Thirty Years of Modeling of Injection Molding. A Brief Review of the Contribution of UNISA Code to the Field

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Abstract:

UNISA code, a software for the analysis and modeling of injection molding, was born at the University of Palermo in Italy in the 1980s. Afterwards, in the 1990s, it was rewritten and expanded at the University of Salerno (Italy) and continuously improved over the years. It is a study code, aimed at understanding rather than simulating. It has the unique characteristic of describing, since the early versions, the morphology of the molded samples. Furthermore, it always implemented the interrelationships among the different material properties (crystallinity, viscosity, density). In this work, the evolution of the software is reviewed, placed in the background, underlining the contribution given to the understanding of polymer processing and morphology evolution. Eventually, the future challenges of modeling are presented.

Introduction

Injection molding is not only one of the most widely adopted techniques for polymer processing, but also one of the most challenging from the modeling point of view. The coexistence of fast cooling rates, high pressures, strong flow fields, makes it extremely difficult to describe in detail the behavior of the polymer during processing. Furthermore, from the very beginning, injection molding is aimed at producing parts having tight tolerances and specific mechanical properties. Thus, the control of internal stresses and morphology distribution inside the moldings is critical. Since the second half of the last century, injection molding has been of interest for the researchers, with the first attempts of simulating the velocity profiles during filling of a cavity. Models and

algorithms continuously evolved, so that at present we have several commercial software able to simulate the main process variables during injection molding in complex molds. The availability of open scholar software is still useful to underline physical aspects which are overlooked and deserve further investigation, to understand details of the process, but also to stimulate the evolution of new routines for the simulation of different conditions. In this work, the contribution given by UNISA Code to the evolution of modeling of injection molding is reviewed. The paper is divided in the following sections: "The 1980s: basic phenomena are described" in which the most significant early works on the simulation of injection molding are introduced; "Crystallization kinetics, morphology development and flow-induced crystallization" in which we report the basic equations adopted for the simulation of crystallization development in injection molding; "Orientation distribution" in which the models adopted for the description of molecular orientation are presented; "Back to flow induced crystallization" in which the model adopted in UNISA Code to describe the effect of flow on crystallization kinetics is described; "Shrinkage and cooling stresses" in which the phenomenon of shrinkage is presented together with the route followed to numerically describe it. The work ends with two sections which try to present possible future issues and development for the modeling and simulation of injection molding.

The 1980s: basic phenomena are described

Despite the firs attempts of describing injection molding can be dated back to 1950s (Spencer and Gilmore 1951), the first simulations which considered filling, packing and cooling were presented in 1980s (a review of the early papers can be found in Huilier 1990). In those years the computing means were obviously not even comparable with those available nowadays. Therefore most of the efforts were spent in the simplification of the equations. We still have benefits from the studies made toward the simplification of balance equations such for instance Lord and Williams' analysis of mold filling (Lord and Williams 1975). In the 1980s, the reference work consisted in a series of papers from McGill University (Kamal and Lafleur 1986, Lafleur and Kamal 1986) which

presented, probably for the first time, a detailed simulation of the complete injection molding process, solving numerically a set of differential equations where many of the relevant phenomena taking place during packing were accounted for locally with reference to a rectangular mold. In particular, the local crystallization rate was described by a non-isothermal modification of the Avrami equation; viscoelasticity was described by the Maxwell-Oldroyd-Gupta-Metzner equation with the effect of temperature on both viscosity and relaxation time. The analysis already included most of the basic knowledge of the phenomena involved. The UNISA Code first appeared in an international journal in 1988 (Titomanlio, Piccarolo and Levati 1988). In that paper, description of the packing-holding stage based on an extension of Lord and Williams' analysis (Titomanlio, Acierno and La Mantia 1980) was implemented in a simulation software. The complete temperature field was considered, and a viscous non-Newtonian rheological equation was adopted. Crystallization was not explicitly accounted for in the energy equation, but the reduction of cooling rate by effect of crystallization heat release was approximately accounted for by means of a suitable reduction of thermal diffusivity (based on the Stefan number). In the introduction of that paper (Titomanlio, Piccarolo and Levati 1988), on commenting the state of the art, the authors underlined some limitations which had to be overcome to improve the simulations: the characterization of the crystallization kinetics and the interactions between the different phenomena, such as the effect of crystallinity on rheology or density changes under simultaneous variations of pressure, temperature, and crystallinity. That paper charted the course for the development of the UNISA code in the following years. Despite of the continuous improvements and enrichment of the routines, the main structure of UNISA code set in that early paper remained unchanged during the years. UNISA code basically relies on a finite different scheme. The geometry is schematized in a series of rectangular or cylindrical elements. The process is separated into two steps: filling and packing stages. The basic equations have been reported in the literature (see e.g. Pantani, Speranza and Titomanlio 2001). During the filling stage the material is considered incompressible and the flow rate is imposed. The position of the flow front is therefore known at each time step. As a default, the

variables at the flow front are averaged on the basis of velocity (i.e. cup-mixing variables are considered at the front). Knowing the flow rate and the rheology, the software calculates the pressure gradients and the temperature distributions. If a value of maximum pressure is reached the flow rate is adequately corrected. During the packing stage, the flow rate at each position is determined by the densification of the material at the downstream positions. At each time step, the software thus starts from the tip of the cavity, imposing a pressure there and calculating the average density due to cooling and thus the flow rate and the pressure drops. Then it proceeds backwards to the injection chamber and finds the requested injection pressure. If this value equals the imposed packing pressure the software passes to the following time step, otherwise a new attempt is made on the pressure at the tip of the cavity on the basis of a Newton-Raphson solution scheme.

