11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
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INTEGRATIVE SIMULATION FOR ASSESSING THE MECHANICAL PERFORMANCE OF A WELD LINE ON INJECTION MOULDED THERMOPLASTIC PARTS

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Key words: Injection moulding, Thermoplastics, Weld line, Reptation theory

Abstract. Weld lines are commonly weak spots in thermoplastic injection-moulded parts. Predicting the healing degree of the polymer matrix at the weld line interface is necessary for enriching the material modelling at the weld line zone. A structural simulation based on such enhanced material modelling would be more accurate and advantageous in terms of product design. In this regard, a physical modelling of the healing degree between polymer interfaces has been developed and used to refine a structural simulation intended to predict the maximal strength of a structure under quasi-static loading. The simulation has been compared to experimental tensile tests performed on specimens injection-moulded with an unreinforced ABS matrix and a 30 wt% glass-fibre reinforced PBT matrix. Strength prediction in the case of the unreinforced polymer has been found satisfactory, proving the capabilities of the model estimating the healing between polymer interfaces. However, large deviations in the strength prediction for the reinforced matrix have been found. Those divergences are probably due to the reduced accuracy of the predicted fibre-orientation at the weld line zone.

1 INTRODUCTION

Injection moulding is one of the most widespread techniques for forming thermoplastic parts at industrial scale. Weld lines constitute one of the main concerns of such transforming process in terms of mechanical performance of the final part. In brief, weld lines are entities formed when two melt flow fronts collide inside a mould cavity. Multiple injection points or complex geometries where flow is split in several melt fronts are causes for the formation of weld lines and are, practically, unavoidable in the framework of the current design of engineering plastic parts [1, 2, 3].

Given the rapid cooling rates imposed during an injection moulding cycle, complete healing between the encountered melt fronts cannot be guaranteed. In addition, weld line formation is normally accompanied by a flow-induced molecular orientation of the polymer chains parallel to the weld line interface that makes more difficult the chain interpenetration [4]. According to Hagerman, weakness of weld lines in unreinforced amorphous polymer parts can be attributed essentially to three factors: 1) incomplete bonding at the weld line interface, 2) the preferential molecular orientation at the interface caused by the fountain flow and 3) the apparition of V-notches around the weld-line because of air entrapment, for example [5]. Using local flow simulation, Nguyen concluded that one of the main sources of weld line weakness is the V-notch, as result of, on the one hand, the poor bonding between polymer interfaces in the zones close to the mould and, on the other hand, the molecular orientation parallel to the weld line that enhances the shrinkage near to the wall [6].

In the case of semi-crystalline polymers, the morphological crystalline distribution along the weld line interface is supposed also to play a decisive role on the weld line strength. In addition, special crystallisation phenomena induced by the particular flow phenomena at the weld line should be taken into consideration. On another note, when injection moulding fibre-reinforced thermoplastics, the flow phenomena during the weld line formation usually induce a microstructure where fibres appear preferentially oriented parallel to the weld line interface. Such microstructures, as flower and volcano-like patterns, are clearly a disadvantage in terms of mechanical performance at the location of the weld line [7]. In consequence, mechanical properties at the weld line interface are mainly dependent on the healing quality and the molecular orientation state at the polymer-polymer interface.

The impact of weld lines on the mechanical performance of injected plastic parts has been extensively studied in literature. Tensile strength, fracture energy and fracture toughness of injected parts with unreinforced polymers are all substantially reduced in presence of a weld line [8]. In addition, the reduction of the aforementioned mechanical properties is more drastic when dealing with short-glass-fibre reinforced specimens [9, 10, 11].

There are two main types of weld lines: stagnating ones and flowing ones. In the first case, once the melt flows are encountered the velocity field at the melt front drops sharply and the weld line interface appears static in the reference system of the mould cavity. On the other hand, we deal with a flowing weld line when a weld line interface is formed but the local flow is not blocked. Then, weld line interface moves inside the cavity until stagnation of the melt flow is reached. Flowing weld line is the most common kind of weld lines founded in industrial applications.

