturization and complexity of objects. The increasing competition in the polymer processing industry makes us looking for new technologies to enlarge the possible applications and enter new markets. An important way for it is to understand and optimize micro-features replications on thermoplastics with the injection molding process. The high rates and low costs, compared to other processes, allow for integrating new markets in micro-electronic, biomedical, optics or cosmetics for example, where micro-structured objects can play an important part.

In this context, the Pôle Européen de Plasturgie (PEP, technical center dedicated to polymer processing) began several years ago a new

research and development project called “Microstructure” which focuses on controlling conception and realization of micro-structured thermoplastic parts. However, the transposition of technology to the micro-scale level is not as direct, because several physical phenomena, usually neglected at macroscopic scale, might have great influence on filling, such as surface tensions, viscoelastic behavior, or complex thermal transfers.

Several 3D softwares do exist for injection molding simulations such as Moldflow[®], Sigma3D[®], Cadmould[®], Rem3D[®], SIMPOE[®], Moldex[®]... They are well suited to help conception and design of molds and parts, but show limits when considering micro-geometries [1-5]. Indeed, some laboratories developed their home made FEM 3D softwares to better consider specific conditions of the micro-injection process, with flow front tracking methods such as pseudo-concentration, Volume Of Fluid (VOF), or Level-Set method. [6-13]

Finally, when considering micrometric geometries, other modeling methods based on molecular dynamics have been studied, and in reference [14] reducing the flow channel size resulted in density fluctuations, an effect which is neglected by the continuum approach.

When looking on the objectives of this “Microstructure” project, the first one considering simulation aspects was to establish surface tension impact on cavity filling, especially when reaching micro-features. The use of Comsol Multiphysics[®] was the best way for us, for two reasons :

- usual modeling softwares dedicated to polymer processing do not consider these effects, and do not allow for integrating other models,
- our goal is definitely not to develop a new software.

In this work, the PEP and SIMTEC, a COMSOL Certified Consultant company, tackle a more theoretical aspect of micro-injection molding, to better understand physics during the process, through numerical simulations of cavity filling. After having made simulations with commercial codes dedicated to injection-molding, we noticed, like others had in the literature, that the obtained results show differences with experiments, mainly because of the simpler models and hypothesis used to facilitate computations.

As a consequence, we have decided to develop a two phase flow approach by the use of Comsol Multiphysics. All the results presented here follow our work done in [15], where we already successfully studied a two-phase flow for Newtonian and non-Newtonian polymer, and in an isothermal or thermal dependant configuration.

In this second step, a Level Set model is applied to several configurations: Newtonian and non-Newtonian fluid (Cross viscosity law), coupled with a thermal equation and a thermal dependence of the viscosity (WLF law). We take into account the unsteady thermal behaviour of the mould while injecting the polymer into the cavity. The viscous thermal dissipation is also integrated in our calculations. Finally, as air – trapping often occurs in the injection molding process, we present some results considering a pseudo-compression law (low Mach number) for the air.

To conclude, we show the ability of the Comsol model to simulate polymer filling in injection molding.

Our simulations are directly compared to :

- experimental results obtained on an industrial injection molding machine,
- other simulations made with Moldflow 3D, the most used simulation software dedicated to polymer processing.

All these results show the extended possibilities of Comsol Multiphysics to deal with multi-phase flow topics.

2. Governing equations

2.1 Coupled Navier-Stokes & Level Set equations

To simulate numerically this model, a level set approach is coupled to the classical Navier-Stokes equations. This method is very well suited to describe the motion of an interface.