Crystallization kinetics, morphology development and flow-induced crystallization

The steps following that first publication were spent in characterizing the crystallization kinetics at cooling rates of interest for injection molding. Indeed, when the crystallization kinetics was introduced in the UNISA code, the parameters of the kinetics were characterized by conventional techniques (i.e. DSC). It soon became clear that crystallization kinetics was too slow to allow a development of crystallinity comparable to what experimentally found.

In the first years of the 1990s, a new technique was presented, which allowed to obtain crystallization data at high cooling rates (Brucato, Crippa, Piccarolo and Titomanlio 1991, Piccarolo, Saiu, Brucato and G 1992). Furthermore, a significant improvement in the prediction of crystallinity development was introduced (Brucato, Piccarolo and Titomanlio 1993) by keeping into account the possibility of the formation of different crystalline phases. This was done by assuming a parallel of several non-interacting kinetic processes competing for the available amorphous volume. The evolution of the relative crystallinity degree of each phase was described as:

$$\frac{\partial \chi_i}{\partial t} = \left(1 - \sum_i \chi_i\right) \frac{\partial k_i}{\partial t} \qquad (1)$$

where the subscript i stands for a particular phase, and k_i is the expectancy of volume fraction of each phase if no impingement would occur.

In 1995 a new, improved version of UNISA Code was presented (Titomanlio, Speranza and Brucato 1995). The crystallization kinetics was implemented by a Nakamura's non-isothermal formulation of the Avrami model, and the parameters were tuned on experimental data collected at cooling rates in the range of interest for injection molding. The crystallization was explicitly considered in the energy equation and the density of the polymer was essentially determined by the crystallinity according to the following equations

$$\rho(T, P) = \rho_c(T, P) X_c + \rho_a(T, P)(1 - X_c) \qquad (2)$$

$$\rho_c(T, P) = \rho_c^0 \left[1 + \alpha_c(T - T_0) - \beta_c P\right] \qquad (3)$$

$$\rho_a(T, P) = \begin{cases} \rho_a^0 \left[1 + \alpha_m(T - Tg) - \beta_m P\right] & \text{if } T > Tg \\ \rho_a^0 \left[1 + \alpha_g(T - Tg) - \beta_g P\right] & \text{if } T \leq Tg \end{cases} \qquad (4)$$

where X_c is the absolute crystallinity. The description of crystallization kinetics in injection molding was rather new. The aim of that work was identifying the most significant phenomena taking place during the process, especially with reference to post filling stages. In particular, it was shown that, by taking account of the effect of pressure on both viscosity and crystallization kinetics, predictions of simulation for pressure, both in the runner and in the cavity, during both mold filling and at beginning of the packing stage improve significantly.

It is worth mentioning that at the beginning of the 1990s the description of crystallization kinetics in injection molding was innovative. For instance, in those years the Cornell Injection Molding Program (CIMP) presented a software able to describe the injection molding of semi-crystalline polymers (Chiang, Hieber and Wang 1991) using a Tait PVT equation of state, thus neglecting the effect of thermal history on crystallization kinetics.

On commenting the description of the simulation results, many aspects of the evolution of the process variables could be clarified. For instance, the presence of an inflection point (Fig. 1) at gate sealing time in the pressure curve soon before the gate was understood and commented thanks to the comparison with simulation results.
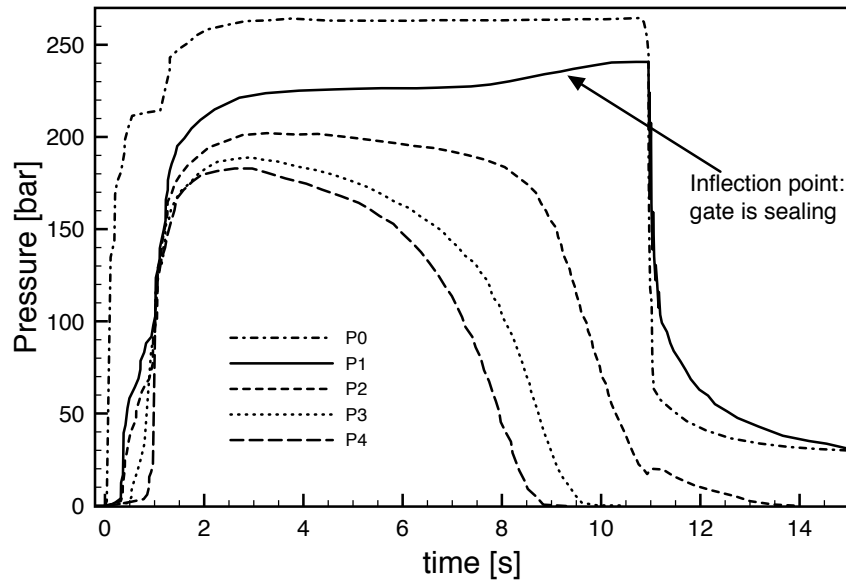

