Simulation of Short Fiber Reinforced Plastics in LS-DYNA® Using Envyo® Mapped Fiber Orientations Obtained from Process Simulation in Moldex3D®

Marcus Gustavsson[1], David Aspenberg[1], Björn Stoltz[2]

[1]DYNAmore Nordic AB
[2]IKEA Components AB

1 Introduction

Accurate representation of materials is an essential part of the quest for realistic and predictive simulation, not least for anisotropic materials such as short fiber reinforced plastic (SFRP). Still, it is common to neglect the anisotropic properties of SFRP components when evaluating the structural performance of the design in FE simulation, thereby often failing to predict a realistic mechanical behavior. Neglecting the anisotropic features of SFRP, especially at an early stage in the design development, may lead to a design that is not viable for the component in question.

A common manufacturing process for thermoplastics components is injection molding. How this process is set up will significantly influence the anisotropic properties for SFRP components; two geometrically identical components using the same material can still have vastly different structural performance and characteristics, given different manufacturing conditions.

Simulation of the injection molding process gives the ability to evaluate and iterate the design of the manufacturing process with relative ease, for instance, gate placement, which greatly influences fiber orientation and weld line locations. Fiber orientations predicted by the process simulation can efficiently be transferred to the structural simulation using a mapping tool such as Envyo®. Working with process simulations can also simplify the simulation-based design process by replacing other techniques for obtaining information about fiber orientation, such as computer tomography (CT).

Ideally, one would like to have the actual fiber orientations in the test specimen when performing material characterization of SFRP materials, e.g., obtained via CT scanning. However, under the assumption that the process simulation provides accurate fiber orientations, a pure simulation-only approach could be used instead.

In this paper, a practical methodology for working with injection-molded SFRP components in LS-DYNA® is presented, where the complete simulation chain from process simulation to structural simulation is performed using commercial software. Injection molding simulations using Moldex3D® provide the fiber orientations that are transferred using Envyo® to an LS-DYNA® model for structural simulation. The study focuses on fiber orientation results and capturing its effect on structural properties by applying the LS-DYNA® material model **`*MAT_4A_MICROMEC/*MAT_215`**.

The aim is to show and evaluate the suggested simulation-only approach under real circumstances, including calibration using test specimens. The focus is on how to work with SFRP, primarily fiber orientation, from a practical point of view, although other aspects of the characteristics inherent to SFRP that should be considered are also discussed. Thus, possibly be the first step in getting started with SFRP simulation in LS-DYNA®.

2 Short Fiber Reinforced Plastic & Injection Molding

To establish some basic understanding for the problem at hand, this section shortly explains some properties and key aspects of short fiber reinforced plastic (SFRP) and injection molding.

Injection molded SFRPs typically consist of a thermoplastic matrix reinforced with fibers out of either glass or carbon. The matrix and fibers have vastly different structural properties, e.g., the differences in stiffness and strength are in the orders of magnitude. Together they make up a significantly stiffer and stronger material than the plastic matrix would make on its own while still offering excellent moldability.

In very simple terms, injection molding is a process where plastic pellets are melted in a feeder screw, which is moved forward, injecting the melted plastic into the mold. It is common that the mold is cooled in some way, often via liquid cooling. After the part has reached a sufficient degree of solidification, the mold is opened, and the part is ejected.

