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Simulation Methodology Accounting for Process Induced Morphology in Short Fiber Reinforced Polymer Matrix Composites

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Abstract **-** Short fiber reinforced plastics (SFRP) are a type of polymer matrix composites processed usually through injection or compression molding technologies, processes that both typically induce important local material morphology variations in the molded component, especially for fiber orientation and length distributions. Designing properly with this type of materials thus requires taking into account these morphology variations, since they determine the final local material thermo-mechanical properties.

In this contribution, a simulation methodology aiming to support mechanical design of injected components made of SFRP is summarized. The proposed methodology consists of a set of integrated experimental and numerical steps covering the material characterization, micromechanical modeling, manufacturing process simulation and component functional behavior analysis.

Most part of the experimental effort is focused on the research of the resulting material morphology after the transformation by injection molding. The main aspect considered is the variation of the fiber orientation and their aspect ratio, which together with the intrinsic nature of the polymeric matrix result in highly anisotropic and non linear stress-strain behavior.

A simulation workflow is shown addressing the prediction of the fiber orientation during the injection molding process and then linking this information with the structural calculation codes through micromechanical mean field homogenization routines, where the parameters of the different models are adjusted from the experimental characterization data through reverse engineering approaches.

Keywords**:** Short Fiber Reinforced Plastics, Process Simulation, Micromechanics.

1. Introduction

Short fiber reinforced thermoplastics benefit from the flexibility and high production rate of the thermoplastic injection molding technologies, although the reinforcing capability of the fibers is affected by the length reduction and orientation that are produced during the injection process. A well known effect is that fibers tend to orient in preferential directions as the melt polymer flows through the feeding channels and fills the cavity of the mould, depending this orientation on the nature of the flow. Shear flows, produced between the solidifying layers in the mould walls and the still flowing molten core, create fiber alignment in the flow direction. On the other hand, orientation tendency in the flowing molten core is different if the flow is convergent, fibers tend to orient in flow direction, or divergent, fibers try to align perpendicular to flow direction. The final result is that every point in the part has different orientation and hence mechanical properties, having little opportunity to control this orientation once the geometry of the part and the position of the injection points have been fixed, since both mostly determine the flow characteristics in the mould.

In order to properly design components made on SFRP it is necessary to account for the process induced morphology variations early in the design stage, so simulation methodologies combining injection process simulations with structural functional analysis are required. In this contribution a numerical-experimental methodology is presented, using cost effective approaches, suitable to be used in engineering applications.

2. Outline of the Methodology

The proposed methodology, represented in Fig.1, starts describing the necessary experimental and numerical characterization activities required to adjust different material models used in the injection process simulation and in the structural analysis. A set of morphological and mechanical characterization tests provide experimental data to be used in a reverse engineering optimization of selected model parameters.

The relevant information from this previous step is a set of material parameters, including orientation model, elastic and failure parameters for the material being studied. Once these parameters have been determined, the same simulation procedure can be applied at the engineering scale to analyze the component under study.

The product simulation workflow is split in two steps. First, the injection molding simulation of the component. It is worth to mention that injection molding simulation can help in designing the mould and process conditions to inject correctly the component, although in this contribution we only pay attention to its use for the prediction of the fiber orientation tensor, required as input for the homogenization routines.

The second step is to perform the finite element simulation to analyze the functional behavior of the component, accounting for the relevant information from the process, as introduced previously.

A final validation step is always necessary, in order to assess the models accuracy, and of course as part of the engineering development process before launching the production process.