Fig. 1 Experimental pressure evolution in several positions along the flow-path for a polypropylene injection molded in a 2mm thick rectangular cavity (Pantani, Speranza and Titomanlio 2001). P0: injection chamber; P1: soon before the gate; P2, P3 and P4 inside the cavity at increasing distances from the gate. The arrow indicates the inflection point at gate sealing time

Despite the attempt to describe crystallization kinetics at rates of interest for injection molding, predictions for gate sealing time still were found larger than the experimental values. It was thus concluded that the effect of flow on crystallization kinetics could not be neglected. Substantial improvements were then included in a new version of the UNISA code (Titomanlio, Speranza and Brucato 1997), in which the effect of flow on crystallization kinetics was explicitly taken into account

$$k(t) = \ln(2) \left[\int_0^t K(T(s)) ds \right]^n \qquad (5)$$

$$K(T) = K_0 \exp\left(-\frac{4\ln(2)(T - T_{max})^2}{D^2} \right) \qquad (6)$$

$$D(\tau) = \begin{cases} D_0 & \text{if } T < T_{\max} \\ D_0 + b\,\tau^s & \text{if } T \geq T_{\max} \end{cases} \qquad (7)$$

Where τ is the shear stress whereas D_0, b and s are fitting parameters; n is the Avrami exponent.

Furthermore, the effect of crystallinity on viscosity was described by the following equations

$$\eta(T, \chi, \dot{\gamma}) = \eta(T, \chi = 0, \dot{\gamma}) h_\chi(\chi) \qquad (8)$$

$$h_\chi(\chi) = 1 + e_1 \exp\left(-\frac{e_2}{\chi^p} \right) \qquad (9)$$

such an hypothesis automatically implies that, for polymers crystallizing during the process, the not flowing condition is determined by a crystallization level (of a few percent) rather than by a value of temperature.

More recently, following a series of more accurate experimental data (Pantani, Coccorullo, Speranza and Titomanlio 2005, Pantani, Speranza and Titomanlio 2015), the effect of crystallinity on rheology was described by a different expression. A shift factor (on both viscosity and shear rate axes) due to temperature, pressure and crystallinity was assumed according to the following relationship

$$\eta(T, P, \chi, \dot{\gamma}) = \frac{\eta_0 \alpha_{TP\chi}}{1 + \left(\frac{\eta_0 \alpha_{TP\chi}}{\tau^*} \dot{\gamma} \right)^{1-n}} \qquad (10)$$

with

$$\alpha_{TP\chi} = 10^{-\frac{C_1(T-T_0-C_3P)}{C_2+T-T_0}} h_\chi(\chi) \tag{11}$$

Although rather rough, the description of the effect of flow on crystallization kinetics according to eq. (7) was innovative for the time since just a few attempts were done for introducing flow induced crystallization in injection molding (Ito, Minagawa, Takimoto, Tada and Koyama 1996). It soon became clear to the researchers working in the field that the phenomenon could not be neglected. A few years later, at the beginning of the 2000s, Zuidema et al. (Zuidema, Peters and Meijer 2001) implemented a model which considered the combined process of quiescent and flow-induced crystallization. For flow-induced crystallization, a modified version of the model presented by Eder et al. (Eder, Janeschitz Kriegl and Liedauer 1990) was adopted. In particular, the shear rate used by Eder as the driving force for flow-induced nucleation and crystallization, was replaced by the second invariant of the deviatoric part of the recoverable strain tensor. This work (Zuidema, Peters and Meijer 2001) was probably the first one which provided a description of morphology in injection molding, in more detail with respect of the amount of crystallinity.

The UNISA code also moved in the direction of the description of morphology. In 2002 (Pantani, Speranza, Coccorullo and Titomanlio 2002) a version of the code was presented, which was able to describe the distribution of the dimensions of the spherulitic crystalline structures. To act out of habit, the software upgrade was introduced after a wide study on the phenomenon of structure development in conditions of interest for processing (Coccorullo, Pantani and Titomanlio 2002). The model for describing the nucleation density assumed heterogeneous nucleation, with a number of nuclei depending on temperature according to the following equation

$$N(T) = N_1 \exp[N_2(T_m - T)] \tag{12}$$

and a spherulitic growth rate provided by the Hoffman-Lauritzen equation (Hoffman, Lauritzen, Passaglia, Ross, Frolen and Weeks 1969)

$$G(T) = G_0 \exp\left[-\frac{U}{R(T - T_\infty)}\right] \exp\left[-\frac{K_g(T + T_m)}{2T^2(T_m - T)}\right] \qquad (13)$$

in both equations (12) and (13) Tm is intended to be the thermodynamic crystallization temperature. Equations (12) and (13) were combined into a kinetic constant, k_α, by adopting the Kolmogoroff's equation for spherical growth

$$k_\alpha = \frac{4\pi}{3} \int_{s=0}^{t} \frac{dN(s)}{ds} \left(\int_{u=0}^{t} G(u)\, du\right)^3 ds \qquad (14)$$