Currently, most of the software simulating the injection moulding process offer the possibility of predicting the formation, the displacement and the final location of weld lines, but the quality of the welding is frequently given only in a qualitative scale. Nevertheless, several attempts for modelling quantitatively the healing of a weld line interface can be found in literature. The free-energy-driven inter-diffusion of polymer chains and the induced molecular orientation at the weld line interface have been usually modelled independently in order to predict the weld line strength [4, 12]. In addition to the classical diffusion models, polymer reptation can be also mentioned among the approaches employed for describing the bridging of polymer interfaces at the weld line [13, 14]. Healing process between two polymer interfaces is basically a temperature-driven phenomenon; hence modelling of the healing is strongly dependent on the thermal history at the weld line interface. Some other modelling approaches are more focused on the flow behaviour at the advancing front in order to take into account the molecular orientation factor [15, 16].

The aim of this work was, on the one hand, to implement a physical model describing the local healing between polymer interfaces, using as input parameters the thermomechanical history of a weld line interface obtained from an injection-moulding simulation carried out with commercial software. On the other hand, the objective was to establish an integrative simulation chain -from process to structural simulation- in order to predict, for example, the maximal strength of an injected thermoplastic part containing weld lines when submitted to a quasi-static loading. Validation of the simulation approach was made in front of the results of experimental tensile tests.

2 MATERIALS AND METHODS

Two commercial engineering polymers were employed in the study: an unreinforced acrylonitrile-butadiene-styrene copolymer (ABS) and a 30 wt% glass-fibre reinforced polybutylene terephthalate (PBT-GF30). Tensile bar specimens with different thicknesses (1.5 mm and 3.0 mm) were injection moulded using one or two in-gates at the extremes of the specimens. In the first case, a specimen without weld line was obtained. In the other case, a specimen with a frontal weld line (stagnating weld line) in the middle of the bar was produced. Different processing parameters (mould and melt temperature) were used to induce different healing qualities at the weld line interface. In the case of the amorphous polymer, the mould temperature was varied between 40 °C and 80 °C, whereas the melt temperature at nozzle was set between 250 °C and 280 °C. For the reinforced semi-crystalline polymer, the mould temperature was varied from 60 °C to 100 °C, whereas the melt temperature at nozzle was fixed at 265 °C. Tensile tests at 1 mm/min (with a 10 mm extensometer placed on the middle of the bar) were performed on the injection moulded specimens in order to characterize the tensile mechanical properties of the materials with and without frontal weld lines. Injection moulding and tensile testing were carried out at the PIMM laboratory (Arts et Métiers ParisTech, Paris, France).

3 SIMULATION TECHNIQUE

3.1 Modelling of the matrix healing at the weld line

In order to model the inter-diffusion of polymer chains at the interface of a weld line we employ the reptation theory, which describes the dynamics of a linear polymer chain (entangled regime) in the melt state. This theory was first stated by De Gennes [17] and, afterwards, enriched by Doi and Edwards [18, 19]. According to the theory, a single polymer molecule in the melt state that is entangled in the middle of other polymer chains can be modelled as a chain embedded inside a tube. The form and the dimensions of that tube would reflect the density of entanglements in the polymer melt. The diffusion of the polymer chain can only occur along the tube, moving forward and backwards. Therefore, the macromolecule is allowed to adopt other configurations only at the extremes of the tube. The time that a given polymer chain requires to escape totally from a tube and adopt a totally new configuration is defined as the reptation time. Reptation time can also be interpreted as the time required by a polymer chain to self-diffuse a distance equal to one radius of gyration.