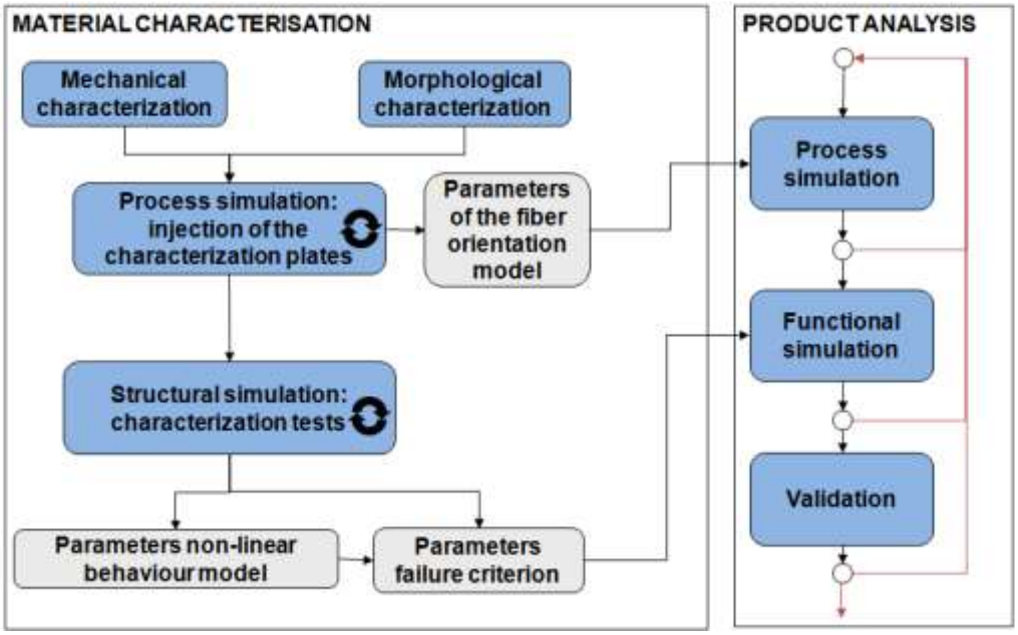

Fig. 1: Simulation methodology.

3. Material Characterization

The objective of the material characterization step is to obtain the required representative experimental data for the subsequent adjustment of the numerical models, both, for the simulation of the injection process and in the functional analysis.

3.1. Mechanical Characterization

Typically, samples are available from the material supplier in the form of injected plates or dumbbells, processed under optimal process conditions. For a complete characterization, specimens with different orientation levels are required. Using just injected dumbbells is not enough because only provide information of the material with high alignment level; extracting specimens from injected plates allow a more diverse orientation states. The plates must have adequate dimensions to allow machining standard specimens to be tested under representative deformation models: tension, compression and shear. As a minimum, here it is suggested to perform at least uniaxial tension and flexural tests under ISO-527 and ISO-178 standards respectively.

In order to obtain the maximum range of variation of the mechanical properties, specimens must be machined in several positions and orientations with regard to the flow direction. Typically 0º, 90º and at least an intermediate angle are selected.

These directions in combination with the fiber orientation distribution existing on the plate, will allow to have different combinations of normal and shear stresses in the material, especially relevant if shear tests are not performed.

In Fig 2 we can observe the important stiffness and strength variation of a PET+36%GF SFRP as a function of the position and orientation the specimen has been machined in the plate.