The comparison between the software predictions and the experimental data, in terms of pressure evolution, crystalline phase distribution, diameters of the spherulites, was good. As stated in the conclusions of that work (Pantani, Speranza, Coccorullo and Titomanlio 2002), further improvements could be introduced only by considering the effect of molecular orientation on crystallization kinetics.

Orientation distribution

The description of orientation of molecular chains is per se quite significant for injection molding, since it can often determine a marked anisotropy of the majority of final properties. Furthermore, molecular orientation and strain cause in semi crystalline polymers an enhancement of crystallization kinetics for both thermodynamic and kinetic reasons: an oriented melt has a higher free energy (and thus a higher melting point), and the kinetic barrier to overcome in the transition from the molten to the crystalline state lowers because extended chains are closer to their condition in the final crystal. The first attempt to predict orientation distribution in injection molded PS samples is due to (Isayev and Hieber 1980), using Leonov viscoelastic constitutive equation. At the beginning of the 2000s, most of the work focusing on simulation of molecular orientation had been carried out by using Leonov model (Douven, Baaijens and Meijer 1995, Kim, Park, Chung and Kwon 1999).

The model used in the UNISA code (Pantani, Speranza, Sorrentino and Titomanlio 2002) was based on a non linear version of the Maxwell model,

$$\frac{D}{Dt}\bar{\bar{A}} - \left(\bar{\nabla}\bar{v}\right)^T \times \bar{\bar{A}} - \bar{\bar{A}} \times \left(\bar{\nabla}\bar{v}\right) = -\frac{1}{\lambda}\bar{\bar{A}} + \left(\bar{\nabla}\bar{v}\right) + \left(\bar{\nabla}\bar{v}\right)^T \qquad (15)$$

in which $\bar{\bar{A}}$ is a tensor representing the deformation of the population of macromolecules with respect to the equilibrium state, and the relaxation time, λ, was assumed to be a function of temperature, pressure, crystallinity (if present) and shear rate:

$$\lambda\left(T, P, \chi, \dot{\gamma}\right) = \frac{\lambda_0 \alpha_{TP\chi}}{1 + \left(\frac{\lambda_0 \alpha_{TP\chi}\dot{\gamma}}{C}\right)^{1-n}} \qquad (16)$$

It is worth mentioning that, despite the fact that the equations for describing viscosity and relaxation time are similar, the parameters can obviously be different.

The model was chosen because, on describing the molecular deformation, it could provide molecular orientation and strain. Furthermore, it was simple enough to be implemented in the code for the simulation of injection molding without delaying too much the computational time and finally it contained a limited number of parameters, which could be determined by means of a standard rheological characterization (Pantani 2005). The model resulted to be able to describe successfully the distribution of molecular orientation in injection molded samples of PolyStyrene, in several molding conditions (Pantani, Sorrentino, Speranza and Titomanlio 2004).

Again, on describing the results of simulations, several insights concerning the phenomena involved in the process were gained. For instance, it resulted clear that, since the mass flow rate crossing each section during packing is determined by the density increase of the material downstream, a larger volume downstream induces a larger packing flow rate and thus a larger convection heat flow which determines longer gate sealing time. This is significant especially for solidification and molecular orientation at gate. This observation, driven by simulation results, was confirmed by an experimental campaign (Pantani, De Santis, Brucato and Titomanlio 2004) from which it resulted clear that, although gate thickness is the most important factor determining the gate sealing time (a thicker gate determines a delayed solidification time), cavity geometry is rather important (increases of both cavity length or thickness induce a delayed solidification time for the same gate thickness).

Going back to orientation, the description of relaxation time given in eq. (16) presented a series of limitations:

– a physical inconsistency, since relaxation time depended on the external flow field (through shear rate) and not on the state of material itself

– a discontinuity in relaxation time taking place in the presence of a discontinuity of shear rate (namely at start-up or during shear steps).

