Through-Process Modelling for Accurate Prediction of Long Term Anisotropic Mechanics in Fibre Reinforced Thermoplastics.

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Abstract. Fibre reinforced thermoplastic (F RTP) materials offer great potential for, among others, weight and cost reduction in a wide range of applications. In this paper, consequences of fiber orientation-induced anisotropy (due to injection molding process) in the development of F RTP parts as well as predictive engineering techniques for part performance evaluation are discussed. A coupled simulation methodology will be used to predict the processing-microstructure-properties relation in F RTP parts, thereby enabling the ability to include fiber orientation-induced anisotropy. In parallel, long term fatigue data was collected on increasingly complex geometries for the purpose of model validation.

1 Introduction

Due to the many advantages of low density, high stiffness and freedom to design geometrically complicated parts, F RTP materials are increasingly replacing metals in a wide range of industrial applications. For instance, metal replacement has accelerated in the automotive industry due to the need for weight reduction to increase fuel efficiency. In water management applications (distribution, measurement, treatment and storage equipment), replacing metals is an approach to meet low-lead regulations, remove system cost and overcome corrosion challenges.

The main process for the production of F RTP parts is injection molding, which gives the engineer freedom to design geometrically complicated multi-functional ribbed parts, needed for robust design, as can be seen in Figure 1.

However, the injection molding process imposes additional complexities to the design and performance of F RTP components by introducing complex glass fiber length and orientation variations in the parts. These variations consequently represent themselves in the form of anisotropic shrinkage during cooling, referred to as warpage, or anisotropic mechanical performance, which might lead to over or under-design in the finished part [1].

One of the important aspects of polymers, either reinforced or non-reinforced, in load-bearing applications is that they display time-dependent response and, ultimately, if not considered in design might lead to failure. It is not the question of whether failure will occur, but rather on what time scale. The assessment of the long-term performance of polymeric products is therefore of the utmost importance. For F RTP components, which are designed for long-term strength, the fiber orientation-induced anisotropy must be taken

into account during the development of such parts, since the long-term response and lifetime of the parts can vary depending on the orientation [2].

With the increasing use of F RTP materials in various applications, virtual product development is also growing extensively, as it is an important drive to reduce time-to-market while minimizing (ideally eliminating) physical prototyping. Simulation of the performance of the final product is one of the key components of the virtual product development. Increasing the accuracy of the simulations requires more detailed modeling, such as the incorporation of the fiber orientation-induced anisotropy variable.

Quantitative prediction of fiber orientation-induced anisotropy and utilization of anisotropy in the design process has been a significant challenge for adoption in the water management industry. In this article, a through-process modeling approach for short- and long-term performance evaluation of F RTP parts is discussed. This approach enables establishing a processing-morphology-property relation and taking into account the effect of anisotropy on the performance. Several predictive engineering techniques, including utilization of both isotropic and anisotropic material properties, are also evaluated.

Fig. 1. A complex injection molded thermoplastic flow block (left) and a hydroblock, assembled with a heat exchanger

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(right), made of NORYL™ resin (short glass fiber reinforced PPO™/PS).

2 Experimental

The material used in this study is a 30% short glass fiber reinforced injection moldable thermoplastic supplied by SABIC (NORYL™ resin, a PPO™/PS material), primarily used in water management applications (Hydro-block, water meter, faucet, etc) due to its good corrosion properties, high temperature resistance, low water absorption and good mechanical performance [3].

Figure 2 shows the geometries molded and used in this study. A so-called shear plaque was used for mechanical testing (tensile and fatigue), (micro) mechanical model creation, and to fit the models' parameters.

Fig. 2. Various geometries moulded and tested in this study.
 (Top left): shear plaque. (Top right): Pressure Vessel.
 (Bottom): Elbow pipe.

Two different geometries with increasing geometrical complexities, i.e. a pressure vessel and an elbow pipe, were also molded for various validation tests (constant internal pressure rate, constant internal pressure and fluctuating internal pressure). The results will be used later to validate the predictive engineering approaches.

