

Innovative Anisotropic Material Modelling Approach for Fiber Reinforced Thermoplastics

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Abstract: Current industrial state of the art for predictive engineering of fiber reinforced thermoplastic materials utilizes nonlinear isotropic material modelling and/or anisotropic linear modelling. Both approaches give inaccurate predictions, since the effect of the orientation and length of the fibers is not taken into account in the former. Whereas, the latter omits the plastic behavior typically observed in thermoplastics. An innovative approach is developed in the last years which takes into consideration the anisotropic nonlinear behavior of the material. This approach which is based on micromechanical homogenization theories that considers both correct processing and fiber orientation, can significantly improve the accuracy of mechanical predictions, but is unfortunately very costly in terms of analysis time. The authors follow the innovative approach of combining the processing conditions of the fiber reinforced materials with obtained fiber length and orientation in the end applications, but couple this with a novel material model which incorporates anisotropic non-linear elasticity, anisotropic hardening plasticity, and multi-layer anisotropic non-linear visco-elastic behavior which can support anisotropy ratios that would cause a numerical breakdown when the Hill yield criterion would be employed. Since thermoplastics have complex fracturing behavior, the material model also incorporates a tailor made damage initiation/damage evolution process. The influence of the processing conditions and fiber orientation on mechanical properties will be elaborated, as well as how the model was calibrated to the large amount of test data available within SABIC.

Keywords: Thermoplastic Materials, Anisotropy.

1. Introduction

The capabilities in terms of material modelling thermoplastic materials have seen a considerable improvement in recent years with the addition of the Parallel Rheological Framework in Abaqus (Abaqus User's Manual, 2014). It contains a plethora of options in terms of capturing the complex behavior that thermoplastic materials exhibit. It includes the possibility to model non-linear elastic behavior mix that with several different large strain plasticity algorithms. To address the viscous behavior of thermoplastics it includes the possibility to add multilayer viscosity, where each of the layers can exhibit non-linear viscosity. Apart from the complexity which has moved into the calibration domain it can be considered the state of the art model for the isotropic modeling of (thermo)plastics.

The limitation on isotropic behavior is the cause of this work, because fiber reinforced thermoplastic material does not behave in an isotropic fashion necessitating the creation of an anisotropic variant with equal capabilities.

Short fiber reinforced thermoplastic material has anisotropic properties which are a result of the injection molding process. The short fibers align themselves with the melt flow into the mold and the resulting distribution strongly influences the overall properties of the part thus created. This fact has been long recognized within the plastics industry and has led to the development of software like Moldflow, Moldex and Simpo. These numerical solvers simulate the injection molding process and deliver as a result the fiber orientation tensor at each point in the part. To perform an accurate FE analysis of the result, this distribution needs to again be represented in the part to be analyzed. Also this has been long recognized, and has led to the implementation of what is the Abaqus from Moldflow translator.

However, so far the only material model in Abaqus, which is capable of using different orthotropic material properties for every integration point is the linear elastic short fiber model, or alternatively using a distribution table for orthotropic elasticity. This is quite far off from the capabilities of the Parallel Rheological Framework. So currently a user that wants to model short fiber reinforced material has two choices: either assume isotropy, and be able to use all the complex material behaviors in the Parallel Rheological Framework or realize that the orthotropic behavior is paramount (why else bother with using injection molding software in the first place) and assume linear elastic behavior.

Now the situation for the linear elastic behavior can be mollified a bit, we could add an anisotropic plastic behavior model like Hill's plasticity. However, what is not often stated is that Hill's plasticity is limited in the anisotropy ratio which it allows. If the anisotropy ratios start to deviate significantly from the isotropic condition, the flow potential is no longer a positive definite function, with non-convergence as a result.

So again we are limited, we may introduce anisotropic plasticity, but only up to a certain amount and not in what is typically observed from experiments. And all this is still ignoring the also very important viscous behavior of the thermoplastic.

Another approach has also come out onto the market which is the field of multi-scale homogenization methods. These look very promising, particularly the Mori-Tanaka based schemes. However, this methodology was developed for linear elasticity, and once we introduce additional mechanical behavior the homogenization schemes become distinctly more involved.

In this paper we set out a new material model that has been added to Abaqus/Standard and Abaqus/Explicit which tries to address the requirements of modeling orthotropic elastic-plastic-viscous materials such as short fiber reinforced plastics. First we illustrate the shortcomings of Hill plasticity in case of large anisotropy ratios. Then we introduce the concept of strain based yield and equivalent uniaxial strain. We then outline the idea of the material model. The material model as shown has been conceived and implemented by Dassault Systemes B.V. and calibrated using material data from SABIC.