These limitations were known at the time the model was developed, but they were accepted in consideration of the simplicity of the model. However, on increasing the demand for more accurate simulations, it was decided to change the dependence of relaxation time on velocity gradient with a dependence upon an internal structural parameter (Pantani, Speranza and Titomanlio 2012). In particular, the difference Δ between the two main eigenvalues of the tensor $\vec{A}$ was chosen as a measure of the "molecular elongation", and thus the relaxation time was described as

$$\lambda\left(T, P, \chi, \Delta\right) = \frac{\lambda_0 \alpha_{TP\chi}}{\left[1 + \left(a\,\Delta\right)^b\right]^c} \tag{17}$$

At the beginning of the 2010s, the UNISA Code was ready to describe the effect of flow on molecular deformation and thus on crystallization kinetics

Back to flow induced crystallization

In a series of preliminary papers, the effect of flow on the crystallization kinetics of an isotactic polypropylene was characterized (Coccorullo, Pantani and Titomanlio 2008, Pantani, Coccorullo, Volpe and Titomanlio 2010, De Santis, Pantani and Titomanlio 2016). If nucleation density under quiescent conditions was found constant at constant temperature, a nucleation rate was observed and measured under steady shear conditions. Also the increase of spherulitic growth rate by effect of steady shear rate was measured and a correlation between the excess of growth rate (with respect to quiescent conditions) and the nucleation rate under the same conditions (of shear rate and temperature) was identified. The existence of such a correlation between Growth rate and nucleation rate is consistent with the fact that also nucleation rate is usually described by Hoffman

and Lauritzen equation (Hoffman, Lauritzen, Passaglia, Ross, Frolen and Weeks 1969) The correlation adopted between the nucleation rate and the excess growth rate (namely the difference between the growth rate measured under flow and in quiescent conditions at the same temperature) is reported in Fig. 2. By adopting the excess growth rate as independent variable, both vertical and horizontal axes are zero in quiescent conditions.
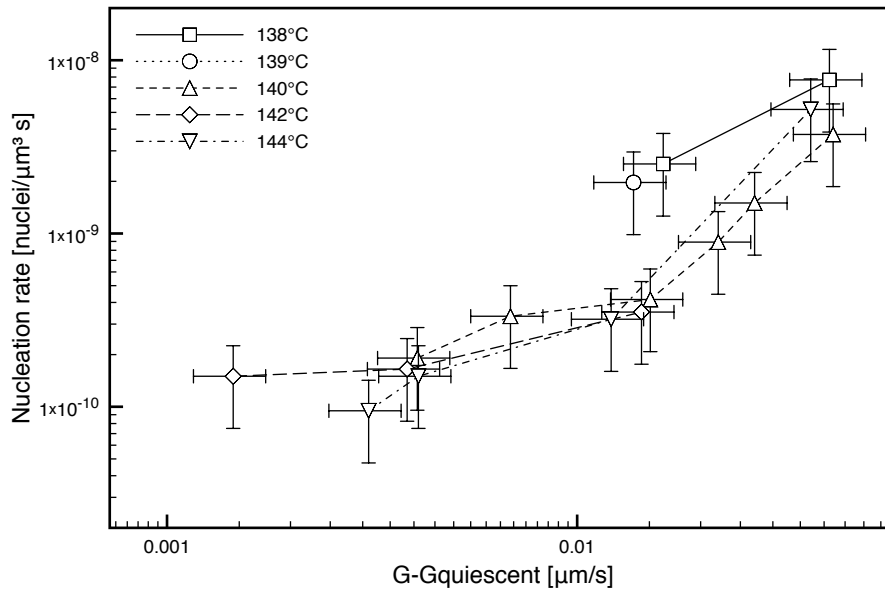

Fig. 2 Correlation between flow induced Nucleation rate and excess Growth rate (Pantani, Coccorullo, Volpe and Titomanlio 2010)

On the basis of this correlation, the nucleation rate can be calculated once the growth rate is known both in quiescent and in flow conditions. It was assumed that in the spherulitic regime, the growth rate could be always described by equation (13), in which only the melting temperature changed by effect of flow. In particular, the melting temperature was assumed to increase on increasing the parameter Δ (Pantani, De Santis, Speranza and Titomanlio 2014).
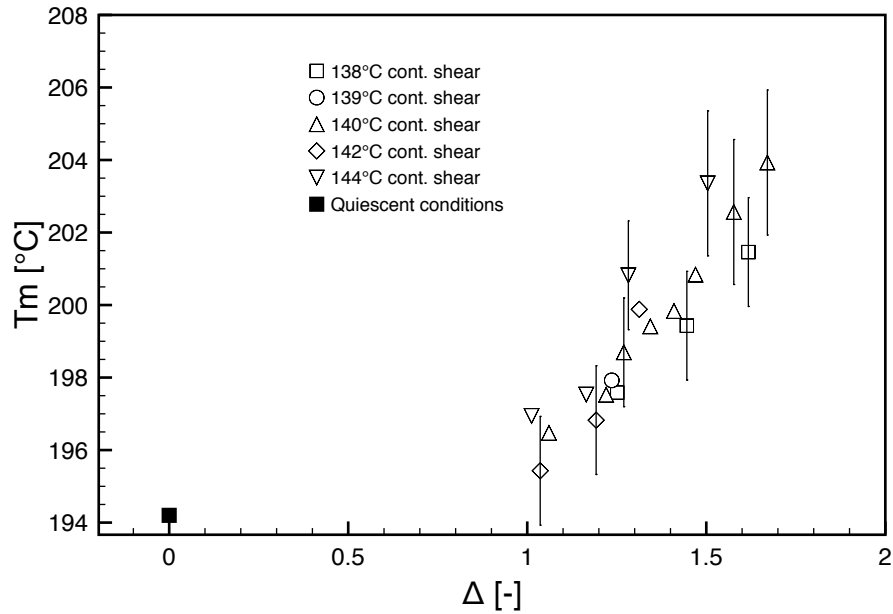
Fig. 3 Correlation between the melting temperature to be used in eq. (13) and the difference Δ

between the two main eigenvalues of the tensor A defined by eq. (15)

