TWO-DIMENSIONAL MOLD FILLING SIMULATION WITH A NON-NEWTONIAN FLUID AND UNSTRUCTURED MESHES

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Abstract. *Injection moulding is one of the most important industrial processes for the manufacturing of thin plastic products. The flow of a fluid characterized by high viscosity in a narrow gap is a problem typically found in injection molding processes. In this case, the flow can be described by a formulation known as Hele-Shaw approach or $2^1/_2D$ approach, referring to limitations of the mould geometry to narrow, weakly curved channels. In this work a technique for the simulation of the filling stage of the injection molding process, using this $2^1/_2D$ approach, with a finite volume method and unstructured meshes, is presented. The modified-Cross model with Arrhenius temperature dependence is employed to describe the viscosity of the melt. The temperature field is 3D and it is solved using a semi-Lagrangian scheme based on the finite volume method.*

Keywords: *injection molding process, finite volume method, free surface, unstructured meshes, semi-Lagrangian formulation.*

1. INTRODUCTION

Nowadays, many products are made by thermoplastics injection, in a process called injection molding. In the injection molding process, molten material is forced into a mold where it cools and hardens. The flow of a fluid characterized by high viscosity in a narrow gap is a problem typically found in the processes of injection molding. In this case, the flow can be described by few suitable simplifications in the three dimensional conservation equations, in a formulation known as Hele-Shaw approach (Bretas and D'Avila, 2000; Kennedy, 1995). Such simplifications can be obtained using a number of assumptions regarding the injected polymer and the geometry of the mold, together with the integration and the coupling of the momentum and continuity equations, so this formulation is also called $2^1/_2$D approach.

In this work a technique for the simulation of the injection molding process of polymer is presented. This technique considers important aspects to guarantee the quality of the part, such

as the heat transference by the walls and the insertion points of the mold, and the influence of the temperature and the shear rate in the polymer fluidity. The implemented numerical method uses the topological data structure SHE – Singular Handle Edge (Nonato et al., 2002), capable to handle boundary conditions and singularities, aspects commonly found in numerical simulation of fluid flow.

The governing equations are resolved using an unstructured mesh, generated by Delaunay triangulation (Shewchuk, 1999) and the discretization method is based on the finite volume formulation (Baliga and Patankar, 1981; Maliska, 1995; Ransau, 2002).

2. THE GOVERNING EQUATIONS

The three-dimensional conservation equations, governing the fluid motion, can be written as follow:

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + (\nabla \cdot \rho \vec{v}) = 0 \tag{1}$$

Momentum Equation:

$$\frac{\partial}{\partial t}(\rho \vec{v}) = \rho \vec{g} + [\nabla \cdot \underline{\sigma}] - [\nabla \cdot \rho \vec{v} \vec{v}] \tag{2}$$

Energy equation:

$$\rho c_p \left(\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T \right) = \beta T \left(\frac{\partial p}{\partial t} + \vec{v} \cdot \nabla p \right) + p \nabla \cdot \vec{v} + (\underline{\sigma} : \{\nabla \vec{v}\}) + \nabla \cdot (k \nabla T) \tag{3}$$

These equations are quite general and hold for all common fluids. For simulating the fluid flow in an injection molding process, during the filling phase, some simplifications can be done on equations (1), (2) and (3), regarding the following assumptions:

1. During the filling phase, the fluid is considered to be incompressible

This assumption means that the density is constant, and allows a simplification on the continuity equation.

2. The thermal conductivity of the material is assumed to be constant

Despite the fact that the thermal conductivity, k, of polymers depends on temperature, this assumption is enforced because of the difficulty in obtaining material data. Therefore, a simplification on the energy equation can be done.

3. Simplification by dimensional analysis

The idea is to obtain estimates of the order of magnitude of each term in the governing equations – terms of sufficiently low order have little influence and, therefore, are neglected. This analysis is made using characteristic values of the variables listed below:

- Cavity thickness, $H = 10^{-3}\ m$
- Cavity length, $L = H/\delta\ m$ where $\delta = H/L << 1$
- Velocity of the fluid, $\vec{v} = 10^{-1}\ m/s$
- Cavity pressure, $p_0 = 10^{7}\ N/m^2$

- Viscosity of the fluid, $\eta = 10^4\ Ns/m^2$
- Expansivity, $\beta = 10^{-3}\ 1/K$
- Thermal conductivity of fluid, $k = 10^{-1}\ W/mK$
- Density of fluid, $\rho = 10^3\ kg/m^3$
- Specific heat of fluid, $c_p = 10^3\ J/KgK$
- Temperature difference between mold and fluid, $T_0 = 10^2\ K$