$$\begin{cases} \rho \frac{\partial u}{\partial t} + \rho u \cdot \nabla u = \nabla \cdot \left[-p Id + \eta (\nabla u + (\nabla u)^T) \right] + \rho g + \sigma \kappa \delta n \\ \nabla \cdot u = 0 \\ \frac{\partial \Phi}{\partial t} + u \cdot \nabla \Phi = \gamma \nabla \cdot \left[\varepsilon \nabla \Phi - \Phi (1 - \Phi) \frac{\nabla \Phi}{|\nabla \Phi|} \right] \end{cases}$$

where ρ is the density, η the dynamic viscosity, Id the identity tensor, g the gravitational field, σ the surface tension coefficient, n the unit normal to the interface, $\kappa = -\nabla \cdot n$ the curvature of the fluid interface, δ a delta function concentrated at the interface between the fluids, u the velocity field (m/s), p the pressure (Pa) and φ is the characteristic function of the polymer ($\varphi(x, y) = 1$ if $M(x, y)$ is located inside the polymer, 0 otherwise). In this equation, the term $\sigma \kappa \delta n$ defines the surface tension forces. Non-slip conditions are applied on each boundary, except of those describing the exit of fluids (above and on the right) where the pressure is set to 0.

2.2 Cross-WLF viscosity law

For a newtonian fluid, the dynamic viscosity is assumed to be constant. For a non-newtonian fluid, the dynamic viscosity is assumed to follow the Cross's law :

$$\eta = \frac{\eta_0}{\left(1 + \left(\frac{\eta_0 \dot{\gamma}}{\tau^*} \right)^n \right)^{\frac{1}{n-1}}}$$

where η_0 is the zero shear rate viscosity at a given temperature (WLF law explained later), τ^* and n are model parameters and $\dot{\gamma}$ is the shear rate ratio, expressed as followed in a cylindrical coordinate system :

$$\|\dot{\gamma}\| = \sqrt{2 \sum_{ij} D_{ij}^2} = \sqrt{\frac{1}{2} \left(2u_r^2 + 2(u_z + v_r)^2 + (2v_z)^2 + 4 \left(\frac{u}{r} \right)^2 \right)}$$

where D_{ij} is the velocity deformation tensor, u and v the velocity components, u_r u_z v_r v_z the velocity derivative on r and z , the cylindrical coordinates.

The influence of temperature on viscosity is taken into consideration by a change in the polymer viscosity following an WLF model :

$$\eta_0 = D_1 \exp\left[\frac{-A_1(T - T_{ref})}{A_2 + (T - T_{ref})}\right]$$

Where T is the considered temperature (K), T_{ref} the reference temperature at which the following experimental coefficients have been determined. N , τ^* , $D1$, $D2$, $D3$, $A1$, $A2$ are experimental coefficients.

2.3 Thermal effects

When the influence of the temperature is taken into account, the temperature is described by the following convection and diffusion equation:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p u \cdot \nabla T - \nabla \cdot [k \nabla T] = 0$$

where C_p is the heat capacity, k the thermal conductivity, and T is the temperature (K) in the medium. The temperature of the boundaries of the mold is set to T_{mold} , except for exit boundaries, where a convective flux condition is applied. Initially, the temperature of the mold is T_{mold} . The temperature of the injected polymer is T_{inj} .

Adding a thermal equation in the mould increases the problem complexity and DOF to be solved.

2.4 Weak compressibility

Till now, both fluids have been considered as incompressible. If this assumption could be valid for the molten polymer (in a first approximation), it is abusive for the air. For low Mach numbers flows, a weakly-compressible model can be used. The air pressure is supposed to follow a perfect gas law :

$$\rho = \frac{pM}{RT}$$

where ρ is the air density, p the pressure, M the molar mass, R the perfect gas constant and T the temperature.

When taking into account the fluid compressibility, fluids dynamics equations move to :

$$\left\{ \begin{array}{l} \rho \frac{\partial u}{\partial t} + \rho u \cdot \nabla u = \nabla \cdot \left[-pId + \eta(\nabla u + (\nabla u)^T) - \left(\frac{2\eta}{3} - \kappa_{dv}\right)(\nabla \cdot u)Id \right] \\ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \end{array} \right.$$

κ_{dv} is the bulk viscosity (fixed to 1E9 Pa.s for polymers according to [16 ;17]). For the air, it is common to take the a value of κ_{dv} corresponding to 2/3 of the dynamic viscosity : it nullifies the new second term, and the density still evolves with time in the mass conservation equation.