To make the model usable, a separate translator was made to interpret Moldflow data for the material model, and to facilitate ease of use and an input file parser was written so that we can add user defined keywords.

2. Fiber Reinforced Plastics and Common Current Practice

The introduction notwithstanding, it is still common practice in the automotive industry to use isotropic material modeling when analyzing the performance of injection molded parts. Although the assumption of isotropy is already a huge simplification, one still needs material data to perform the analysis.

It may come as a surprise, that despite this widespread usage of isotropic modeling, that there is no standardized way on how the isotropic material data is to be obtained for reinforced plastics. Thus, depending on the measurement of the data, either obtained from a datasheet, or testing from directly molded specimens, or specimens cut from parts, one obtains different values for stiffness and strength. One of the prime reasons for this are the differences in fiber orientation.

The European Alliance for Thermoplastic Composites (EATC) has devised a method to properly measure isotropic properties from specimen cut from injection molded plaques (Schijve, W and Rüegg, 2008). Samples are cut in three directions (0° , 45° and 90°) with respect to flow front direction. Subsequently classical laminate theory is used to calculate isotropic properties based on a 0° , 45° , 90° , -45° stacking. For an illustration see Figure 1

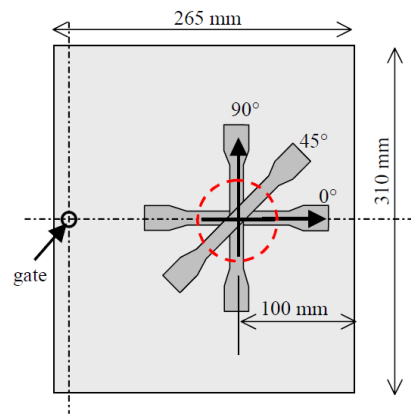


Figure 1. Schematic overview of plaque and samples used in EATC method for determining isotropic material properties

It is common practice to use “datasheet” values of materials for isotropic modeling. These values are usually generated with directly molded tensile specimens, which exhibit high fiber alignment. By consequence, the strength and stiffness of the material are significantly higher compared to what is typically observed in actual applications. Designs based on these values typically encounter failure below the expected values.

Doing isotropic analysis with the EATC values are on the other hand usually conservative compared to reality, which in turn yields parts that are heavier than they need to be.

It should then be clear, that going the isotropic route is not the most ideal approach, and we should consider attempting to do an anisotropic analysis of injection molded parts. To see an illustration of typical value ranges consult Figure 2.

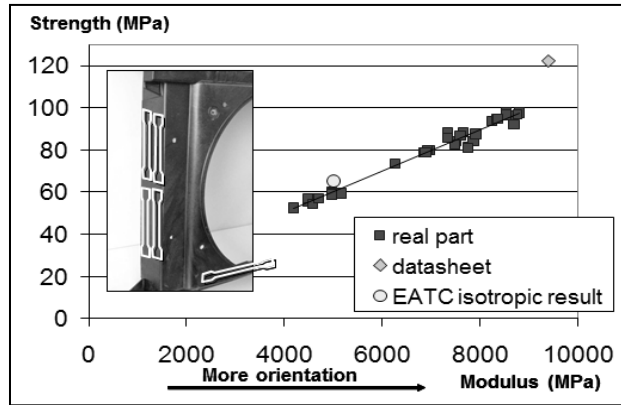


Figure 2. Mechanical performance of front-end part molded in 40% PP-LGF (SABIC®STAMAX™ 40YM240)

3. Strain Based Yield

The go to model once orthotropic plasticity is shown to be a factor is Hill's plasticity or one of its derivations. Before we can discuss the concept of Hill's plasticity we need some terminology in place. We denote by σ the stress, and ϵ the strain as usual. We assume that an orthonormal basis for our space of interest is in place, so that vectors can be written as $x = x_1 e_1 + x_2 e_2 + x_3 e_3$. In that case $E_1 = e_1 \otimes e_1$, $E_2 = e_2 \otimes e_2$, $E_3 = e_3 \otimes e_3$, $E_4 = e_1 \otimes e_2 + e_2 \otimes e_1$, $E_5 = e_1 \otimes e_3 + e_3 \otimes e_1$ and $E_6 = e_2 \otimes e_3 + e_3 \otimes e_2$ form a basis for the symmetric tensors, so that we can for example write $\sigma = \sum_{i=1}^6 \sigma_i E_i$. Writing then $\sigma = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz})$ is then termed Voigt notation, which is merely interpreting the symmetric tensors as a vector space and choosing a particular basis. In Abaqus the basis for the strains differs from the basis for the stress in that the last 3 base tensors are halved. In this way we can think about the stress as a 'vector' as being a member of a vector space.