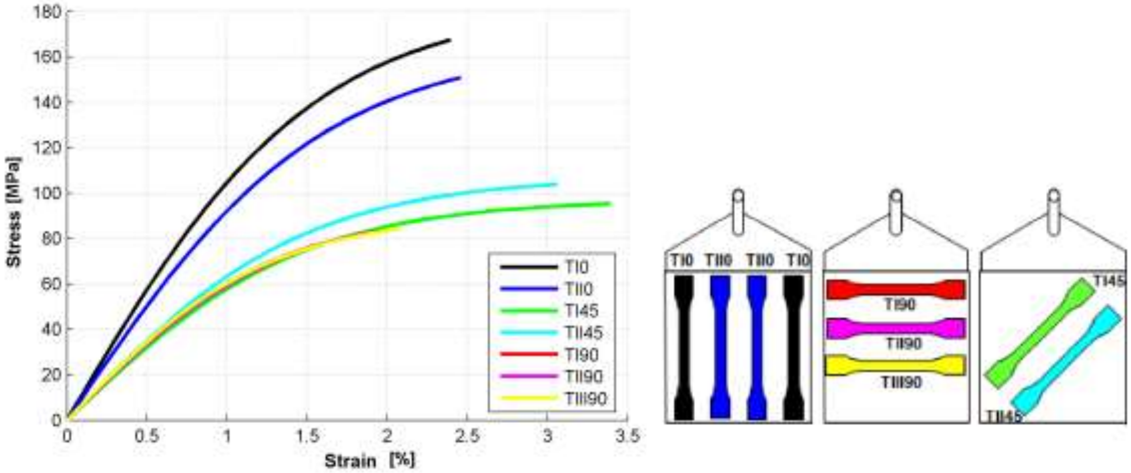

Fig. 2: Uniaxial tension tests.

3.2. Morphological Characterization

Differences in mechanical properties are caused by changes in the material morphology. In order to relate both of them, the microstructure of the material must be analyzed. The fiber orientation must be measured at least in the central positions of the selected specimens for mechanical testing. Several techniques are available, among them a section analysis is selected in this work, using just one inclined section with regard to the thickness direction of the plates, as proposed by Mlekusch [1].

The procedure requires extract a piece of material and its encapsulation in resin for the materialographic preparation, consisting on progressive rough to fine polishing and posterior ultrasound cleaning. Then the sample is inspected in a SEM microscope, allowing having good contrast for glass fibers in polymeric matrix materials. The obtained images are then treated by means of a image treatment software (IMAGEJ) in order to determine the parameters of each cut fiber, represented by an ellipse (see Fig.3). Although the treatment process has some tools for the counting and fitting ellipse parameters, the user intervention to separate close fibers and eliminate partial ellipses is necessary to some extent (see Fig.4).

Other relevant microstructural aspect to be considered is the fiber length distribution. In particular, the reinforcement capacity of the fibers depends on their length/diameter ratio. The diameter distribution is extracted from the orientation analysis since the minimum axis of the ellipse actually is the fiber diameter. For the fiber length distribution, it is common to isolate the fibers from the material by burning or digesting in acid the polymer matrix. Once this is done the fiber residue is weighed to determine the fiber content and carefully dispersed to be observed in an optical microscope. With the aid of image treatment software the length of each fiber in the photograph is measured and a statistical representation is used. Typically diameter distribution fits well in a normal distribution whereas the length fits properly to a log-normal distribution.

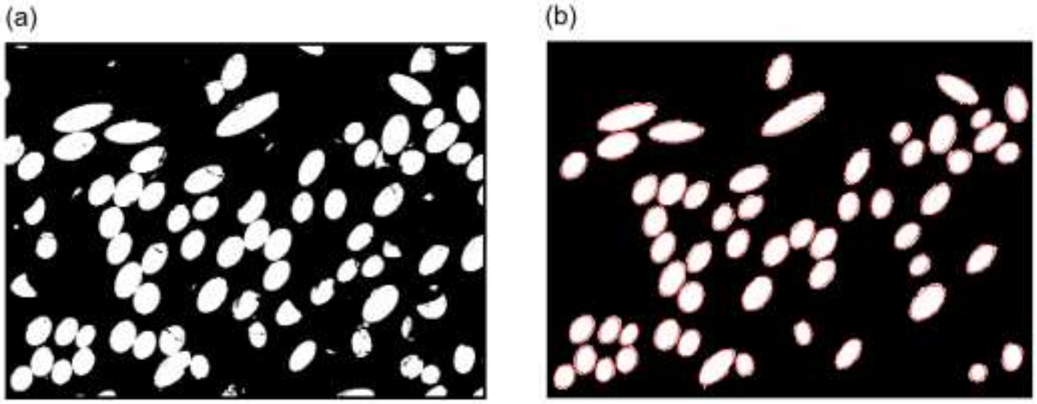

Fig. 3: Image treatment of sections. (a) initial SEM image, (b) treated image.