The results using a compressible model will only consider an isothermal newtonian flow. Indeed, we encountered many numerical convergence problems due to the time-dependent density, and a lack of experimental data on bulk viscosities.

2.5 Micro-features

Different sizes of micro-channels are present on the plastic parts (see description of the plastic parts), leading to adapted and detailed meshes.

2.6 Transversely work

We finally developed a complex model, where several phenomena interact :

- fluids mechanics,
- thermal effects,
- biphasic flow

Best results have been obtained working on :

- i. Solvers : direct solvers (UMFPACK and PARDISO) are the most efficient, but after a benchmark of many solvers, it appears that the GMG solver was the best iterative solver, with pre-smoother and Vanka post-smoother associated to the pressure.
- ii. Mesh : it has a direct influence on the solution quality. Several mesh have been tested (triangle, quadrangle), and each sub-domain had its own mesh.
- iii. Study on γ : The use of the Level Set equation requires the addition of a stabilizing parameter, γ , on the interface transport equation : if it is too small, the solution is not enough stabilised. If it is too high, the results can be physically unreal. Three possibilities : γ local (depends of flow front velocity at a given point), γ homogeneous (depends of the

mean flow front velocity) and finally, we opted for a partially homogeneous parameter, where the flow front velocity is calculated in function of the micro/macro subdomains.

- iv. *Fluidic equation simplifications* : as we met sometimes difficulties with the numerical convergence, we tried to simplify the fluidic part of the model, using Stokes (negligible inertial term compared to viscosity effects) or simplest Darcy model (the velocity is calculated from the pressure gradient). But it did not have enough effect on convergence, still due to the level set equation. So we kept a full Navier-Stokes equation.

3. Methods

Our mold has been drawn as shown on Fig.1. A picture of the axi-symmetrical part is presented in [15].

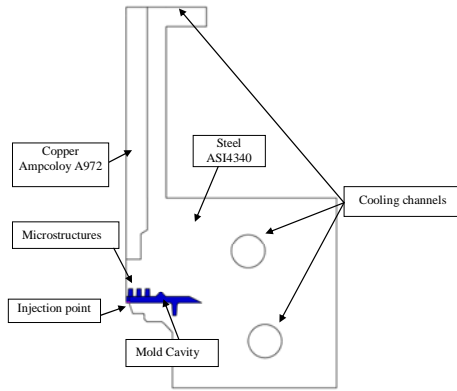


Fig. 1. Illustration of the mold geometry

The following table describes the numerical values of functional parameters used in this paper, considering injection molding of a polypropylene PP 86MF97 from the Sabic company. As an indication, in injection time is 0,84s.

Parameter	Unit	Num. Value for air	Num. Value for polymer
Density: ρ	Kg/m ³	1.199	833
Dynamic viscosity (for Newtonian calculations) : η	Pa.s	1e-5	50
Gravitational field: g	m/s ²	-9.82	
Surface tension coefficient: σ	N/m	0.073 N/m	
Reinitialization	m/s	0.1 ; 1	

parameter: γ			
Parameter controlling interface thickness: ϵ	m	h_{max}	
Cross model parameter: n	-	-	0.2614
Heat capacity: C_p	J/(Kg.K)	1100	2800
Heat conductivity: k	W/(m.K)	0.03	0.18
Initial temp. of cooling channels and air: T_{mold}	K	303	
Temp. of polymer: T_{inj}	K	493	
Injection flow rate	m ³ /s	$4 \cdot 10^{-6}$	

Table 1 : Numerical values of functional parameters used in our simulations.