This process has great influence on how the part turn out in just about every aspect. For SFRP, one aspect is the resulting fiber orientation. Many flow characteristics will affect the orientation, with the most general case probably being the through thickness fiber orientation anisotropy that occurs when the melted SFRP flow through a relatively thin cross section. Without dwelling into the details of the flow mechanisms behind it, the resulting fiber can be said to tend to orient itself in a manner that makes it possible to identify mainly three characteristic layers through the thickness; two outer layers where the fibers tend to be oriented primarily in the direction of the flow and a core region where the fibers tend to be oriented in-plane transversely to the flow [1], see figure 1.
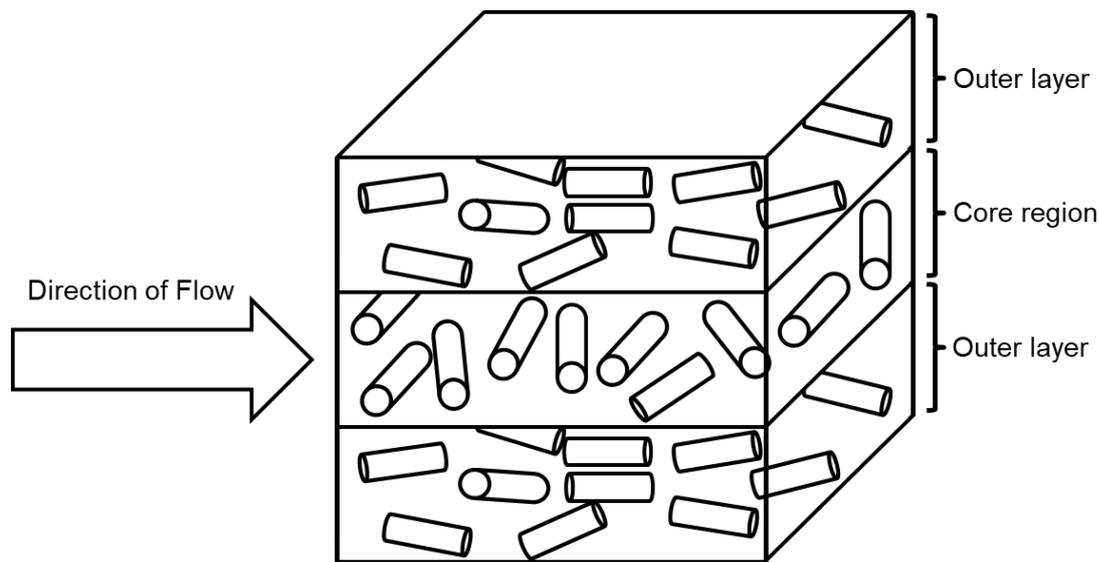
Fig.1:   *Simplified depiction of the flow induced through thickness anisotropy in fiber orientation*

In reality, there is also an outer most skin layer where generally the orientation is more uniformly random, this skin layer is thin in relation to the other layers and for the purpose of this discussion it is ignored, however, it is observed and included in the simulations. For a test geometry such as the plate used in this study, this pattern in the fiber orientation gives a material that have more or less transversely anisotropic properties.

The material used in this study is a short fiber reinforced thermoplastic with a polyamide 6 matrix and with 30 % glass fiber by weight (PA6GF30). For reference, this material has a Young's modulus and yield strength approximately 3 respectively 2 times that of the same but unreinforced polymer according to the manufacturer's datasheet.

The inclusion of fiber alters the mechanical properties in many aspects, however, not all of them are desirable and there are some possible downsides that come with adding fiber reinforcement to a plastic. The obvious one is the anisotropy, the fibers do not increase strength isotropically, which also means the fibers can add less strength than expected if comparing with a material's datasheet.

In addition to affecting the orientation of fibers, injection molding can produce local variations in fiber concentration as well as fiber length, which also contribute to the fiber induced anisotropy. It is common to assume these properties as constant, as in this study. However, it is important to be aware that these phenomena are present to some extent; to what degree can depend on material composition, part complexity, process conditions, etc.

Further, even unreinforced injection molded thermoplastics are vulnerable to process induced local anisotropy, such as weld lines, also known as knit lines. This is relevant because the inclusion of fibers can amplify the effects of the weld lines that create stress concentrations. One study has shown that while an unreinforced plastic might lose about 17 % of its yield strength, a fiber reinforced equivalent can lose up to 80 % of its yield strength [2]. In short terms, this is mainly due to the fact that the fibers tend to orient themselves parallel to and not across the weld line, thus not adding stiffness perpendicular to the weld line.

Aside from the properties added by the inclusion of fiber, these materials obviously inherit traits from thermoplastics, for example viscoelasticity and viscoplasticity or different behavior in tension and compression. Thermoplastics are also very susceptible to environmental factors such as humidity and temperature. All these factors must be considered during testing, material model calibration and when using the material card.

3 Methodology

The steps of the suggested methodology for producing, transferring, and using fiber orientations in LS-DYNA are described in this section. While the method only deals with fiber orientation, other aspects that are relevant for simulation of SFRP in the context of the software are highlighted for the reader's consideration.