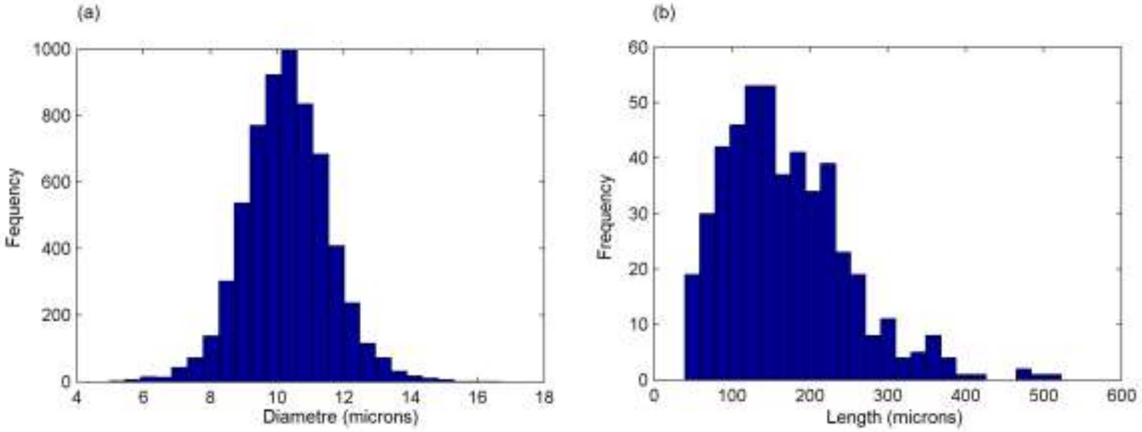

Fig. 4: Diameter distribution (a) and length distribution (b).

4. Process Simulation

This section consists of applying injection simulation tools to predict relevant morphological aspects produced during the process, such as fiber orientation, fiber breakage and concentration. Among them the most relevant when dealing with short fiber reinforced plastics is the fiber orientation.

Based on the original work of Jeffery about hydrodynamics of ellipsoidal rigid particles in dilute suspensions, Folgar and Tucker [2] developed an orientation model applicable to short fiber concentrated suspensions, incorporating an isotropic rotary diffusion term to account for the fiber interactions. Advani and Tucker [3] expressed this model in the form of the evolution equation for the second-order orientation tensor that together with a closure approximation for the fourth-order orientation tensor, is the form still today incorporated in most commercially available injection simulation software. Further improvements of this model were introduced by Tucker et al.[4] through the concept of reduced principal rate, that retards the orientation dynamics to correct the observed mismatch between numerical predictions and experimental measurements when the flow length is significant. The latest evolutions incorporated the concept of anisotropic rotary diffusion (ARD) from Phelps and Tucker [4], specially developed to improve predictions for long fiber reinforced plastics. This model is currently incorporated in the software Moldflow and requires the specification of 5 parameters. Tseng et al. [5] improved the ARD model reducing the number of parameters to 3 being incorporated in the Moldex3D software.

Common industrial practice is to use the default values for the parameters considered by the injection simulation programs, usually giving acceptable results. But having performed orientation measurements, in this methodology is proposed to perform an optimization of these parameters for the material being considered. Fig.5 shows a comparison of predicted and experimental orientation tensors after optimization of the interaction coefficient of the Folgar Tucker model.

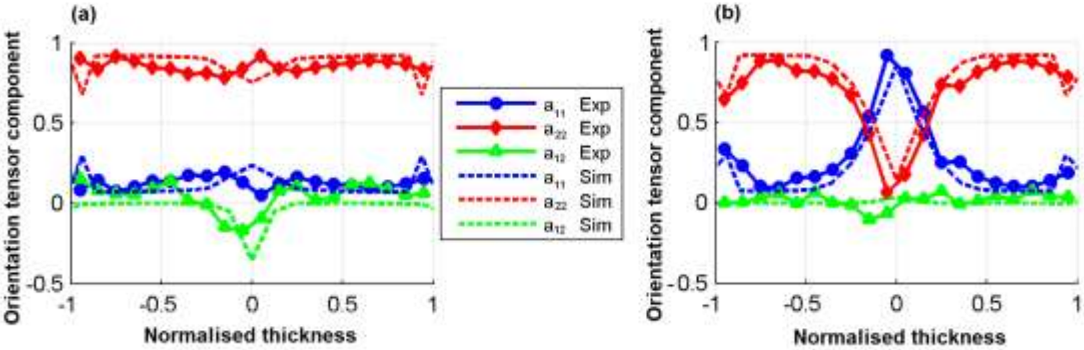

Fig. 5: Correlation orientation tensor, (a) lateral point, (b) central point.