Parameter	Unit	Num. Value for polymer
n	[]	0,2614
τ^*	Pa	42419,7
D1	Pa.s	$1,6497 \cdot 10^{14}$
D2	K	263,15
D3	K/Pa	0
A1	[]	30,999
A2	K	51,6

Table 2 : Cross-WLF experimental parameters used for PP Sabic 86MF97

The domain is meshed by 47895 nodes and 95427 triangle elements, corresponding to more than 550.000 DOF (quadratic Lagrange elements). Computations have been performed with the direct solver UMFPAK, COMSOL MULTIPHYSICS[®] version 3.4.

4. Results and discussion

4.1 Pseudo-compressibility

Those effects are extremely difficult to take into account, even simplifying the model (newtonian isothermal. The solution always diverges when reaching the last third of the cavity (at about 0,18s). No adapted solver are available to study compressible fluids. Nevertheless, interesting first results show vortices in the air (Cf Fig. 2) and a effective evolution of the air density during injection (Cf. Fig. 3).

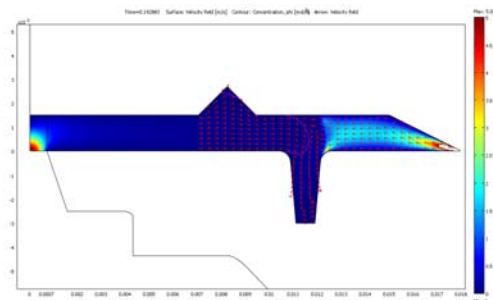


Fig. 2 Velocity field at 0,18s ; vortices appear in the air.

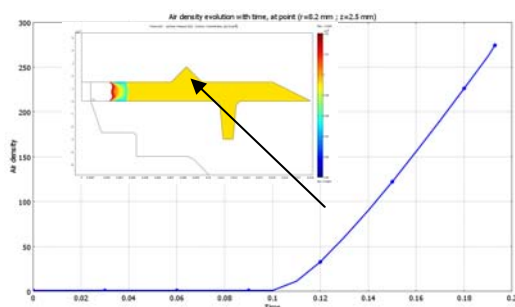


Fig. 3 Evolution of the air density at a given point during the injection.

We will thus keep the incompressible assumption for the air.

4.2 Thermal and pseudo-plasticity effects

As our equations are coupled and non-linear, we can have sometimes convergence difficulties, so the calculation times are long (several hours). In a first step, we worked with a flat surface (no microstructure on the top).

As expected using Cross-WLF and viscous dissipation equations, the viscosity goes down to 70 Pa.s near the walls, where shear is maximum. Fig. 4 points out the potential of our code : it represents the temperature field after 0,29s of injection, both in the cavity and within the mould. We can see heat fluxes (normed red arrows) evacuating calories towards cooling channels (white disks).

In this example, the hot runner is supposed poorly thermally insulated, and that is why the mould is warmed up next to it.

If we look at the molten polymer temperature, we find an increase of several degrees in the high shear areas due to viscous dissipation.

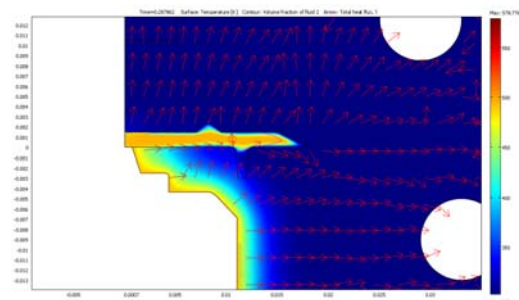


Fig. 4: Temperature field in the mould and flow front position in the cavity (in red) at t=0,29s

4.3 Filling micro-features

4.3.1 Moldflow® simulations

If we only consider the filling phase, the main difference between Moldflow® software and our calculations is that we consider a biphasic fluid, and that we simulate the transient thermal effects within the mold.

For the Moldflow study, we chose 3D tetrahedra. Because of too small geometries, we could not mesh correctly the part. We used Hypermesh® finite element pre-processor to build the mesh, and then imported it in Moldflow, but we were not able to take into account all the micro-features (software and memory capacities). Then we decided to study only a few turns, in front of the injection point.

