# On the simulation of the Filling Stage of Thermoplastic Injection Molding using the Open-Source Solver *openInjMoldSim*

João Pedro, Bruno Ramôa, João Miguel Nóbrega, Célio Fernandes

*Institute for Polymers and Composites, University of Minho, Campus de Azurém, 4800-058 Guimarães, Portugal; b8389@dep.uminho.pt (J.P.); bruno.ramoa@dep.uminho.pt (B.R.); mnobrega@dep.uminho.pt (J.M.N.); cbpf@dep.uminho.pt (C.F.)*

## 1. Introduction

In the present study, the simulation of the three-dimensional (3D) non-isothermal, non-Newtonian fluid flow of polymer melts is investigated. In particular, the filling stage of thermoplastic injection molding (IM) [ROS] is numerically studied with a solver implemented in the open-source computational library OpenFOAM® [KRE, MOL].

## 2. Governing equations

In the approach employed, the air and the polymer melt phases are assumed to be immiscible and compressible, unless otherwise stated. During the filling stage, the flow is governed by the mass, momentum, and energy conservation equations, which can be written as follows:

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

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = \nabla \cdot \boldsymbol{\sigma},$$

$$\frac{\partial (\rho c_P T)}{\partial t} + \nabla \cdot (\rho c_P \mathbf{u} T) = \beta T \left( \frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p \right) + p \nabla \cdot \mathbf{u} + \boldsymbol{\sigma} : \nabla \mathbf{u} + \nabla \cdot (k \nabla T),$$

The simulation of the IM filling stage requires solving the fluid flow equations and

capturing the melt front location at every time step. For that purpose, an advanced free-surface capturing model, based on the volume-of-fluid (VoF) [HIR] method is used. In this method, a species transport equation is used to track the relative volume fraction of the two phases, or phase fraction, α, distribution. The phase fraction ranges from zero to one, zero being for air and one for the polymer melt. In this way, the fluid interface is located in regions where 0 < α < 1, and the physical properties can be calculated as an average weighted by α, as follows:

$$\psi = \psi_m \alpha + \psi_a (1 - \alpha),$$

where the subscripts *m* and *a* denote the melt and air phases' properties, respectively, and $\psi$ represents all the relevant fluid properties, namely $\rho$, $\eta$, $c_P$, and $k$. The governing equation for the phase fraction, $\alpha$, is defined as:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) + \nabla \cdot [\alpha(1 - \alpha)\mathbf{u}_r] = \mathrm{S_p} + \mathrm{S_u},$$

where $\mathbf{u}_r$ is the relative velocity vector, commonly denominated by "compression velocity". $S_p$ and $S_u$ represent two terms that arise from considering a compressible material.

The rheological behavior of the melt and air phases is defined by a single-fluid two-phase model. For the air phase, the kinematic viscosity is assumed to be constant, i.e., a Newtonian fluid. For the polymer melt, the Cross-WLF constitutive model is employed. This constitutive model is widely adopted for studying both the filling and packing stages of the IM process and is given by:

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

In this work, we adopted the Williams-Landel-Ferry (WLF) model to describe the dependence of $\eta_0$ on $T$ and $p$, given by:

$$\eta_0(T, p) = \mathrm{D_1} \exp\left[\frac{-\mathrm{C_1}(T - T_0)}{\mathrm{C_2} + T - T_0}\right]$$

where $\mathrm{T_0} = \mathrm{D_2} + \mathrm{D_3} p$ and $D_1$, $D_2$, $D_3$, $C_1$, and $C_2$ are parameters determined by experimental characterization.