This study uses Moldex3D® 2021 R1 for injection molding simulation and procuring fiber orientations for the test plate, and Envyo® v2.0.15 for mapping the fiber orientations to an LS-DYNA® R13 mesh and material. Characterization is done using tensile tests results and reverse engineering simulation aided by LS-OPT, method flow chart shown in figure 2.
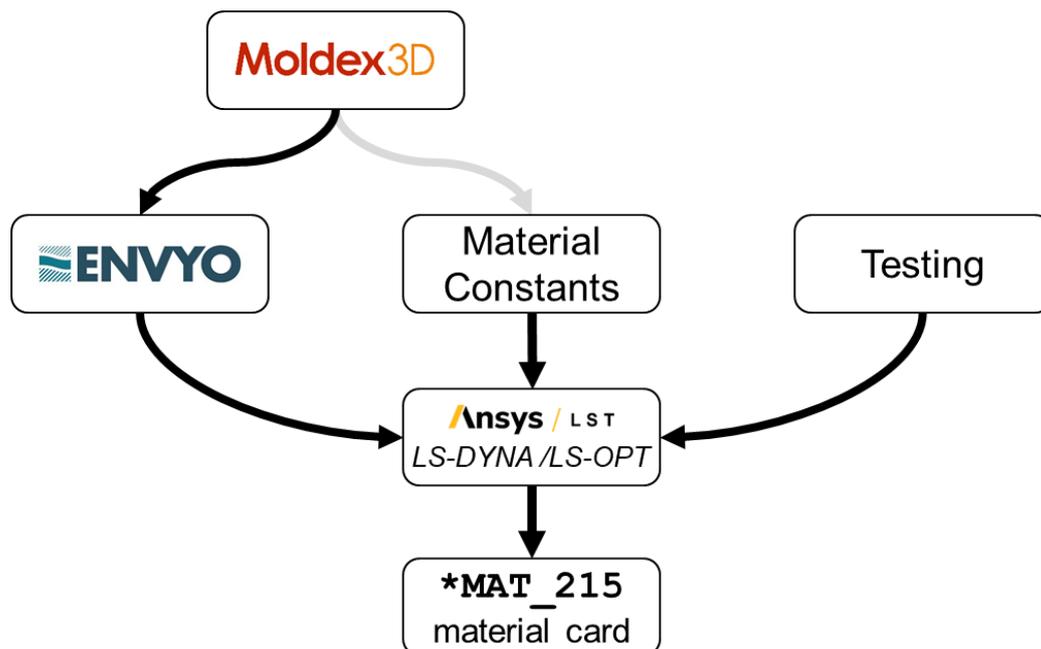
Fig.2: *Flow chart of the methodology for characterization of the material*

3.1 Process Simulation in Moldex3D®

Moldex3D is a simulation software that allows for simulation of a variety of plastic molding processes where the foremost is injection molding of thermoplastics [3]. One main use of Moldex3D is to predict fiber orientation in fiber reinforced plastic parts. It does so by calculating the flow pattern during the filling stage, the flow's influence on the fiber orientation is then predicted, usually in a one-way coupling, as was done in this study using Moldex3D's patented iARD-RPR model [4]. More reading about the governing equations for flow and fiber orientation prediction can be found in other publications [1,4]. Additionally, Moldex3D can also predict other defects caused in the injection molding process, such as weld lines.

The material in question is available in Moldex3D's material database. If the wanted material is unavailable, it is possible to select an alternative material using Moldex3D Material Hub Cloud [5]. It is also possible to input custom material parameters.