Using assumptions about material behavior and dimensional analysis to estimate the magnitude of the terms in each equation, the equations (1) to (3) are reduced to the following:

Continuity Equation:

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0 \tag{4}$$

Momentum Equations:

$$\frac{\partial p}{\partial x} = \frac{\partial}{\partial z}\left(\eta \frac{\partial v_x}{\partial z}\right), \quad \frac{\partial p}{\partial y} = \frac{\partial}{\partial z}\left(\eta \frac{\partial v_y}{\partial z}\right), \quad \frac{\partial p}{\partial z} = 0 \tag{5}$$

Energy Equation:

$$\rho c_p \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y}\right) = \eta \dot{\gamma}^2 + k \frac{\partial^2 T}{\partial z^2} \tag{6}$$

Further simplification is available by integrating the momentum and continuity equations.

4. Simplification by mathematical analysis

In order to obtain an expression for the pressure, which is a function of x and y only, it is convenient to integrate the momentum and continuity equations across the thickness. The resulting equation is a single equation for the pressure, called Hele-Shaw equation:

$$\frac{\partial}{\partial x}\left(S_2 \frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial y}\left(S_2 \frac{\partial p}{\partial y}\right) = 0 \tag{7}$$

where S_2 is called fluidity and it is defined by:

$$S_2 = \frac{1}{2}\left\{ \int_{h^-}^{h^+} \frac{z'^2}{\eta} dz' - \frac{\left(\int_{h^-}^{h^+} \frac{z'}{\eta} dz'\right)^2}{\int_{h^-}^{h^+} \frac{dz'}{\eta}} \right\} \tag{8}$$

The equation (7) can be further simplified by assuming that the flow field is symmetric and the equation (8) can be written as:

$$S_2 = \int_0^h \frac{z'^2}{\eta} dz' \tag{9}$$

In this case, the calculations need only to be performed for one half of the cavity thickness, enabling both considerable gain in computational speed and reduction of storage requirements.

2.1. Resulting Equations

After those assumptions, the governing equations for the average quantities of the fluid flow, during the filling of a mold, can be written as:

$$\frac{\partial}{\partial x}\left(S_2\frac{\partial p}{\partial x}\right)+\frac{\partial}{\partial y}\left(S_2\frac{\partial p}{\partial y}\right)=0 \tag{10}$$

$$\rho c_p\left(\frac{\partial T}{\partial t}+v_x\frac{\partial T}{\partial x}+v_y\frac{\partial T}{\partial y}\right)=\eta\dot{\gamma}^2+k\frac{\partial^2 T}{\partial z^2} \tag{11}$$

The modified-Cross model with Arrhenius temperature dependence is employed to describe the viscosity of polymer melt (Chang and Yang, 2001):

$$\eta(T,\dot{\gamma})=\frac{\eta_0(T)}{1+\left(\eta_0\dfrac{\dot{\gamma}}{\tau^*}\right)^{1-n}} \tag{12}$$

with

$$\eta_0(T)=B\exp\left(\frac{T_b}{T}\right) \tag{13}$$

where n is the power law index, η_0 is the zero shear viscosity, τ^* is the parameter that describes the transition region between zero shear rate and the power law region of the viscosity curve.

For polystyrene, the material constants are $\tau^* = 1.791\,10^4\,Pa$, $B = 2.591\,10^{-7}\,Pas$, $n = 0.2838$, and $T_b = 11680\,K$. The density, the specific heat and the thermal conductivity are $\rho = 940\,Kg/m^3$, $c_p = 2100\,J/KgK$ and $k = 0.18\,sW/mK$, respectively (Chen et al., 1998).

In this work the fluid flow is considered symmetric, so the equations for the velocity components are given by:

$$v_x=-\frac{\partial p}{\partial x}\left(\int_0^z\frac{z'}{\eta}\,dz'-\int_0^h\frac{z'}{\eta}\,dz'\right) \tag{14}$$

$$v_y=-\frac{\partial p}{\partial y}\left(\int_0^z\frac{z'}{\eta}\,dz'-\int_0^h\frac{z'}{\eta}\,dz'\right) \tag{15}$$

The equations (10) and (11) will be solved with the finite volume method using an unstructured mesh, generated by a two-dimensional quality mesh generator based on Delaunay triangulation called EasyMesh (Niceno, 2001).