Fourth order tensors can be thought of as linear operators mapping a second order tensor into another second order tensor. Once we have selected a basis for the second order tensors, every fourth order tensor thus takes a matrix representation. We will write fourth order tensors with calligraphic letters, for example $\mathcal{P}$.

3.1 Hill's plasticity

Hill's yield criterion (Hill, 1948) can then be written as

$$\sqrt{\sigma : \mathcal{P} : \sigma} - \sigma_y \leq 0,$$

Where σ_y is the equivalent uniaxial yield stress, and $\mathcal{P}$ is the fourth order projection tensor. Now take $A_{ij} = \frac{\bar{\sigma}}{\sigma_{y,ij}}$, which are the inverses of the relative yield ratios for each direction. In the basis given as above, we can write this fourth order tensor as

$$\mathcal{P} = \frac{1}{3} \begin{bmatrix} 2A_{11}^2 & A_{33}^2 - A_{11}^2 - A_{22}^2 & A_{22}^2 - A_{11}^2 - A_{33}^2 & 0 & 0 & 0 \\ A_{33}^2 - A_{11}^2 - A_{22}^2 & 2A_{22}^2 & A_{11}^2 - A_{22}^2 - A_{33}^2 & 0 & 0 & 0 \\ A_{22}^2 - A_{11}^2 - A_{33}^2 & A_{11}^2 - A_{22}^2 - A_{33}^2 & 2A_{33}^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2A_{44}^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2A_{55}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2A_{66}^2 \end{bmatrix}$$

Now assume we have large anisotropy, in which case we could have relative yield ratios of 0.1, 1 and 10. If you fill in these numbers in the above, we find a negative eigenvalue in the matrix representation. This means that there is a stress σ so that $\sigma : \mathcal{P} : \sigma$ is negative, no matter how small we take that stress.

We can thus conclude that for large anisotropy ratios, the Hill criterion breaks down. Unfortunately for short fiber reinforced plastics, we usually are dealing with large anisotropy ratios. From this we can conclude that yet again we are left with either choosing a clearly incorrect isotropic approximation or limiting the anisotropy ratios.

It is clear that neither is desirable. We are now going to try and move around this limitation from moving our yield potential from stress space to strain space.

3.2 Poisson Free Strain

To see the equivalence, let us start with the Mises yield criterion. In this case we have similarly to the Hill criterion that

$$\sqrt{\sigma : \mathcal{W} : \sigma} - \sigma_y \leq 0,$$

but here we have

$$\mathcal{W} = \frac{1}{2} \begin{bmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix},$$

now to move from a stress based yield law to a strain based yield law, we simply multiply our flow potential by $\frac{1}{E}$, which gives us

$$\sqrt{\sigma/E : \mathcal{W} : \sigma/E} - \sigma_y/E \leq 0,$$

where we will coin the term yield strain as $\epsilon_y = \sigma_y/E$. For the isotropic case let us investigate what σ/E brings us. Now $\sigma = \mathcal{D} : \epsilon$. Thus $\sigma/E = (\mathcal{D}/E) : \epsilon$. So if we now introduce $\mathcal{U} = \mathcal{D}/E$, then we can introduce the Poisson free strain as $\hat{\epsilon} = \mathcal{U} : \epsilon$. In which case our yield function becomes

$$\sqrt{\epsilon : \mathcal{R} : \epsilon} - \epsilon_y \leq 0,$$

Where $\mathcal{R} = \mathcal{U}^T : \mathcal{W} : \mathcal{U}$ which is now fully posed in strain notation. We also note that this formulation is identical to the isotropic stress based one.