UNISA code was then ready to describe the effect of molecular elongation on crystallization kinetics, according to the following scheme:

- flow induces orientation according to eq. (12), and thus Δ can be calculated

- according to Fig. 3, Tm increases and can be determined

- the growth rate can be thus calculated by eq. (13)

- the nucleation rate can be then determined by Fig. 2

- the kinetic constant is finally given by eq. (14)

Preliminary simulations of the injection molding of an iPP were carried out accounting of the effect of flow on spherulitic growth rate and nuclei density (through a flow induced nucleation rate). These first results (Pantani, De Santis, Speranza and Titomanlio 2014) showed that although the effect of flow has an enormous effect on the crystallization kinetic functions, it does not modify significantly the results for the distribution of average spherulites diameters with respect to the case in which flow induced crystallization is neglected. This overall result, which may appear macroscopically inconsistent, is due to the fact that the increase of spherulitic growth rate and of

nucleation rate have an opposite effect on the final spherulite diameters. On the other hand, the enormous increase of the crystallization functions by effect of flow reduces significantly the thickness of the layer where the alpha crystalline phase of polypropylene is quenched. Software outputs show a reduction of about one order of magnitude of the thickness of this layer by effect of flow induced crystallization. This is consistent with the experimental observations.

In a forthcoming paper, the effects of flow induced crystallization on the distribution of morphology in injection molded polypropylene parts will be further discussed.

Obviously, the effect of flow is not limited to the enhancement of nucleation and growth rates of the spherulitic structures. On increasing the intensity of flow, fiber-like structures are found. The formation of these structures was described in different ways in the literature. Zuidema et al. (Zuidema, Peters and Meijer 2001) considered a competition between the spherulitic structures and the fibrillar structures (shish-kebabs). Kennedy and Zheng (Zheng and Kennedy 2004) considered an Avrami index gradually decreasing from 3 to 1 on increasing the intensity of flow. The UNISA Code has not presented so far a routine for the prediction of oriented crystalline structures, but an attempt of modeling was recently presented (Pantani, Nappo, De Santis and Titomanlio 2014).

Shrinkage and cooling stresses

The prediction of dimensional changes and residual stresses in injection molding was implemented in the UNISA Code at the end of the 1990s. The basis of the model were presented in a series of papers (Jansen and Titomanlio 1996, Titomanlio, Brucato and Kamal 1987, Titomanlio and Jansen 1996)

- the evolution of shrinkage from the moment of first solidification is determined by a balance between restraining and constraining forces

- when a molten slab is cooled inside a mold from lateral surfaces, it can be considered as made by a series of layers in mechanical equilibrium overlapped in the thickness direction which solidify at different times

- each layer would like to shrink according to density increase related to its temperature, pressure and, if present, crystallization history

- deformation is forced to be the same for all layers, and it has to be consistent with the balance of forces acting on the object surface, both while the slab is inside the mold and after its ejection from the mold

- stresses arise in each layer (in case, relaxation also occurs) according to material behavior (stress build-up was described by an elastic constitutive equation)

- if in-mold shrinkage can be taken into account, instantaneous dimensions are regulated by mechanical equilibrium between internal stresses and external forces acting on solid layers (i.e. melt pressure, friction and any other interaction with mold wall)

- if the molding is constrained inside the mold, the in-plane dimension of the molding is fixed until de-molding;

- if at the ejection there is contact of the polymer on the mold walls, thickness shrinkage is regulated by release of pressure at ejection, Poisson effect in relation to in-plane shrinkage and thermal (and, in the case of crystallization or reaction) contraction to room temperature.

In the same years, a similar approach was developed by Bushko and Stokes (Bushko and Stokes 1995a, Bushko and Stokes 1995b) and Douven and co-workers (Douven, Baaijens and Meijer 1995, Zoetelief, Douven and Ingen Housz 1996) who proposed a model for analyzing residual stresses and shrinkage in injection molding. They assumed a viscoelastic constitutive equation for the polymer, rather than the viscous-elastic approach adopted in the UNISA Code. At least for cooling rates typical of injection molding, it can be demonstrated that with a careful choice of a solidification criterion the viscous-elastic model is at least as accurate as the viscoelastic model. In Fig. 4 a comparison is reported between the calculations for stress distribution in an injection molded PS sample calculated by Zoetelief et al (Zoetelief, Douven and Ingen Housz 1996) by using both a viscous-elastic and a viscoelastic approach, and the simulations for the same case done by UNISA Code considering different choices for the solidification criterion. In particular, the polymer