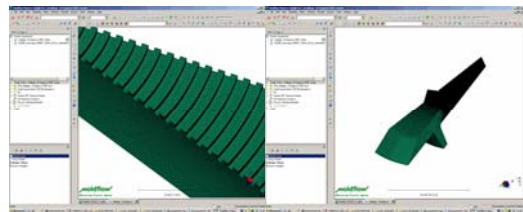


Fig. 5: Illustration of a full 3D Hypermesh mesh with all the micro-features

4.3.2 Example with channels of 1x1mm²

The following pictures show the flow front profile : when considering incomplete injections (we stop the injection before the end), the channels are progressively (along x-axis) and partially filled (along y-axis): our Comsol model underestimates filling of structures because of the air (incompressible), as experiences show a filling of the structures up to 90% during the dynamic step of the injection molding process. Unsurprisingly, on one hand Moldflow® provides a full filled part (monophase model), which is not the case. On the other hand, it well

predicts filling times and pressure, and indicating that air trapping “could” occur in micro-features (can’t predict of course what will be reached depth).

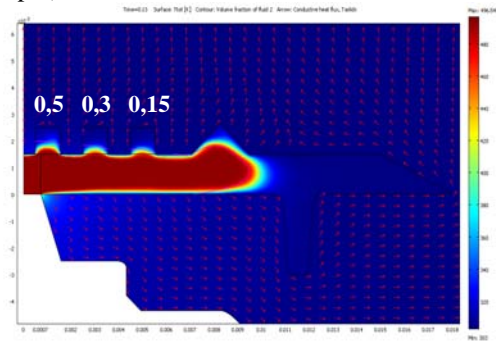


Fig. 6: Incomplete injection stopped at 0,16s simulated with Comsol.

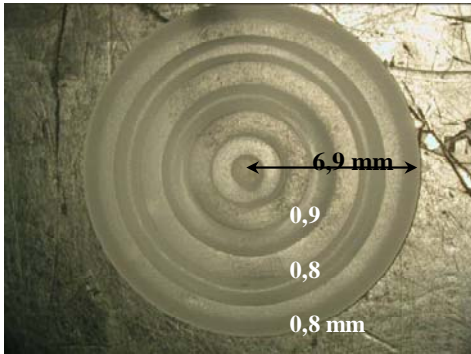


Fig. 7: Incomplete injection stopped at 0,16s obtained experimentally.

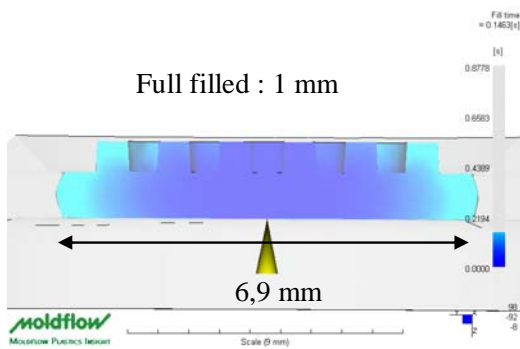


Fig. 8: Incomplete injection stopped at 0,15s with Moldflow®

Other examples will be shown during conference with micro-features down to 0,05 mm with an aspect ratio of 1 or 2, as illustrated on following pictures.