For an orthotropic material we typically have $E_1, E_2, E_3, G_{12}, G_{13}, G_{23}, \nu_{12}, \nu_{13}$ and ν_{23} . We are going to first construct an E_4, E_5 and E_6 . The construction is based on taking an average Poisson ratio. We give the result for E_4 and assume the rest follows similarly. For this stiffness we have.

$$E_4 = G_{12}(2 + (\nu_{12} + \nu_{21})).$$

Note that the definition is given such that in the isotropic case all the stiffnesses are identical. We now use the exact same logic as before, where we introduce an Poisson free strain by $\hat{\epsilon} = \mathbf{U} : \epsilon$, but now we define $\mathbf{U} = \mathcal{E}^{-1} : \mathcal{D}$, where $\mathcal{E}$ is basically the fourth order tensor where in matrix representation the diagonal consists of the stiffness terms E_i . Note that for the isotropic case this just reverts to the definition we gave before. We will now not change the yield strain, but rather leave it at the form that we found, thus our strain flow potential looks like:

$$\Phi(\epsilon) = \sqrt{\epsilon : \mathcal{R} : \epsilon} - \epsilon_y \leq 0.$$

Note that this has some very interesting consequences, because we now have that the yield point in the first direction in terms of stress is $E_1 \epsilon_y$. And similarly the yield points in terms of stress in the second and third directions are $E_2 \epsilon_y$ and $E_3 \epsilon_y$. The strain yield potential is also positive semi-definite in terms of the strain tensor, so we have now circumvented the Hill degeneration problem. We term $\sqrt{\epsilon : \mathcal{R} : \epsilon}$ the equivalent uniaxial Poisson free strain.

However, we now have that the yield points are directly related to the stress. We could again work around this by making a similar assumption as Hill did, by allowing the weighting tensor to take Hill's form, but it turns out that isotropic strain as a predictor in yield point turns out to be a very good predictor, so for the materials at hand we have chosen not yet to do this.

There is a simple motivation for this, and that is that it is the matrix which is responsible for the yielding behavior. If we assume homogeneity of the continuum, and make the assumption that the matrix and the fiber see approximately the same strain, then it is the matrix that deforms in a plastic and/or viscous manner and not the fiber, which only deforms elastically. So we observe yield at just about the same level of strain all the time. The contribution to the stress however is wildly different, which is mostly caused by the orientation of the reinforcements. This observation is given credence by looking at experimental results.

3.3 Strain Based Generalized Maxwell Model

At this point, we can take the idea of Poisson free strain and equivalent uniaxial Poisson free strain and unite it into a nonlinear version of the generalized Maxwell model. The idea of which is illustrated in Figure 3.

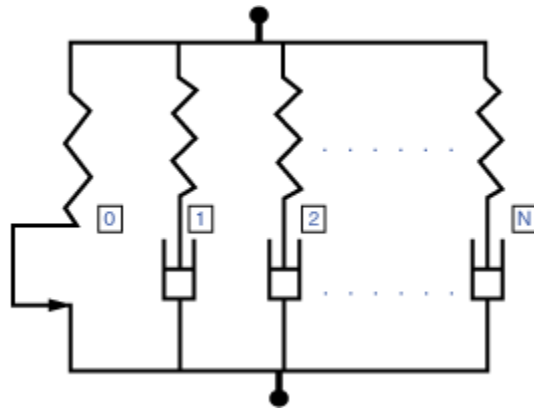


Figure 3. Generalized Maxwell Model (picture courtesy of Abaqus User's manual)

This is conceptually the same concept as was employed for the PRF, which is the reason we can use the same figure again. We are going to assume an arbitrary amount of layers, where the zeroth layer is called the equilibrium layer. It consists of a spring in series with a friction element which denotes the plasticity behavior. On top of that we can have several different layers which model the viscous behavior. The current version of our implementation of the model several viscosity laws (one of them which degenerates to linear viscoelasticity when the coefficients are chosen correctly) All these laws are implemented in a strain based manner, so they all behave in an orthotropic fashion. On top of this we also allow non-linear elasticity.

The complete material model thus described is implemented in a UMAT and a VUMAT for both shells and solid elements.

4. Setting up the Material Model with Injection Molded Data

We have now seen what the material model entails, but we still need to feed the results of the injection molding analysis into it. We have only written a utility that uses the data from a Moldflow analysis on a shell mesh into Abaqus, but other formats could also easily be incorporated.

So for simplicity we can assume that **abaqus moldflow** was run as a tool. When the translator was run on a shell mesh, this will present us with two files:

1. The shf file, which contains the orthotropic data for a certain number of section points through the thickness of a shell element. Each section point may have a distinct set of orthotropic material coefficients, and have a distinct material orientation.
2. The str file, which contains the initial stresses due to thermal shrinkage.

Both these files are read by a small tool, which reads the data and writes it into a binary file, which takes the extension sdv. The tool is written in C++. Essentially the sdv file contains the data which is given in both files, but takes a more convenient directly digestible format to be used by the subroutine.