was considered an elastic solid when below a solidification temperature (normally the glass transition temperature) which can be taken a function of pressure and of cooling rate (Pantani and Titomanlio 2006).
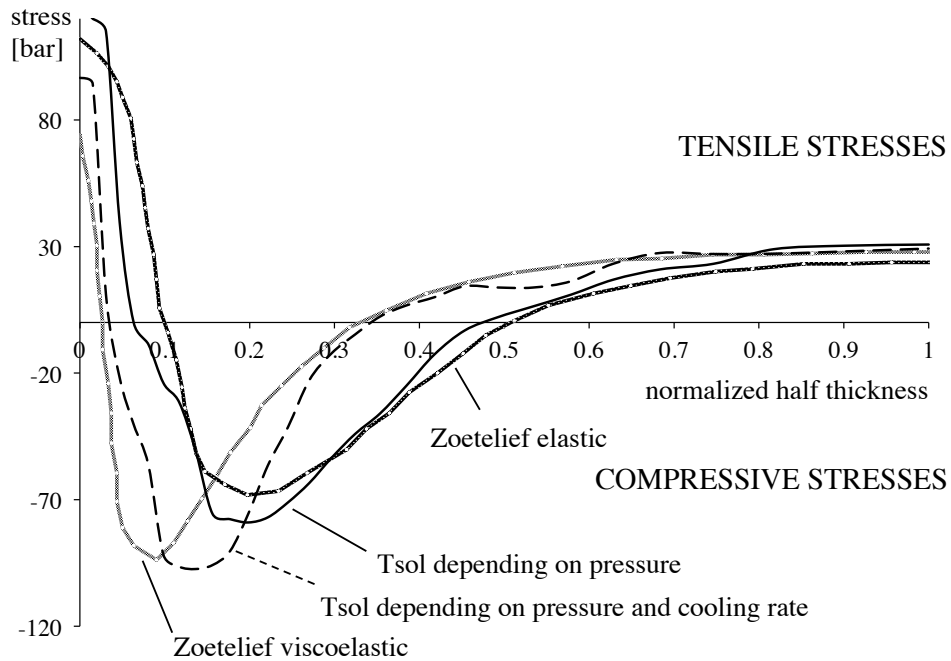

Fig. 4 Comparison between the results reported by Zoetelief et al(Zoetelief, Douven and Ingen Housz 1996) and the predictions of the UNISA Code, with different options for the solidification temperature, Tsol.

The model implemented in the UNISA Code can be applied to both amorphous and semi-crystalline polymers once the solidification condition is identified. For semi-crystalline polymers a solidification condition based on a crystallinity value is assumed (De Santis, Pantani, Speranza and Titomanlio 2010) similarly to what done for the no-flow condition; the solidification crystallinity value has to be larger than the no-flow crystallinity value .

Boundary conditions and future developments

As mentioned above, the main equations for describing most the significant phenomena involved in injection molding were already collected and simplified in the 1980s. However, some details in the boundary conditions were still subject to improvements, and resulted to be quite significant on the

accuracy of simulations. One example is the mold rigidity. When modeling the process, the dimensions of the cavity are considered constant. However, due to the high pressures, a deflection of the mold can take place, and this determines a different evolution of pressure curves during processing (Delaunay, Le Bot, Fulchiron, Luye and Regnier 2000b). It was shown (Pantani, Speranza and Titomanlio 2001, Vietri, Sorrentino, Speranza and Pantani 2011) that the effect of mold deformation on pressure evolution inside the cavity can be described by using an apparent volumetric compressibility given by

$$\beta_{v,app} \simeq \beta_v + \frac{K_M}{S_0(x)} \qquad (18)$$

in which K_M is the mold compliance, usually in the range 10^{-5}-10^{-4} mm bar^{-1}, and S_0 is the local cavity thickness. This simple description of mold deformation allows to significantly improve the results of simulations (Costa 2014).

Another significant aspect of simulations, which is often overlooked, is the thermal boundary condition at polymer-mold interface. Already in 1995 (Titomanlio, Speranza and Brucato 1995) UNISA Code implemented a heat transfer coefficient depending of the reciprocal of the square root of time, in order to keep into account the heat penetration inside the mold. Later on (Pantani, Speranza and Titomanlio 2001), the description of the heat transfer coefficient was improved by considering a contact resistance between the polymer and the mold

$$h(t_c) = \max \begin{cases} h_0 \sqrt{\frac{t^*}{t^*+t_c}} \\ h_l \end{cases} \qquad (19)$$

where t_c is the local contact time between polymer and mold wall, h_0 and t* are constants taken as standard contact polymer-mold heat transfer coefficient [2 10^4 W/(m^2 K)] and a very short time value (0.1s). Such a small value for t* ensures that the heat transfer inside the mold soon becomes the controlling mechanism. The lower limiting value h_l is the ratio between the mold conductivity and the distance between the mold surface and the cooling channels. By adopting this description of the thermal boundary condition, it was demonstrated that a detailed thermal history close to the

mold wall could be reproduced (Kim, Park, Chung and Kwon 1999), with consequent better description of the evolution of morphology in the skin layers of the moldings (Hieber 2002) .