3. THE NUMERICAL METHOD

Cartesian and structured meshes, in general, present little flexibility of refinement, producing, in many applications, an extreme resolution in some regions of the domain, while in other more critical regions the resolution is insufficient to find satisfactory results. This problem is more critical for transient problems. The application of unstructured meshes can, in these cases, result in great reduction of the computational cost, since the used meshes are adequate to the precision requirements of the problem: they allow to apply boundary conditions in complex geometries without an additional effort and offer great flexibility in the definition of the spacing in each region of the domain. This flexibility can be explored in order to obtain methods which

are more computationally efficient.

The search for adequate methods, which simultaneously deal with complex geometries and are conservative, has motivated the development of methodologies that have two characteristics: the use of the integral conservation equations of the properties in elementary volumes and the use of unstructured meshes to obtain elementary volumes. Methods based on this strategy, as the ones developed by Baliga and Patankar (Baliga and Patankar, 1981), have been called Control Volume Based Finite Element Method (CVFEM).

One of these methods based on triangular meshes consists in building the control volume by connecting the geometric center of the triangles to the medians of their sides (Maliska, 1995). The methodology developed in this work is based on this method.

Equations (10) and (11) are solved as follows:

1. For a given time t_0 and a given free surface position, a finite volume approximation of equation (10) is solved, thus obtaining the pressure distribution p at t_0;
2. Using equations (14) and (15) the velocities components v_x and v_y are obtained;
3. The temperature distribution at t_0 is obtained by a semi-Lagrangian approximation of equation (11);
4. The free surface position at $t_0 + dt$ is found.

The steps above are repeated until the mold is completely filled.

3.1. Finite Volume Discretization of the Pressure Equation

The equation (10), using the flux notation, can be written in its conservative form, also called divergence form, as follow:

$$\nabla \cdot \vec{J} = 0 \tag{16}$$

where the flux $\vec{J}$ is given by $\vec{J} = S_2 \nabla p$.

The discretization of equation (10) is obtained by the integration of the differential equation in the conservative form (16) in the elementary volume as the ones shown in figure 1(a). Therefore,

$$\int_V \nabla \cdot \vec{J}\, dV = 0 \tag{17}$$

Applying the Gauss Divergence Theorem to the equation (17), the contribution of the integral over the elementar volume V is given by:

$$\int_V \nabla \cdot \vec{J}\, dV = \int_S \vec{J} \cdot \vec{n}\, dS \tag{18}$$

where S is the closed boundary of V and $\vec{n}$ is a unit outward normal to S.

Considering a control volume like the one illustrated by figure 1(b) and integrating equation (16) over the control volume of vertex 1, restricted to element $\overline{123}$, the equation (18) can be written as:

$$\begin{aligned} \int_{S_{\overline{123}}} \vec{J} \cdot \vec{n}\, dS_{\overline{123}} &= \int_a^c \vec{J} \cdot \vec{n}\, dS_{\overline{123}} \\ &= \int_a^0 \vec{J} \cdot \vec{n}\, dS_{\overline{123}} + \int_0^c \vec{J} \cdot \vec{n}\, dS_{\overline{123}} \end{aligned} \tag{19}$$

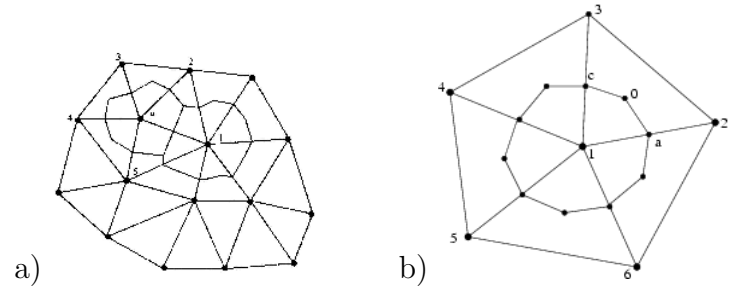

Figure 1: Control volumes for the median method

The integration given by equation (19) requires the values of the derivatives of p through the lines $\overline{a0}$ and $\overline{0c}$, however, the values of p are known only over the mesh vertices. Hence, it is necessary to interpolate p. A suitable linear interpolation of p is given by $p = Ax + By + C$ where the constants A, B and C, for the element $\overline{123}$, can be found. Organizing conveniently this terms, the equation (19) can finally be written as follow:

$$\int_a^0 \vec{J} \cdot \vec{n} dS + \int_0^c \vec{J} \cdot \vec{n} dS = C_{11}p_1 + C_{12}p_2 + C_{13}p_3 \tag{20}$$

where coeficients are given by:

$$C_{11} = \frac{S_2}{D}[(y_a - y_c)(y_2 - y_3) + (x_a - x_c)(x_2 - x_3)] \tag{21}$$

$$C_{12} = \frac{S_2}{D}[(y_a - y_c)(y_3 - y_1) + (x_a - x_c)(x_3 - x_1)] \tag{22}$$

$$C_{13} = \frac{S_2}{D}[(y_a - y_c)(y_1 - y_2) + (x_a - x_c)(x_1 - x_2)] \tag{23}$$

and

$$D = (x_1y_2 + x_2y_3 + x_3y_1 - y_1x_2 - y_2x_3 - y_3x_1) \tag{24}$$

The contribution to the control volumes of vertices 2 and 3 can be analogously computed. Considering

$$p_e = [p_1 \quad p_2 \quad p_3]^t \tag{25}$$

the element vector of the pressures at element $\overline{123}$, the contribution to element control volumes $\overline{123}$,

$$u_e = [u_1 \quad u_2 \quad u_3]^t \tag{26}$$

can be computed by

$$u_e = C\, p_e \tag{27}$$

where C is a 3×3 matrix constituted by the coeficients C_{ij}, with $1 \leq i, j \leq 3$.

After adding the contributions of the others elements, an algebraic system of equations for

the control volume centered on each vertex is obtained. This linear system is solved using the Conjugate Gradient Method, and its solution gives values for p at the triangle vertices, that is, at the center of the control volumes in which the conservation balances of the pressure p have been made.

3.2. Moving the Free Surface

For identification and advancement of the free surface of fluid, one technique called Volume of Fluid (VOF) (Ransau, 2002) is used. This strategy consists, basically, in applying the mass conservation, in the integral form, to the control volume which involves a vertex and in the discretization of the equation using the finite volume method.

In this way, an equation for the filling factor, *fill*, of the control volume is obtained. This filling factor varies in the interval $[0, 1]$, that is, if *fill* of a vertex is equal to 1, means that the control volume associated with the vertex is completely full of fluid and if *fill* of the vertex is equal to 0, then the control volume associated with the vertex is completely empty. Intermediate values of *fill* indicate that the control volume is partially full, or, in other words, they indicate the position of the free surface.

After computation of the *fill* factor in time variation ($\frac{\partial fill}{\partial t}$), for all mesh vertices, it is possible to calculate the time step, dt, that is necessary to accurately fill one control volume associated with a vertex whose $0 \leq fill \leq 1$, considering only contributions from control volumes that are filled. At each time step, the time interval is chosen such that only one control volume is filled. This strategy results in a scheme without numerical diffusion.

3.3. Solving the Equation for the Temperature

The contributions for the temperature are found by a semi-Lagrangian method. The basic idea is to follow a particle during its trajectory over the mesh. This technique consists in writing the energy equation (11) in terms of the material derivative, as follow:

$$\frac{DT}{Dt} = f \quad \text{where} \quad f = \frac{1}{\rho c_p}\left(\eta\dot{\gamma} + k\frac{\partial^2 T}{\partial z^2}\right) \tag{28}$$

which can be evaluated as

$$\frac{T(p, t+dt) - T(p,t)}{dt} = f \tag{29}$$

where p is an arbitrary particle.

Choosing a particle that occupies the position of a vertex at time $t + dt$ and writing this expression in terms of coordinates $\vec{x} = (x, y)$, we have:

$$T(\vec{x}, t+dt) = T(\vec{x} - d\vec{x}, t) + dt\, f \tag{30}$$

where $d\vec{x} = \vec{v} \cdot dt$. Expanding $T(\vec{x} - d\vec{x}, t)$ using a truncated Taylor serie, we obtain:

$$T(\vec{x}, t+dt) = T(\vec{x}, t) - dt\, \vec{v} \cdot \nabla T + \frac{dt}{\rho c_p}\left(\eta\dot{\gamma} + k\frac{\partial^2 T}{\partial z^2}\right) \tag{31}$$

where the convective term, $\vec{v} \cdot \nabla T$, is computed at the element that contains the particle p at time t and $\vec{v}$ is the velocity at the vertex. The condutive term, $k\frac{\partial^2 T}{\partial z^2}$, is computed using a difference finite scheme in the z-direction.