2.1 Morphology characterization

Fiber orientation and length distributions were characterized to provide input for micromechanical modelling, including fiber aspect ratio and local fiber orientation distribution. A dynamic image analysis technique, developed within SABIC, was used for fiber length measurement [4]. This technique is a semi-automated approach using Camsizer particle size analyzer for fiber length analysis. It is statistically more robust and faster than the static imaging method.

Local fiber orientation distribution was measured at the location from which tensile specimens were cut. Computed tomography scanning (CT-Scan) was used to directly measure microstructure. Raw data was then analyzed to calculate components of local orientation tensors along the thickness of the test specimen [5]. The process is depicted in Figure 3-4.

Fig. 3. Left: The shear plaque and the specimen used for CT-Scan. Right: CT-scan images at the region of interest. A distinct difference can be observed in local fiber orientation distributions in the skin (marked as blue) and in the core (marked as red). Arrows indicate flow direction. Right: Diagonal components of local fiber orientation tensor, obtained by post processing of CT-scan images.

Fig. 4. Diagonal components of local fiber orientation tensor, obtained by post processing of CT-scan images.

2.2 Mechanical testing

In order to characterize the anisotropic performance of NORYL™ resin and create (micro) mechanical models, tensile specimens were cut at 0°, 45° and 90° from a fixed location of the shear plaque. Tensile (constant strain rate) and fatigue (fluctuating stress) tests were performed at various orientations, temperatures and load levels.

Fig. 5. Geometry of the injection-moulded shear plaque used for mechanical testing and microstructure characterization with location and orientation of tensile specimens.

2.4 Validation test

To evaluate various simulation methodologies, different mechanical tests have been performed on the pressure vessel and the elbow pipe, subject to internal water pressure at 90°C including:

- Constant pressure rate, representing short-term response.
- Fluctuating pressure, representing fatigue performance.

In order to record the evolution of strain under internal pressure, a 12M ARAMIS system was employed. Figure 6 shows the test setup. ARAMIS is a non-contact measuring system, which enables an optical 3D deformation analysis for statically or dynamically loaded test objects.

Fig. 6. Top: Experimental setup, utilizing ARAMIS camera system. Bottom: The strain evolution, averaged over the area of interest on the surface of the pressure vessel subject to internal constant pressure rate.

3 Predictive Engineering Approach

In this section, various modelling and simulation methodologies for performance evaluation of FRTP parts are discussed together with their advantages and drawbacks.

3.1 Isotropic approach

The use of isotropic material data for part performance prediction is still common practice in industry, especially for early stages of an application development. There is not yet a standard way on how isotropic material

properties are obtained for FRTP materials. Depending on how data is measured (directly injection-molded tensile specimen, tensile samples milled out of injection-molded plaques with various geometries and processing conditions, specimen cut from actual parts, etc.), a wide range of properties are found due to differences in fiber orientation distribution [5].

Measuring material engineering data on a directly injection-molded (DIM) tensile specimen (also referred to as Datasheet values) leads to unrealistically high stiffness and strength values due to an extremely high fiber alignment in a long narrow geometry. This approach could potentially lead to an overestimation of performance and, consequently, under-design of the part in real application [1].

To address this issue, the European Alliance for Thermoplastic Composites (EATC) has developed a methodology to convert the anisotropic mechanical properties, measured on injection molded plaques, into effective (quasi)isotropic properties. This methodology utilizes the classical laminate theory [6], as shown schematically in Figure 7. This method enables having unique isotropic material properties, independent of fiber orientation and processing conditions [5].

Fig. 7. Schematic illustration of quasi-isotropic properties generation using classical laminate theory.

Engineering datasheets of quasi-isotropic stress-strain and fatigue curves were created based on 0°, 45° and 90° stress-strain curves and fatigue curves.

3.2 Anisotropic approach

However, Using the isotropic modeling approach for FRTP materials does not fully represent actual performance, since fiber orientation-induced anisotropy is not taken into account. Micromechanically based constitutive models [7, 8] are powerful tools, which enable establishing a relation between mechanical properties of FRTP materials and their underlying morphology including being fiber volume fraction, aspect ratio and orientation. Recently, some of these models have been adapted and implemented in several commercial software, which allow their utilization in industrial applications.