One of the strengths of the reptation theory is the identification of a clear relationship between the phenomena at the microscopic scale (polymer chain diffusion) and the thermo-mechanical behaviour at the macroscopic scale (rheological properties of the polymer melt). According to the theory, the reptation time or the characteristic time required by a polymer chain for reaching a new topological configuration can be estimated from the spectra of terminal relaxation times identified by rheological characterization of the polymer melt. The crux of the matter lies on the methodology for quantifying such characteristic times based on experimental rheological data. More detailed information about the different approaches for identifying the reptation time from rheological data can be found elsewhere [13, 14].

In this work, reptation time is supposed to be associated with the shear rate at which the melt starts exhibiting rheo-thinning behaviour. In practice, the aforementioned characteristic time can be calculated using the classical models describing the shear-thinning behaviour of a Cross-fluid in function of the shear rate (Cross model). Reptation time is therefore estimated as the longest relaxation time of an ideal Cross fluid, as given in the next equation:

$$t_R \approx \frac{\eta_0}{\tau^*} \tag{1}$$

where t_R is the reptation time, τ^* is a critical shear stress (characteristic for each polymer) and η_0 is the Newtonian shear viscosity. The Newtonian shear viscosity of the polymer melt can be also modelled in function of the temperature and the pressure following a WLF model or an Arrhenius model. In consequence, the reptation time estimated with equation (1) is, at the same time, dependent on temperature and pressure.

The previous quantitative estimation of the reptation time is clearly a simplification approach because, on the one hand, it is constrained by the mathematical structure of the Cross-fluid model and, on the other hand, it averages the actual spectra of relaxation times found in a commercial polymer matrix, where the molecular weight distribution is generally not mono-disperse.

By supposing that the polymer chain diffusion at the weld line interface is driven by reptation, it can be stated that the weld line interface disappears (i.e. the polymer configuration distribution at the weld line is indistinguishable from that one at the bulk melt) when the polymer chains are allowed to diffuse during one reptation time. In consequence, by over passing this critical diffusion time the mechanical behaviour of the material at the weld line interface would be the same as that one in the bulk. In that context, the local healing degree at the weld line interface can be then quantified as the ratio between the physical and the reptation time, integrated for a given local thermo-mechanical history at the weld line interface. Mathematically, the local healing degree of the polymer matrix would read as follows:

$$Q = \int_{t_0}^{t_f} \frac{dt}{t_R(T,P)} \tag{2}$$

where Q is the local healing degree (that can goes from 0 until ∞), t_0 is the time when the first local contact between melt fronts is established during the weld line formation and t_f corresponds to the time when the local temperature falls down to a level in which reptation can be neglected. Reptation is strongly hindered below glass transition temperature for an amorphous matrix and below crystallisation temperature for a semi-crystalline polymer.

In the framework of the present modelling approach, the thermo-mechanical history at the weld line interface was obtained using commercial software simulating the injection moulding process. In this case, the required analysis sequence for the injection-moulding simulation was the following: filling, packing, in-mould cooling and out-of-mould cooling. For the sake of simplicity, t_0 in equation (2) was fixed at the time of end of filling, independently of the position of the weld line. Previous hypothesis is supported by the fact that the time for filling the cavity is very short in comparison with the time required to cool down the part below the glass transition or the crystallisation temperature. In this modelling approach, the spatial resolution of the local healing degree at the weld line depends on the mesh density employed in the injection moulding simulation.

3.2 Finite-Elements structural simulation

In this study, the structural simulation was intended to mimic the experimental tensile testing carried out on the injection-moulded specimens with and without weld line. The Abaqus®/Implicit code was selected in this work to perform the simulations of the tensile tests. The tensile test was simulated in the framework of a quasi-static loading, i.e. the rate of loading was not considered in the simulation. Fundamentally, we applied to two different simulation techniques depending on the existence or not of glass-fibre reinforcement. In addition, for each kind of material, two different structural simulations were performed: tensile test on a specimen without weld line (reference case) and tensile test on a specimen with weld line.