4. RESULTS

The solution of the pressure distribution has been validated considering analytical solutions against constant fluidity. The energy equation solution has been validated against the analytical solution of the transport of a sharp temperature discontinuity by a constant velocity field and other one-dimensional analytical solution for the temperature field. In this section we present two representative results of solving equations (10) and (31) for general situations. In these simulations, we use prescribed velocity and prescribe temperature boundary conditions at the mold inlet. The input data for this simulation are: inlet temperature $T = 513\,K$, wall temperature $T_w = 313\,K$, prescribed velocity $v_0 = 10^1\,m/s^2$ and reference pressure at inlet mold $p_0 = 10^5\,N/m^2$. The material properties are the same at the described on Section 2.1.

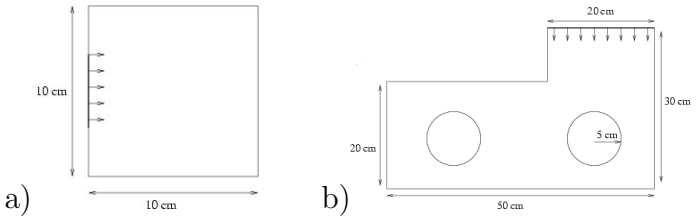

Figure 2: Molds used in the simulations: 2(a) - retangular mold and 2(b) - complex l-shaped mold with two circular insertions

The first the simulation was conducted using a rectangular mold, whose dimensions are shown in Figure 2(a). The unstructured triangular mesh built on the rectangular mold has 313 elements. This relatively coarse grid was chosen for this test because it produces better visualization of results. The figures 3, 4 and 5 show the pressure, the velocity vector and the temperature fields at the center plane of the cavity, respectively. They show four stages of the mold filling, ordered as follow: right after the flow had started, at $t = 0.51s$; at two intermediate times, $t = 1.82\,s$ and $t = 3.16\,s$; and near the end of the injection, when $t = 4.68\,s$. The predicted injection time is $4.97\,s$, and the exact time, based on mass conservation is $5\,s$, resulting in a 0.6% error. For the temperature field, only the completely filled elements are shown with the aim of illustrating the advance of the free surface.

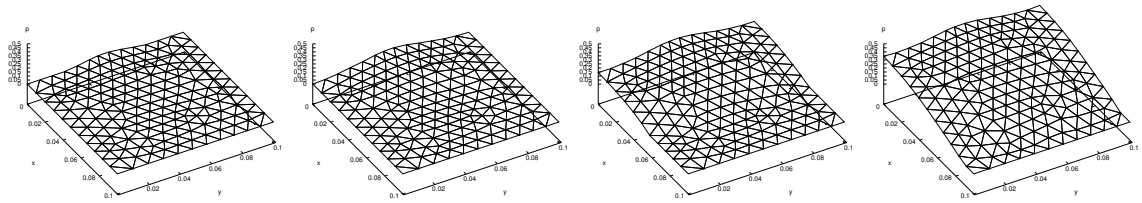

Figure 3: Four stages of pressure solution for a rectangular mold. The values are scaled by p_0

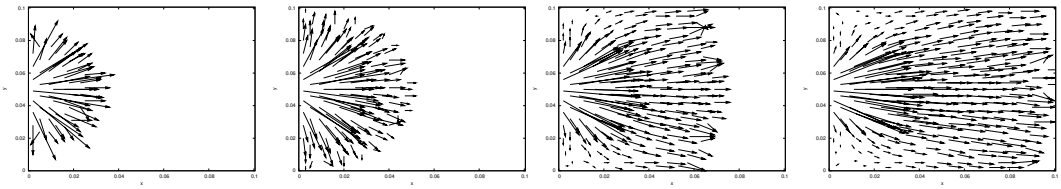

Figure 4: Velocity vectors obtained after the calculations for the pressure distribution

A l-shaped mold with two circular insertions, whose dimensions are shown in Figure 2(b) was used in the second simulation. The unstructured triangular mesh built on the mold has 563 elements.