5. Structural Simulation

To estimate resulting thermomechanical properties from the fiber orientation predictions, a micromechanical homogenization procedure is required. Among the existing approaches, the only ones nowadays computationally admissible for industrial application are the ones based on the mean field homogenization approach, which formulates the constitutive material relations for the constituents (fibers and matrix) from the phase averaged stress and strain micro fields. In the field of short fiber reinforced plastics, probably the most extended model was the formulated by Mori-Tanaka [6], that estimate the properties of a fully aligned composite of fibers of a given aspect ratio, from the properties of the constituents and the respective volume fractions. The consideration of the fiber orientation and fiber length distribution is typically introduced by a Voigt second homogenization step. In case of fully elastic constituents and perfect bonding, this mathematical scheme provides an exact solution of the homogenization problem. For the consideration of non linear plastic behavior, usually the former scheme is formulated in an incremental framework, in terms of strain and stress rates, using consistent tangent stiffness tensors [7-8].

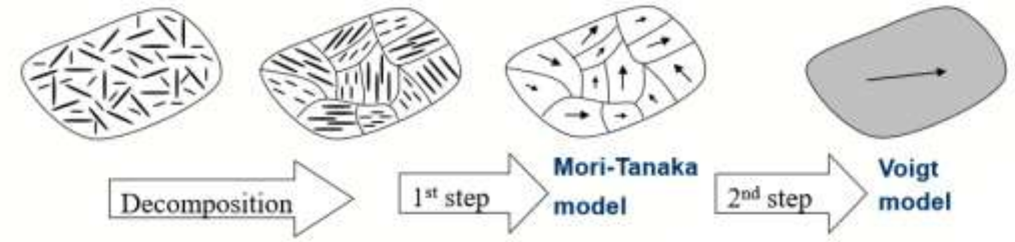

Fig. 6: Two steps homogenization scheme.

The structural material model is completed by a failure indicator. For SFRP the most commonly used are quadratic failure criteria (Hill type) in the stress or strain states, applied at composite level, whose strength coefficients are dependent on the local fiber orientation states through specific averaging procedures [9].

The approach followed in this work is to implement a reverse engineering simulation work flow, where finite element simulations of the performed mechanical characterization tests, fed with the predicted fiber orientations and measured length distributions, and using as material constitutive model the aforementioned 2 steps homogenization scheme, are performed to estimate the stress-strain composite overall behavior. The differences with the experimental stress-strain curves and ultimate stress or strains values are minimized in a least squares sense through the optimization of the parameters of the matrix constitutive model and the unidirectional composite failure parameters. This optimization process is represented in Fig.7.The obtained results for the PET+36%GF SFRP shows average errors of around 7% in modulus and ultimate strength, being the maximum error below 20% (see Fig.8).