3.2.1 Unreinforced ABS material

The mechanical response of the amorphous polymer matrix was simulated using an isotropic elasto-plastic model with isotropic hardening. The yield stress was identified from the true tensile stress - logarithmic strain curve at the off-set yield strength at 0.05 % of deformation (as approximation of the onset of the non-linear stress-strain behaviour). Using this criterion, yield stress for the ABS material was set equal to 26 MPa.

In order to consider the weld line on the structural simulation, the local healing degree Q of the elements (process-simulation mesh) belonging to the weld line was calculated using the equation (2). The required local thermo-mechanical history at the weld line was obtained from a process simulation performed in Moldflow®. As result, each element marked as weld line was characterized by a local healing degree that quantifies the quality of the polymer inter-diffusion. Theoretically, a welding interface of an amorphous polymer with a mono-disperse molecular-weight distribution should completely heal by diffusing during one-reptation time. In other words, the matrix with a local healing degree equal or greater than one ($Q \geq 1$) would be indistinguishable from the bulk matrix and should exhibit the same mechanical behaviour. On the other hand, the matrix with a local healing degree lower than one ($Q < 1$) would have not reached the same density of entanglements as the bulk matrix and would exhibit a brittle behaviour. Nevertheless, we deal here with a poly-disperse molecular-weight distributed matrix and, therefore, the Q-threshold representing the complete healing of the polymer matrix could be different from one. In this work, we have employed a security factor SF for taking into account this deviation. The mechanical behaviour of the polymer matrix with a local healing degree equal or greater than the security factor ($Q \geq SF$) would be then the same of the bulk material. On the other hand, the elements with a local healing degree lower than the security factor ($Q < SF$) were mapped from the process-simulation mesh to the structural simulation-mesh and sub-modelled using an ideal elasto-plastic material law. Previous material law is clearly a simplification hypothesis. In this case, the behaviour at rupture was not taken into account and the simulation should be evaluated only in the framework of a strength-criterion design; in other words, the simulation is supposed to give an estimation of the maximal stress that the structure can load. The Young's modulus was assumed not to be affected by the presence of the weld line and the yielding stress was fixed at 26 MPa (as in the bulk material).

3.2.2 Reinforced PBT material

The mechanical behaviour of the semi-crystalline matrix was described using an isotropic elasto-plastic material law with isotropic hardening. The corresponding model parameters were identified by reverse engineering on tensile curves measured on bars cut from injection-moulded 2 mm plaques. The reverse engineering process in Digimat® was performed using the tensile data obtained from bars cut in the longitudinal, transversal and 30° (with respect to the injection) directions and the experimental 3D fibre-orientation measured on the plaque with computed tomography.

The tensile test of the specimens without weld line were simulated then using Abaqus® coupled with Digimat®CAE in order to take into account the anisotropy induced by the fibre orientation. Prediction of the fibre-orientation was obtained in Moldflow® using the in-built Folgar-Tucker orientation model with auto-calculated interaction coefficient. Simulated fibre orientation was mapped from the process-simulation to the structural-simulation mesh using Digimat®MAP.

Simulated tensile tests on the specimens containing a weld line were also performed using Abaqus® coupled with Digimat®CAE. Nevertheless, additional information was required in order to take into account the presence of the weld line. In this case, the mechanical behaviour at the weld line was simulated by considering two independent effects: healing degree of the polymer matrix and the particular fibre orientation in the surroundings of the weld line. The mechanical behaviour of the bulk polymer matrix was represented by the identified isotropic elasto-plastic model with isotropic hardening. In analogy with the simulation of the unreinforced material, the weld line elements with a local healing degree lower than the security factor ($Q < SF$) were mapped from the process-simulation to the structural-simulation mesh and sub-modelled with a penalized matrix material model (ideal elasto-plastic material law with yielding stress at 23.5 MPa). On the other hand, the fibre orientation was also obtained from the Moldflow® simulation (Folgar-Tucker model with auto-calculated interaction coefficient) and transferred, in a standard way, to the structural simulation mesh employing Digimat®MAP.