The figures 6, 7 and 8 show the pressure, the velocity vector and the temperature fields at the center plane of the cavity, respectively. They show four stages of the filling of the mold: right

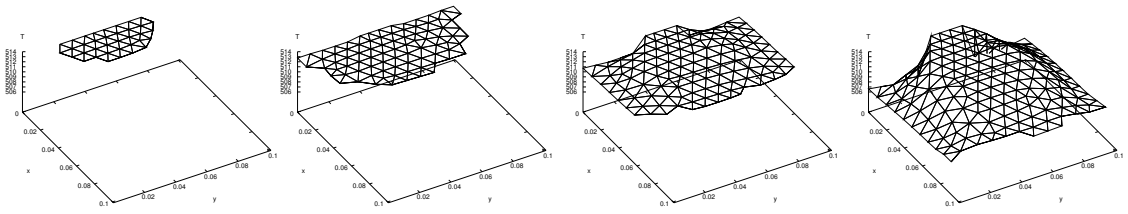

Figure 5: Four stages of the temperature distribution at the cavity center plane, ie, $z = 0$

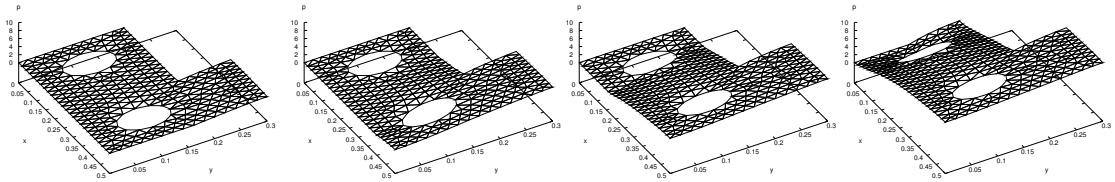

Figure 6: For stages of the pressure solution for a mold with two circular insertions. The values are scaled by p_0

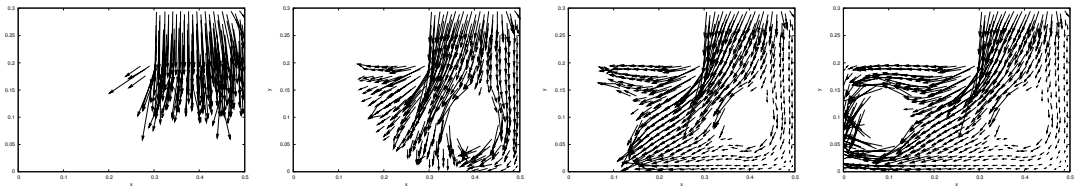

Figure 7: Velocity vectors obtained after the calculations for the pressure distribution

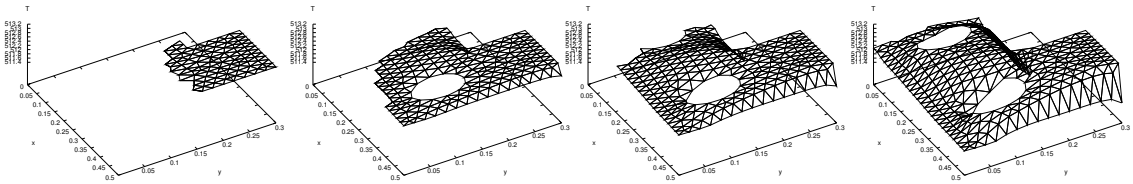

Figure 8: Four stages of the temperature distribution at the cavity center plane, ie, $z = 0$

after the flow had started, at $t = 15.38\,s$; at two intermediate times, $t = 37.21\,s$ and $t = 46.41\,s$; and near the end of the injection, when $t = 56.53\,s$. The predicted injection time is $57.48\,s$, and the exact time, based on mass conservation is $52.5\,s$, resulting in an 8.41% error which is quite large. However, using a finer mesh with 5546 elements, the predicted injection time is given by $52.61\,s$, resulting in a 0.20% error. For the temperature field, only the completely filled elements are shown with the aim of illustrating the advance of the free surface.

In this second simulation, it is possible to observe the capability of the present model to deal with splitting and remerging of the free-surface/melt front during the filling process. The prediction and localization of this effect are essential to guarantee the final quality of the part since the remergin regions are one of the most fragile areas of the molded part.

5. CONCLUSION

This work presented a finite volume method over an unstructured mesh for solving the governing equations of fluid flow during the filling phase of injection molding. This methodology allows to simulate complex geometries without excessive computational efforts, producing temperature

and shear stress distributions and real injection times. Thus, the proposed method may be considered an useful tool for the design, analysis and troubleshooting of injection molding process. This fast and simple prediction tool provides a 3-dimensional temperature distribution, including heat transfer and viscous dissipation effects, which is sufficiently accurate for most applications.

6. ACKNOWLEDGEMENTS

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