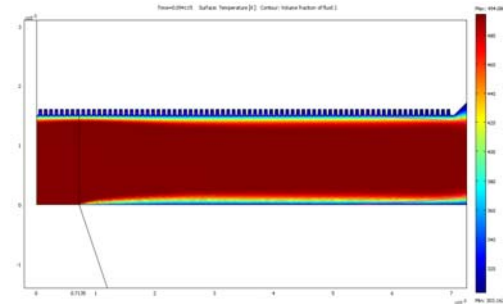


Fig. 9: Filling micro-features of 0,05x0,1 mm

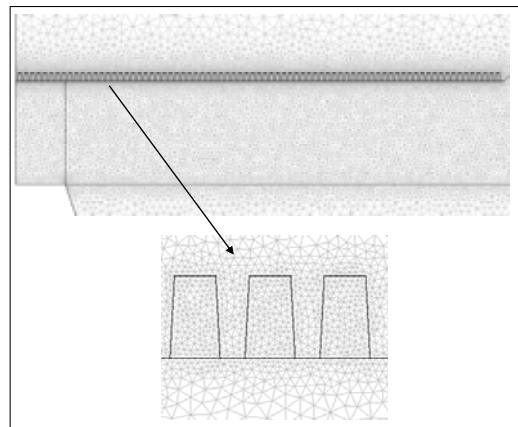


Fig. 10: Example of Comsol mesh for 0,05x0,1 mm microstructures.

4.3.3 Influence of transient thermal effects

Our model gives us the means to study the mould temperature evolution during injection, and especially the influence it can have on the flow. Indeed, at the beginning of the project we put forward a hypothesis that the polymer could be fluidized by a temperature rise of the mould surface (could heat transfer inside the mould be faster than fluid transfer ?).

In our case, the mould is very well temperature regulated : as shown on Fig. 11, where the evolution of transient temperature is represented at a given point of the mould surface. Before the molten plastic reaches the point, mould surface at this given point only heats 1° more than the initial temperature.

The effect of transient thermal on flow can then be neglected in our case. But other applications, our model is able to predict if the mould is well regulated or not.

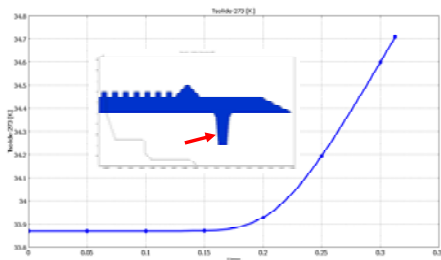


Fig. 11: Temperature evolution with time at a given point of the mould

4.3.4 Influence of surface tension

The assumption of surface tension as a factor influencing the filling of micro-features can be ruled out here despite the low velocities. Fig. 12 indicates that the filling is perfectly identical whatever its value between 20 and 60 mN / m, which corresponds to the values usually encountered in polymers.

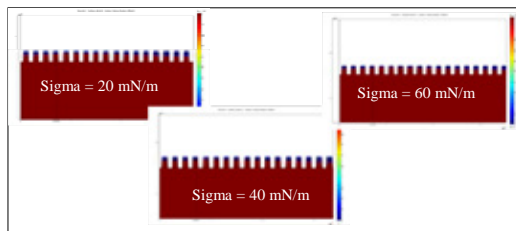


Fig. 12: Effect of the surface tension (between 20 et 60 mN/m) on 0,1x0,2mm microstructures filling

5. Conclusions

In this work we managed to build a fully thermal-mechanical coupled model with a Level-Set method, for the injection moulding process. When considering micro-features, for a small aspect ratio, Moldflow® does not take into account the air, its predictions (total filling) are very close to reality (where air is compressed). Comsol takes into account an incompressible air: whatever the aspect ratio (or almost), our model predicts a partial filling, and quite far from reality (half).

The trend is likely to be identical, no matter the size of the geometry. What is noteworthy is that both approaches are complementary and gave us the means to address physics of the filling of microstructures, while keeping a critical eye on some results. The ideal solution has not been found: we can say that the surface tension or the

thermal transient (with mould properly regulated) had no effect on the filling. On the other hand, there are three major physical phenomena in our view, neglected so far, and very difficult to incorporate into the code:

- Compressible fluids (air, but also and especially polymer): extremely complex to incorporate in the code because of convergence difficulties.
- Slipping walls: the need to conduct experimental measurements beforehand.
- And of course the viscosity law of the polymer: simplified in our case (pseudo-plastic), the polymer has a much more complex behaviour related to its viscoelasticity.

6 Acknowledgements

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