4 RESULTS AND DISCUSSION

4.1 Unreinforced ABS material

The results of the experimental tensile tests on 1.5 mm specimens (unreinforced ABS) with and without frontal weld line are presented in Figure 1. As theoretically expected, Young's modulus was not compromised by the existence of a weld line (2.9 GPa $\pm$ 0.2 GPa without weld line in front of 2.7 GPa $\pm$ 0.1 GPa with weld line), but the mechanical behaviour at rupture was strongly affected by the presence of the weld line (plastic failure without weld line in front of brittle failure with weld line).

In addition, the structural simulation results can also be observed in Figure 1. The result of the virtual tensile test on a specimen without weld line was found in agreement with the experimental data for strains lower than 3%, range in which the maximal tensile stress is found (onset of necking). As mentioned before, the structural simulations performed in this work are intended to be used in the framework of a strength-criterion design.

In the simulation workflow for specimens containing a weld line, three main factors affecting the final results can be clearly identified: the geometry of the weld line predicted by the process simulation, the security factor SF defining the threshold value of the local healing degree Q and the material model of the penalized weld line elements in the structural simulation. In terms of prediction of the weld line geometry, the capabilities of the process simulation software are limited. In Moldflow®, for example, the predicted location of the weld line is restricted to the outer-surface of the plastic part, i.e. no

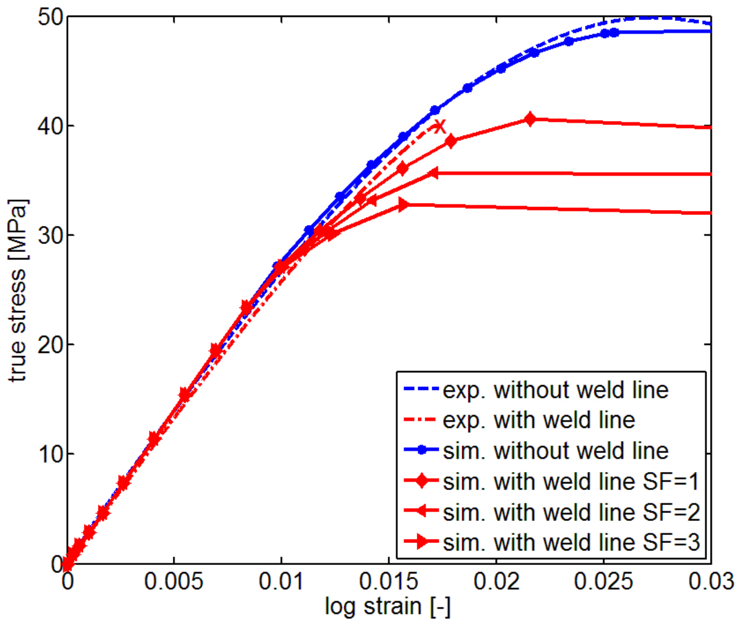

Figure 1: Experimental and simulation results of a tensile test on a 1.5 mm specimen injected with an amorphous polymer (with and without frontal weld line)

information about the weld line position through the thickness is given. As the position and form of the weld line could be easily predicted in this study, the weld line was supposed to be formed at the mid-plane of the tensile bar and the local healing degree Q was calculated for all the elements cut by such cross section.

The material model for the penalized weld line elements is obviously a factor playing a role on the structural simulation results. Here, nevertheless, the matrix material model for the penalized matrix elements was defined in a physical basis in order to keep it constant and reduce the degrees of freedom of the simulation. By defining the maximal stress of the penalized elements (yield stress in the elasto-plastic material law without hardening) at the same stress-level from which a true stress - log strain tensile curve starts exhibiting a non-linear behaviour, we intended to mimic the maximal strength of a poorly healed weld line interface. In fact, we assumed that the maximal strength of a poorly healed weld line interface (i.e. polymer matrix with a lower density of entanglements than the one in the bulk matrix) cannot be greater than the critical stress which triggers the localized plasticity phenomena in the bulk matrix. In front of the previous statement, we additionally supposed that the onset of the macroscopic non-linearity in the true stress - log strain tensile curve is associated with the development of localized plasticity phenomena (microscopic shear plastic bands, for example).