The idea is to put the orthotropic material parameters, not as material constants, but as state variables for the material. Even though they are not really state variables in the sense that they would change as a function of deformation, they are still local to each integration point. We cannot use a distribution with a user defined material for properties, and a field would be not ideal either, since we would need to give nodal properties. We could of course circumvent this again by implementing a USDFLD, but that would still entail the same amount of memory as is required for defining them as state variables.

The initialization is then performed through implementation of the subroutines SIGINI and SDVINI. We also use an ORIENT subroutine to set up the integration point orientations from 6.14 onwards.

The reason we do not also use a `*Initial Condition, type=solution` is because these values can only be given on an element basis, and are then uniformly applied throughout the thickness. Where it should be clear that the distribution through the thickness for a fiber distribution is typically not constant.

Apart from these procedures we also implement the user subroutine UEXTERNALDB to control the initialization process. The total analysis goes as follows.

- At the start of the Abaqus run, UEXTERNALDB is called, which opens the sdv file that was created and reads the contents into memory. If there is no sdv file present, the routine assumes that the data is given through initial conditions statements in the input file.
- At the beginning of the first increment SIGINI and SDVINI as well as ORIENT read the data which was read into memory and places those in the appropriate state variables in the Abaqus data structure.
- At the end of the first increment UEXTERNALDB is called again, which deallocates the allocated memory. At this point initialization is complete, and the UMAT has access to all the data.

This implementation was made prior to availability of VUEEXTERNALDB, so initialization is done through Abaqus/Standard, after which an import needs to be made.

The next issue is dealing with specifying all the constants that need to go into the material model. Abaqus has a strict rule of specifying the material constants with 8 variables per data line. If we want to change the material data slightly, this would mean all the data would need to be rearranged.

To this end, we created a small script which can parse arbitrary input files, and write them out again. The utility will create a hierarchical dictionary of all the keywords encountered in the input file. Once an input file is in the internal data structure, it can also write it out again.

We will now introduce fictitious keywords. These fictitious keywords can then be removed from the dictionary through a small add-on function, which will then add a `*User Material` card and also a `*Depvar` card with the correct data lines. Subsequently calling the write methodology will then create a valid input file for execution.

5. Results

5.1 Uniaxial tensile behavior

The model has been validated using simple 1-element tests for the material fitting, and dog bone specimens to see its behavior in multiple element tests.

SABIC has provided all the required material data for performing a rate dependent fit. The result of which is illustrated in Figure 4.

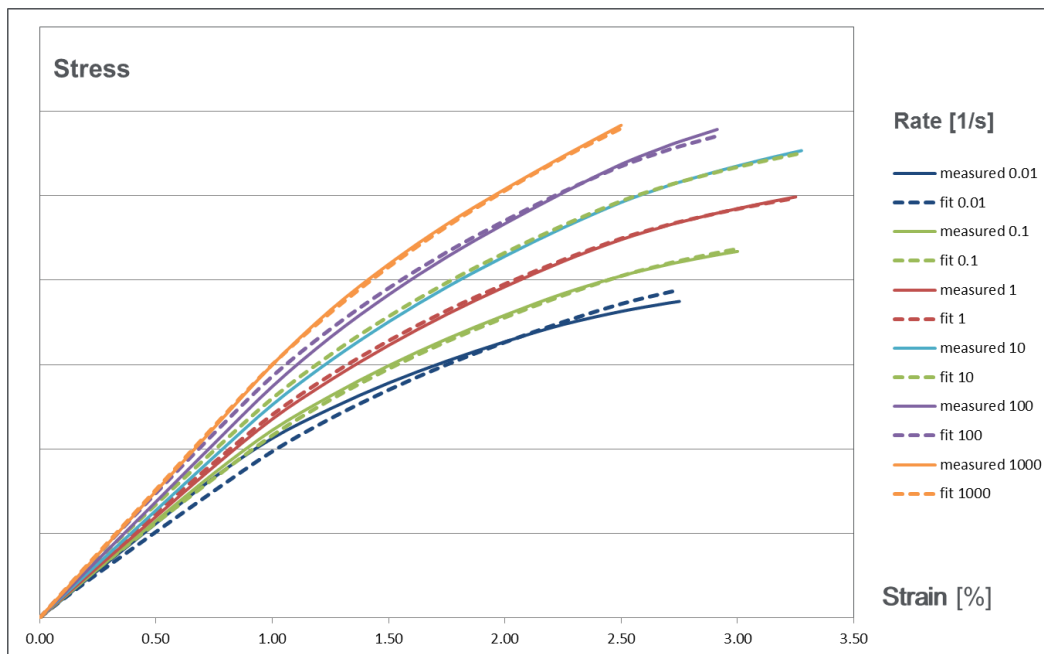


Figure 4. Results of Fitting Material Model

The fit for the rate dependency is done on the equivalent isotropic data. It is then assumed that the anisotropic results follow the same behavior, but the actual scale of the curve will scale with the stiffness in the respective direction.