A two-step mean-field homogenization procedure [9, 10] is employed here to relate the local mechanical properties of the FRTP part to its processing-dependent morphological features. In this technique, the real representative volume element (RVE) of the reinforced material is replaced with a model RVE of an aggregate of so-called pseudo grains. In each pseudo grain, fibers having similar shape and orientation are grouped together and embedded in the matrix phase. The first homogenization step estimates the properties inside each

pseudo-grain using a mean field homogenization scheme, appropriate for basic two-phase composites, e.g. Mori-Tanaka model [11]. Then, a second homogenization step averages these properties, applying fiber orientation distribution, and derives the effective response of the aggregate of homogenized pseudo-grains.

In this study, Digimat software suite is utilized to perform micromechanical modelling. Figure 8 gives the general overview of the micromechanical modelling workflow

Fig. 8. Schematic overview of Digimat workflow for creating anisotropic material models [12].

Inputs needed are morphology information (local fiber orientation tensor, fiber content, fiber aspect ratio) and per-phase (matrix and fiber) material properties. Morphological information of the RVE required for mean field homogenization are obtained experimentally, as explained in the previous section.

The parameters of the micromechanically based constitutive models of each phase (matrix and fiber) are characterized based on the measurements on the matrix and fiber reinforced material at 0°, 45° and 90° load angles. An elaboration of the material models and reverse engineering procedure for characterization of micromechanical model parameters can be found in [12].

3.2.1 Anisotropic fatigue failure criteria

The fatigue modelling is based on combination of the elastic constitutive model and a macroscopic fatigue failure indicator. The fatigue failure criteria is a modified Tsai-Hill 3D transversely isotropic failure indicator. But in the case of fatigue, strength parameters are function of the number of cycle. This criterion has three input arguments (as it assumes identical strengths in tension and compression) and outputs one indicator. The inputs are:

1. Axial fatigue strength depending on the number of cycle to failure, $S_L(N_c) > 0$.
 2. In-plane fatigue strength depending on the number of cycle to failure, $S_T(N_c) > 0$.
 3. Transverse shear fatigue strength depending on the number of cycle to failure, $S_{LT}(N_c) > 0$.
- and the output is a fatigue failure indicator FC in the form of:

$$FC(N_f) = \frac{\sigma_L^2}{S_L(N_c)^2} - \frac{\sigma_L(\sigma_{T1} + \sigma_{T2})}{S_L(N_c)^2} + \frac{\sigma_{T1}^2 + \sigma_{T2}^2}{S_T(N_c)^2} +$$

$$\left(\frac{1}{S_L(N_c)^2} - \frac{2}{S_T(N_c)^2} \right) \sigma_{T1} \sigma_{T2} + \frac{\sigma_{LT1}^2 + \sigma_{LT2}^2}{S_{LT}(N_c)^2} + \left(\frac{4}{S_T(N_c)^2} - \frac{1}{S_L(N_c)^2} \right) \sigma_{TT}^2 \quad (1)$$

where σ_L , σ_{T1} and σ_{T2} are the longitudinal and the two transversal stress amplitudes, respectively. Furthermore, σ_{LT1} and σ_{LT2} are the shear stress amplitude between the longitudinal and transverse directions and σ_{TT} is the shear stress amplitude in the plane normal to the longitudinal direction.

Failure occurs when the indicator reaches or exceeds the value of 1.

Like for the short term failure modelling, the problem with these criteria is that you need to enter the fatigue failure stresses in different directions (Digimat notations: X, Y and S). That can be done for a general composite material with known properties. However, for an injection molded material with an arbitrary fiber orientation distribution, this is not known beforehand, as the orientation distribution function will be different for each element. To solve this issue Digimat use a progressive failure mechanism that is called the First Pseudo-Grain Failure (FPGF) model [12].