In such framework, the factors influencing the structural simulation of specimens containing a weld line were simply reduced to the security factor SF. As mentioned before, the security factor SF is intended to correct the deviation between the estimated mean reptation time and the spectrum of reptation times that is particular to a polymer with a multi-disperse molecular-weight distribution. For that reason, the simulation results of the tensile test on specimens with weld line in Figure 1 are given for three different values of security factor SF. It was found that the actual maximal strength of the specimen with weld line (39.7 MPa $\pm$ 0.9 MPa) can be predicted by using a security factor SF between 1 and 2, where $SF = 1$ gives the most accurate prediction (40.6 MPa). This result means either that the mean reptation time estimated with equation (1) describes correctly the global polymer dynamics of the ABS (with a given spectrum of reptation times) or that the poly-dispersity of the amorphous polymer is close to one.

4.2 Reinforced PBT material

The experimental tensile tests on 3.0 mm specimens (PBT-GF30) with and without frontal weld line are presented in Figure 2. Reinforced specimens exhibited a brittle behaviour independent of the presence or not of a weld line. Nevertheless, the frontal weld line had a dramatic effect on the Young's modulus and the maximal strength of the specimen. In terms of rigidity, Young's modulus was reduced in 46% by the presence of the weld line, falling down from 9.1 GPa $\pm$ 0.1 GPa to 4.9 GPa $\pm$ 0.1 GPa. Given the fact that the elastic response of the matrix at the weld line interface should not be substantially compromised (a slight change of matrix rigidity could occur by a modification of the crystalline content and microstructure); the radical diminution in Young's modulus should be related to a severe change in glass fibre orientation in the zone of the weld line. On the other hand, maximal strength was decreased in approximately 55% from 113.6 MPa $\pm$ 1.5 MPa without weld line to 50.6 MPa $\pm$ 1.0 MPa with weld line. To infer the possible causes of such decrease in strength is more delicate because of the multiple phenomena involved in failure, but certainly such reduction in strength was mainly induced by the diminution in rigidity.

The result of the coupled structural simulation (Abaqus® coupled with Digimat®CAE) on the specimen without weld line is also shown in Figure 2. Here, the linear elastic response was correctly described, i.e. for strains lower than 0.7%. This fact probably indicates that the fibre orientation predicted by Moldflow® was in agreement with the reality, at least in terms of averaged orientation in the cross-section of the specimen. Simulated non-linear stress-strain response was, however, slightly underestimated. In the range of strains lower than 3% (classical limit-deformation for this kind of reinforced compounds), the simulated strength was approximately 5% smaller than the experimental maximal strength. We should recall that the structural simulations in this study are intended to be used in the framework of strength-criterion design. Failure behaviour is not simulated here.

In the case of the specimen containing a frontal weld line, the mechanical response at the weld line was simulated by considering two independent effects: on the one hand, healing degree of the polymer matrix and, on the other hand, the induced fibre orientation