The relation of specific volume, pressure, and temperature is designated by the pressure-volume-temperature behavior (PVT). In this work, we have employed the modified Tait model where the specific volume, $\widehat{V}$, is given by:

$$\widehat{V} = \widehat{V_0}\left[1 - C\ln\left(1 + \left(\frac{p}{B}\right)\right)\right] + \widehat{V_t}$$

## 3. Case studies

### *3.1. Case Study 1: Filling of a Rectangular Cavity with a Cylindrical Insert*

This case study covers the filling of a rectangular cavity with a cylindrical insert, illustrated in Figure 1. The cavity geometry has a constant thickness of 4 mm, a width of 40 mm, and a length of 150 mm, while the cylindrical insert has a diameter of 15 mm, and its center is located at 55 mm from the inlet.

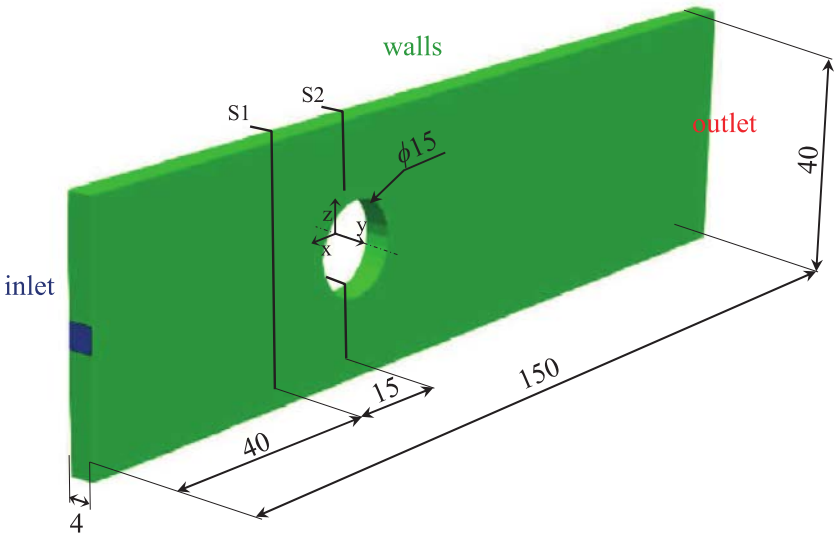


**Figure 1.** Geometry and boundary patches for Case Study 1 (dimensions in mm).

Figure 2 shows the distribution of the pressure field on the mold cavity, computed for both compressible (C) and incompressible (I) formulations, at the switch-over point (98% of volume filled cavity). These results showed that the maximum pressure required to fill the cavity, predicted by both formulations, was quite similar, with a difference of approximately 3.7%, and the computational cost is 5% smaller for the incompressible formulation.

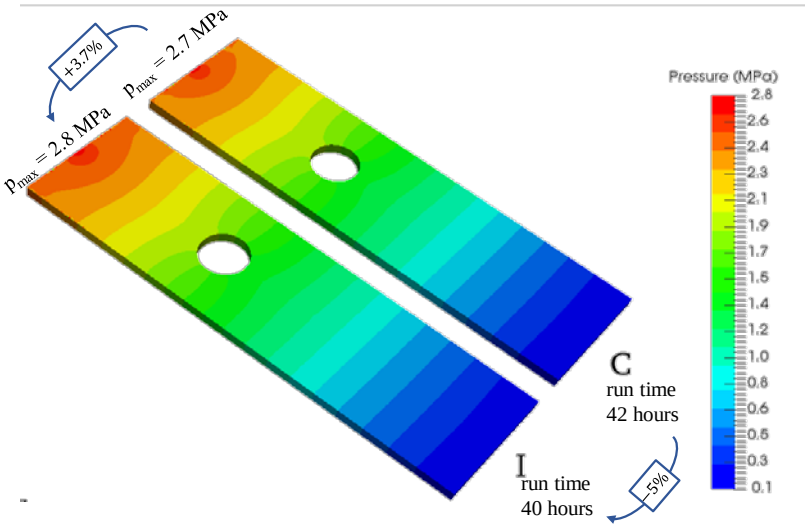


**Figure 2.** Distribution of the pressure field on the mold cavity, for the two formulations, compressible (C) and incompressible (I), at the switch-over point.