Required Fiber orientation as input for anisotropic simulations has been obtained from commercially available injection molding simulation software Autodesk Moldflow Insight.

5.2 Real application example

The accuracy of isotropic, linear anisotropic and non-linear anisotropic simulation methods (see Figure 5) have been evaluated by simulating a lock stiffness experiment on an existing frond-end module carrier made of 40% long-glass fiber filled Polypropylene.

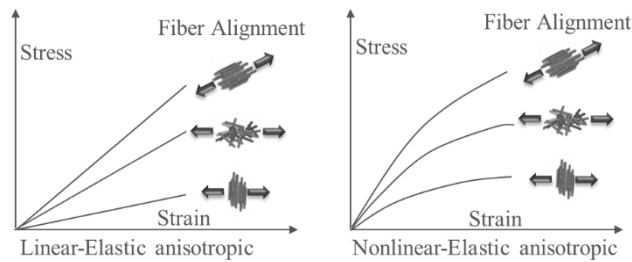


Fig. 5: Two main anisotropic modelling methods.

The carrier was subjected to a 2 kN load at room temperature and the resultant displacement was measured, Figure 6. It was observed that the lock stiffness was under predicted by ~20% when EATC isotropic values were used. When linear elastic anisotropic material data from Moldflow were directly applied, predicted stiffness was ~30% too high, while the results, obtained with developed non-linear elastic plastic anisotropic model, were very close to the experiments (-4%) (See Figure 6). It should be noted however, that for direct Moldflow-Abaqus simulation only linear integrated triangular elements could be used. Other predictions could be done using quadratic triangular elements. This will influence the results to some extent.

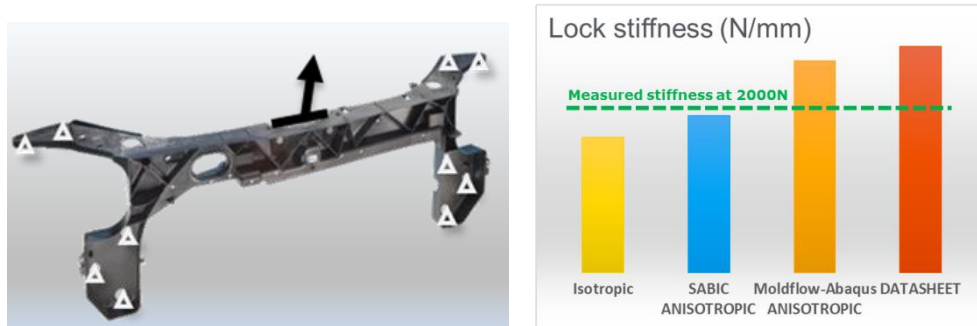


Figure 6. Simulated versus measured lock stiffness on an existing front-end module made of 40% PP-LGF (SABIC®STAMAX™ 34YM240). Left: schematic setup of lock stiffness test. Triangles indicate constraints, a 2 kN force was applied in

lock direction (arrow). Right: Predicted stiffness. Isotropic properties according to EATC method.

6. Conclusions

Accurate prediction of mechanical performance and dimensional stability of the part is the key for reaching the desired light weight design and minimized development time.

Current industrial state of the art for predictive engineering of fiber reinforced thermoplastic materials relies in most cases on isotropic material modeling, where fiber orientation is not taken into account. This approach gives contradictive predictions.

Anisotropic performance prediction, which considers fiber orientation in the end applications delivers the best accuracy in performance prediction, which is only a few percent off from reality. However, the anisotropic predictive engineering approach using multi scale homogenization methods require significantly more computational resources compared to the current state of the art approach which is isotropic modelling. Analyses take longer time and in general more memory is required.

Sitting inbetween the simplified isotropic modeling, and the homogenization methodology is the phenomenological framework we have presented in this paper that yields significantly improved results compared to the isotropic modeling, but does not have the high analysis cost required for the full scale homogenization approach.

7. References

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