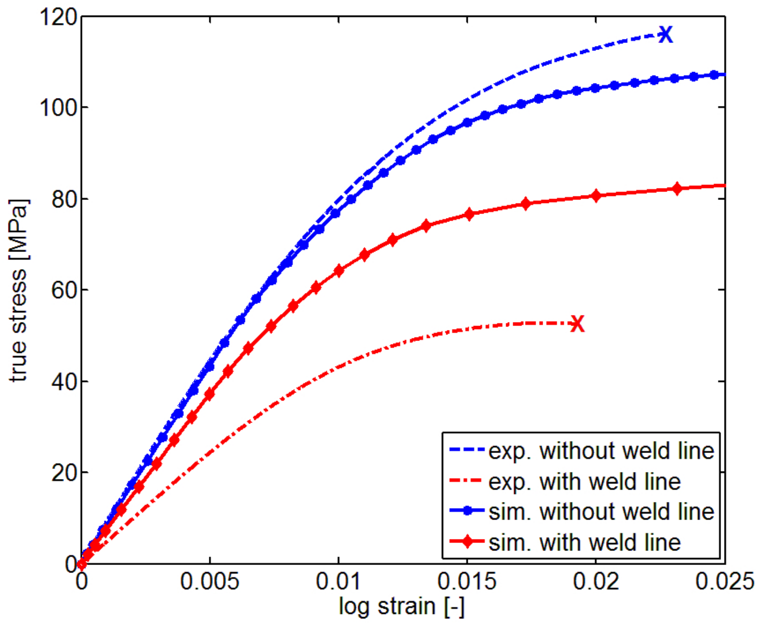

Figure 2: Experimental and simulation results of a tensile test on a 3.0 mm specimen injected with a glass fibre reinforced semi-crystalline polymer (with and without frontal weld line)

in the weld line zone. As in the simulation case of the unreinforced ABS, the weld line was supposed to be located at the mid-plane of the tensile bar. Estimation of the local healing degree Q for the elements cut by such cross-section brought that no element was critical in terms of matrix healing, even when considering a security factor $SF = 4$. This means that the semi-crystalline polymer matrix under the current injection-moulding conditions had enough time to diffuse and vanish away the polymer-polymer interface in all points of the weld line cross-section. Previous result is in agreement with the viscosity data of the neat PBT matrix that exhibits, for example, a terminal relaxation time of about 1.7 ms at 240 °C. In consequence, the simulated mechanical response at the weld line was only dependent on the predicted glass-fibre orientation. However, the rigidity obtained from the coupled structural simulation (Abaqus® coupled with Digimat®CAE) on the specimen with weld line was approximately 55% overestimated in comparison with the measured value. At the same time, predicted maximal strength was overestimated in about 65%. Such excessive deviations are certainly a proof of the inaccuracy of the standard fibre-orientation models implemented in the process-simulation software for predicting the induced fibre-orientation when two melt fronts collide inside the mould. In consequence, a better prediction of the mechanical strength of weld lines formed with fibre-reinforced materials is strongly dependent of an improvement of the fibre-orientation models, which should take into account, for example, the viscoelastic effects during the melt fronts collision.

5 CONCLUSIONS

Quality of the polymer healing at the weld line interface has been modelled based on the reptation theory, which describes the inter-diffusion of macromolecules. An estimation of the local healing degree can be calculated then from the thermo-mechanical history of the polymer matrix in a given point of the weld line. The strength contribution of the polymer matrix in the macroscopic mechanical response of a weld line has been simulated by defining that the maximal strength of a poorly healed polymer interface is equal to the critical stress triggering the localized plastic phenomena in the bulk matrix (estimated as the onset of the non-linear behaviour of a macroscopic true stress - log strain tensile curve). In the case of the unreinforced ABS, the threshold of local healing degree which establishes the passage from a poorly healed to a completely healed interface (bulk polymer matrix) has been found close to 1 (theoretical value according to the reptation theory). For a reinforced matrix, the mechanical response of a weld line not only depends on the polymer matrix, but also on the fibre orientation. In the particular case of the 30 wt% glass-fibre reinforced PBT matrix, strength contribution of the semi-crystalline polymer has been found no compromised by an eventual incomplete healing at the weld line interface, i.e. polymer matrix has been modelled as bulk material even at the weld line interface. In consequence, the simulated mechanical response of the weld line was exclusively dependent on the predicted fibre-orientation. The excessive deviation found between the measured and simulated strength of the weld line would reveal an inaccurate prediction of the fibre-orientation in the vicinity of the weld line. Such inaccuracy could be explained by the fact that the standard fibre-orientation models do not consider the additional flow phenomena occurring during the collision of melts fronts (e.g. viscoelastic contribution).

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