3.3 Through-process modelling workflow

A through-process modeling methodology (coupled Moldflow-Digimat-Abaqus) is employed here to establish the processing-morphology-property relation in FRTP parts and predict their anisotropic mechanical performance. Moldflow[®] software is used to simulate the injection molding process and to predict the local fiber orientation distribution in the part. Digimat software suite is utilized to establish a relation between local mechanical properties of a FRTP material and processing-dependent morphology. Structural simulation is then performed in a finite element analysis software, like Abaqus. Workflow of such methodology is depicted in Figure 9.

Fig. 9. Workflow of the through-process modelling methodology, employed here for predicting the anisotropic mechanical performance of fibre reinforced thermoplastic parts

For fatigue lifetime prediction, an additional step is required, to relate the stress distribution on the part to the anisotropic time-to-failure.

4 Results and Discussion

In order to evaluate the accuracy of the through-process modeling methodology, validation tests are performed on different geometries, i.e. the pressure vessel and the elbow pipe. Performed tests are burst pressure test

(constant applied pressure rate, representing the short-term failure) and fatigue test (fluctuating internal pressure).

4.1 Burst pressure

Burst pressure simulations have been performed on the pressure vessel and the elbow pipe at constant burst pressure rates of 0.01 and 0.1 [bar.s⁻¹], using both isotropic and anisotropic simulation approaches. The results are shown in Figure 10. As can be seen, isotropic prediction using DIM tensile data underestimates the strain evolution, i.e. a much stiffer behavior. It is observed that results can be improved by using quasi-isotropic data for simulation.

However, none of the isotropic approaches can capture the realistic performance of the pressure vessel. Only by taking into account fiber orientation-induced anisotropy via through-process modeling methodology, one can more accurately predict the strain evolution in the part.

Fig. 10. Burst pressure simulation results on (top): a pressure vessel at a constant pressure rate of 0.01 [bar.s⁻¹] and (bottom): an elbow pipe at a rate of 0.1 [bar.s⁻¹]. The red areas on the surface of the parts, show the location of area of interest, over which strains are measured.

4.2 Fatigue with fluctuating pressure

Fatigue simulations have been done with an internal water pressure oscillating at a constant pressure ratio of 0.1. Figure 11 shows the predicted cycle-to-failure as a function of maximum applied internal pressure, using isotropic and anisotropic approaches.

As can be seen, the isotropic approach strongly overestimate the real cycle-to-failure. For a pressure vessel, with an injection location on top, the first principal direction of stress (Hoop stress) is

perpendicular to the fiber alignment at skin. Therefore, fiber reinforcement becomes less effective. This design situation could happen in many of water management applications due to commonality in geometric consideration, in which failure occurs due to an internal water pressure. The anisotropic simulation approach can capture this effect, enables providing a more realistic prediction.

It is worth pointing out that for the case of the pressure vessel, there is a factor of 200 difference in cycle-to-failure prediction of isotropic and anisotropic approaches for a same maximum applied internal pressure. For the elbow pipe, the prediction difference is a factor of 100. As can be seen, fiber orientation-induced anisotropy has a significant influence in the long-term performance and lifetime of FRTP parts and using isotropic approach can lead to a significant overestimation of the durability of the part.

Fig. 11. Fatigue simulation and cycle-to-failure prediction using isotropic and anisotropic approaches at a stress ratio of 0.1. (Top): pressure vessel. (Bottom): elbow pipe.

5 Conclusion

A through-process modeling methodology has been established and evaluated for accurate prediction of short- and long-term performance of short fiber reinforced thermoplastic parts. This methodology establishes a relationship between the processing-dependent morphology of FRTP part and its anisotropic mechanical performance. Simulation results show that anisotropic simulation via the through-process modeling approach can more accurately represent the performance of a FRTP part. An in-depth knowledge and accurate characterization and modeling of material properties is key in this approach.

Quantitative prediction of the performance of FRTP parts via anisotropic simulation and incorporation

of that in the application development process is crucial towards sustainable design solutions. Capturing realistic performance of FRTP parts can potentially result in:

- Improved simulation accuracy, leading to accelerated development cycle.
- More weight reduction possibilities via optimum material use, enabling thinner and lighter structures.
- Reliable lifetime prediction, and consequently design for durability.

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