As also mentioned above, the analysis of simulation results often allow to clarify physical aspects of the process. With reference to the thermal boundary condition at the polymer-mold interface, some anomalies in the evolution of the temperature in the layers close to mold surface could be understood. If the pressure inside the mold goes to zero, in that position the contact with the mold wall becomes not efficient, the heat transfer at the mold wall decreases and the thermal profile inside the sample flattens; if the sample even detaches from the mold wall, the temperature history can dramatically change: the heat transfer coefficient at the mold wall undergoes a dramatic decrease, and , as reported in fig.4, the sample surface temperature can even rise again (Delaunay, Le Bot, Fulchiron, Luye and Regnier 2000a).
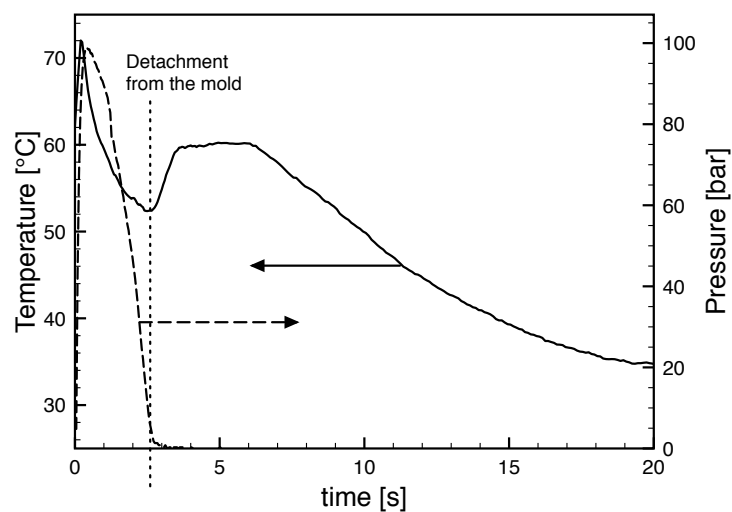

Fig. 5 temperature history measured inside the polymer sample at a distance of about 0.03mm from mold wall and pressure history measured at the same position. The material is a polystyrene (Pantani, Speranza and Titomanlio 2001)

The capability of describing the details of the thermal profile inside the mold opens new possibilities for the applications of injection molding simulation software.

Injection molding is currently being utilized in a wide variety of new applications. The current desire for smaller, cheaper, highly integrated, and more versatile products has spurred its increased use and acceptance in fields where more expensive and time-consuming techniques are currently applied. The possibility to obtain objects with particular dimensions spanning from meter to micron ranges and with good replication of micro-features allows its application to a host of productions such as electronics apparatus, medical devices and optical systems.

It is clear that such applications require a fast, good and repeatable control of all the processing parameters. In particular, the mold surface temperature is probably the most important one. This is the reason why the methods for the fast control of mold surface are currently a target for technologists and researchers. Simulation software cannot be found unprepared under these aspects. It is necessary to have the possibility of implementing a mold surface temperature depending on time. Even better, it is desirable to attain a description of the temperature evolution inside the mold.

When a replication of the surface is aimed at, it is necessary to have an accurate description of the conditions of the polymer when it gets in touch with the mold surface. This cannot be attained without considering fountain flow, an aspect which was investigated in the past (Gogos, Huang and Schmidt 1986, Mavridis, Hrymak and Vlachopoulos 1986), but has recently been set aside.

Final remarks

The simulation of injection molding is continuously evolving (Zhou 2013). The increasing computing power reduces the limitation in the description of the domain and of the behavior of the material. The classical goal of injection molding simulation, namely the prediction of pressure fields, flow rates and temperature evolution can thus be extended to very complex geometries, or cavities containing micro-features. However, the evolution of the state of the art in the field charts the route toward a much more ambitious goal: the prediction of material properties, such as the distribution of product dimensions (shrinkage), of internal stresses and of morphology (orientation, crystallinity, dimensions and shape of crystalline structures). These features are strongly dependent on details of the thermo-mechanical history experienced by the material during processing.

On reviewing the contribution of the UNISA Code to the field of modeling and simulation of injection molding it was shown that, in order to achieve a reliable description of morphology evolution during polymer processing, one needs:

• a thermo-mechanical model which accounts for the main phenomena that take place

• a good description of geometry and thermal boundary conditions

• an accurate and comprehensive material characterization as far as:

– rheological behavior: viscosity and viscoelasticity (for orientation distribution) and effect of crystallinity

– crystallization kinetics, including the effect of flow on the morphology development.

It is clear that the characterization of material properties cannot be carried out without an effort in the collection of experimental data in the range of process variables of interest for injection molding. This constant comparison with the behavior of the material and with the experimental results obtained during well characterized molding tests was a "trademark" of the UNISA Code.

Finally, it should be pointed that the continuous comparison between simulation results and experimental data is the key to the understanding of all the physical phenomena taking place during the processing. Without this comparison, no development, neither in the technology nor in the modeling, can be attained.

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