### 3.2. *Case Study 2: Filling of a Tensile Test Specimen*

This second case study comprises the simulation of the filling stage of a tensile test specimen. The aim of this case study is to compare the accuracy and performance of *openInjMoldSim* with the proprietary software *Moldex3D*®. This case study geometry is illustrated in Figure 3.

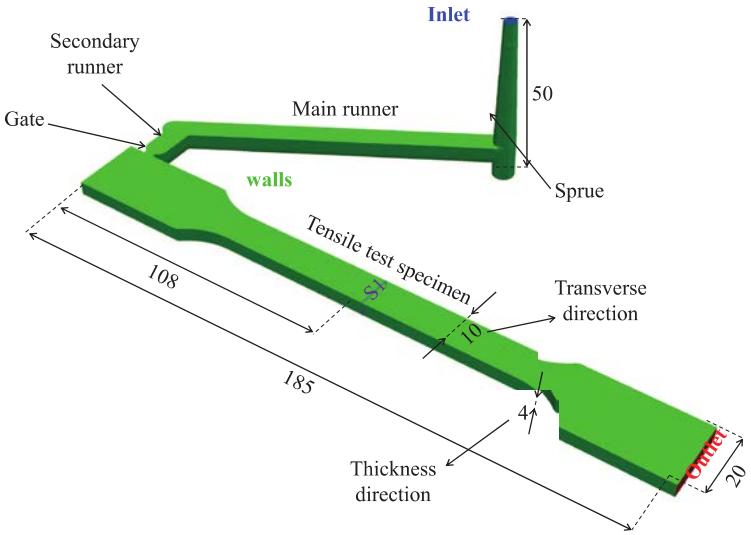


**Figure 3.** Geometry and boundary patches for Case Study 2 (dimensions in mm).

Figure 4 shows the contour of the pressure field distribution in the cavity at the switch-over point. The pressure profiles obtained in both software are qualitatively identical. However, as also shown in Figure 4, the melt flow front predicted by the open-source software seemed more realistic than that of the proprietary counterpart, which present a plug-like surface.

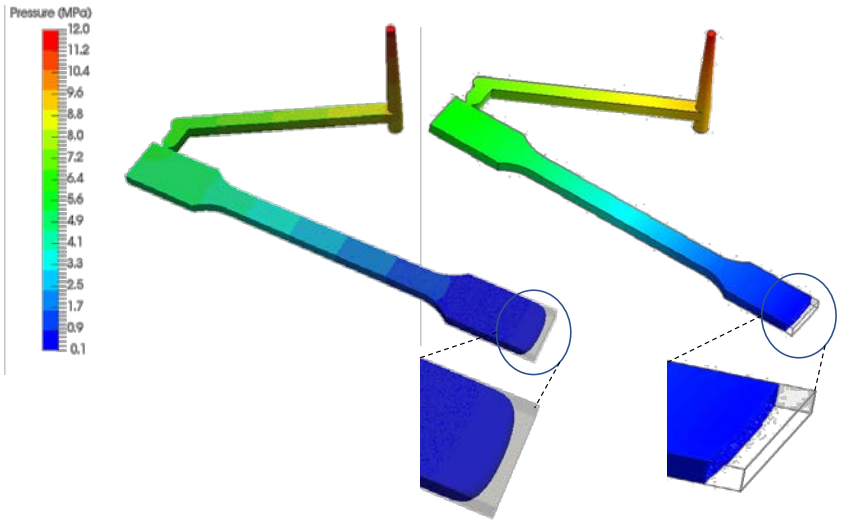


**Figure 4.** Pressure distribution at the switch-over point and melt flow front shape predicted by the most refined mesh of both software.

## 4. Conclusions

A numerical formulation available in the open-source computational library OpenFOAM®, the *openInjMoldSim* solver, was assessed in different test cases related to the simulation of the filling stage of the injection molding process.
In summary, the results presented here showed that the injection molding code can be used to model the filling stage of injection molding processes accurately.

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