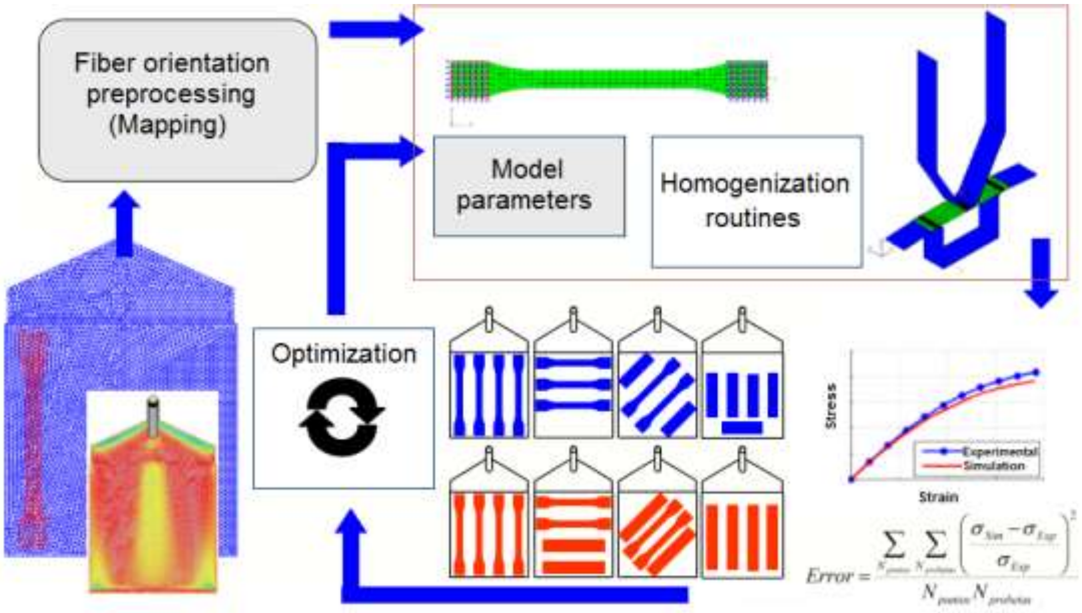

Fig. 7: Constitutive model and failure criterion adjustment.

Although in this work all the micromechanical homogenization routines for the non linear elasticity and failure have been in-house developed, commercial solutions like DIGIMAT provides a powerful interface between different injection simulation software and structural codes, having available a wide range of constitutive models, including plasticity, viscoelasticity and fatigue.

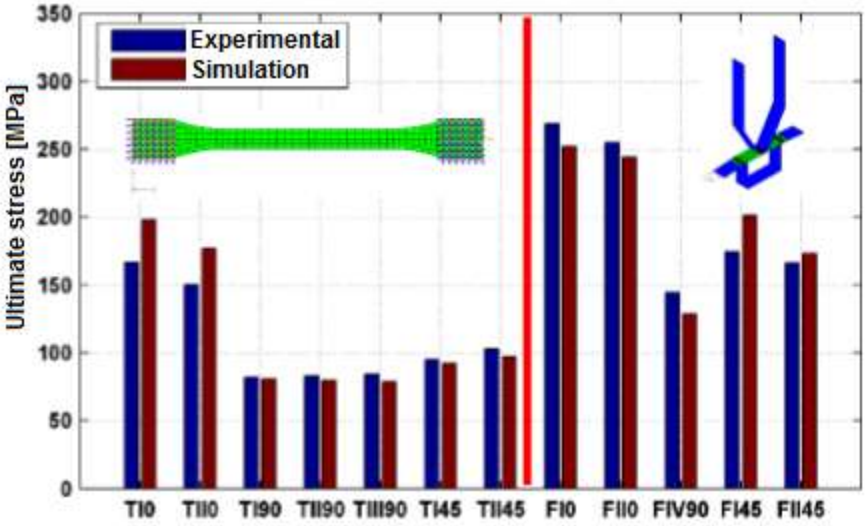

Fig. 8: Numerical-experimental correlation. Specimens ultimate stress.

6. Methodology Application

Having completed the material characterization, the simulation tools are ready to be applied to help the design process of the component to fulfill the required specifications. A validation of the proposed methodology is performed on a component of high responsibility, a valve of an automotive brake booster. With the fitted model the injection process is simulated and the orientation tensors predicted. It should be mentioned that a good practice when working repeatedly with the same material on similar components is to measure orientation on some of these components and re-optimize the orientation model parameters.

The FEM simulation reproducing the function of the component is performed, where every iteration at each integration point call the homogenization routines to update the stress state. The failure indicator informs about the material integrity, being informative, that is, no post failure material properties degradation or element removal is included.

In this example, a validation test was performed and the simulation results correlated with the experiments in terms of force-deflection and strength, showing differences below 10%.

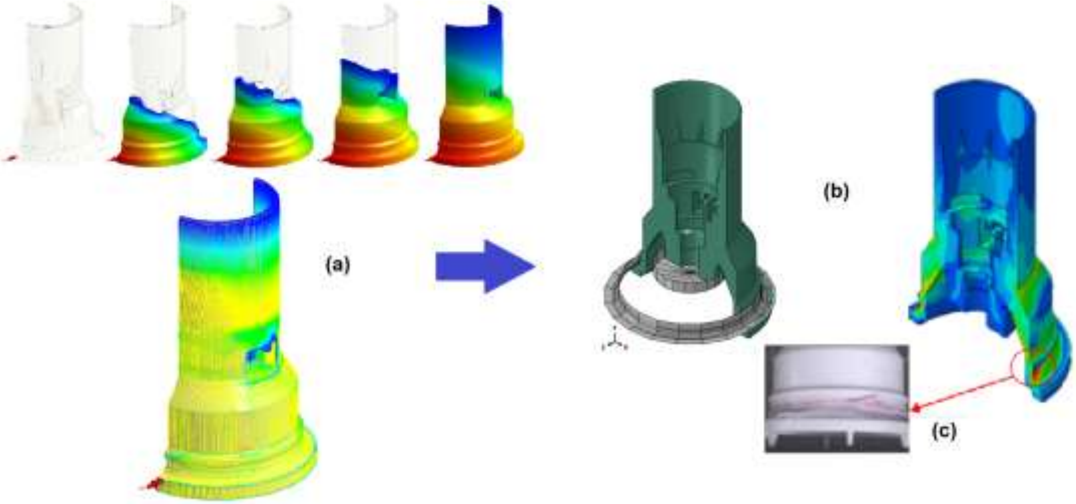

Fig. 9: Application to industrial component: (a) process simulation, (b) functional simulation and (c) validation.

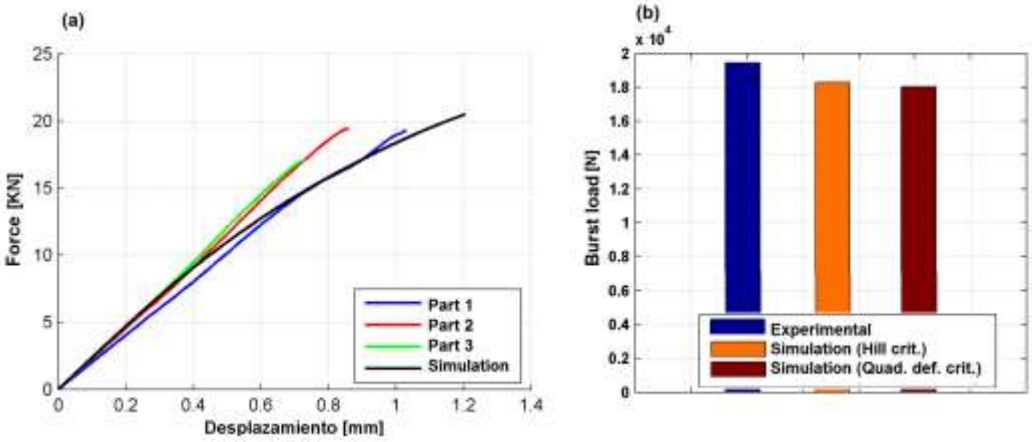

Fig. 10: Numerical-experimental correlation.

7. Conclusions

- The applied methodology allows a better estimation, on the design step, of the resulting mechanical properties after the manufacturing process, allowing a more realistic approach against other basic approaches that neglect morphology variations assuming isotropic and homogeneous material models.
- Supports the idea that injection molding and structural simulations must be sequentially coupled in the design loop, since not only part geometry conditions mould design and process feasibility, but at the same time, injection process strongly affects part performance.

- Early adopters, especially in the automotive sector, are using similar methodologies in their engineering departments, thanks to the emergence on the market of commercial codes (like DIGIMAT) for linking injection and structural simulation codes. However the massive extension is still far from been produced.

Acknowledgments

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