The simulation was set up using the process parameters dictated by the sample plate manufacturer concerning injection speed and pressure as well as plastic melt temperature. It was assumed that the surface on the mold was the same temperature as the cooling agent. This ideal cooling assumption is assumed to have little effect on the fiber orientation in this instance due to short injection time, part size, and moderate cooling agent temperature. The sample plate geometry and melt front time results are shown in figure 3.
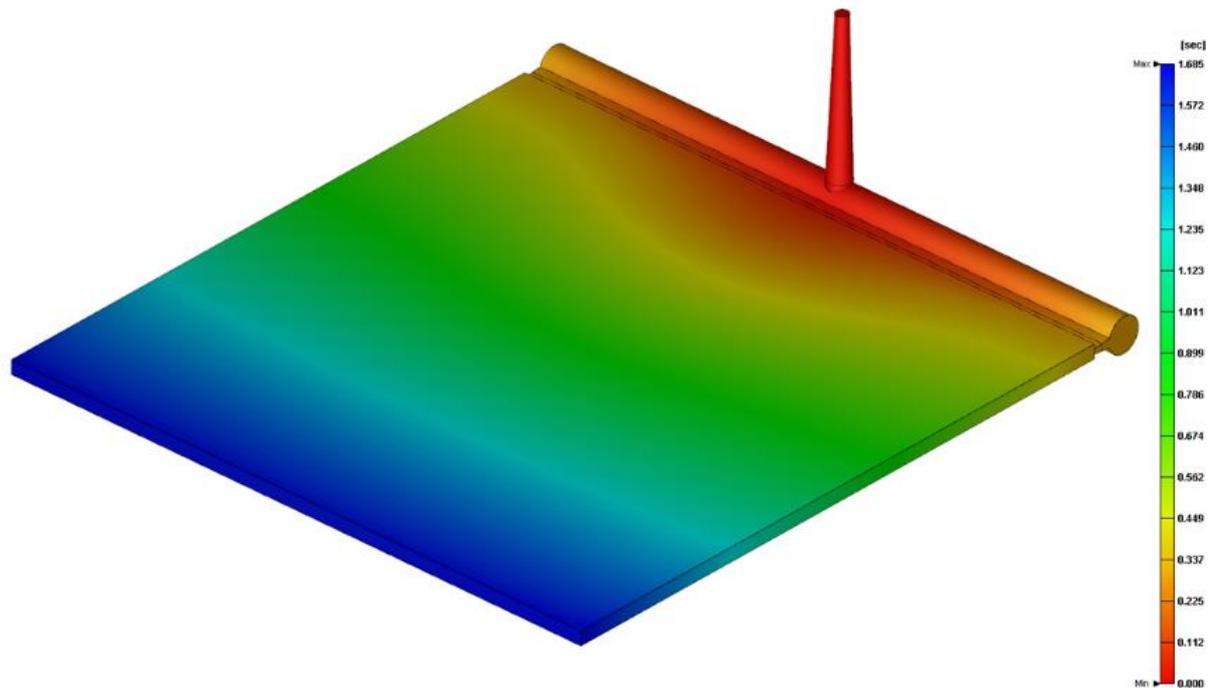
Fig.3:   *Melt front time, time for melt front to reach a certain position, injection gate and runner also visible*

The 175 x 175 x 4 mm plate is discretized with a mesh size of 0.7 mm and 20 layers through its thickness. A sufficient number of elements through the thickness is required to capture the gradient in fiber orientation accurately. Figures 4 – 5 show the resulting fiber orientation. In the outer layers, fibers align with the flow, whereas in the core region, fibers tend to be transversely oriented relative to the flow. The less oriented skin layer, mentioned in section 2, can also be observed in figure 6. The triangle shaped artifacts seen in core region clippings, figure 4, is due the interpolation between elements.
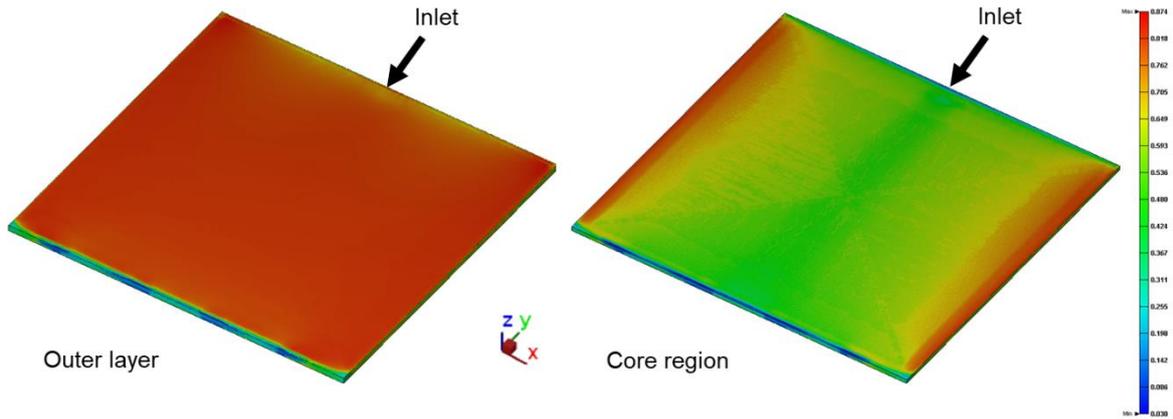
Fig.4: *Degree of fiber orientation in the Y direction, cut at 75 % thickness (outer layer) and at 50 % thickness (core region)*
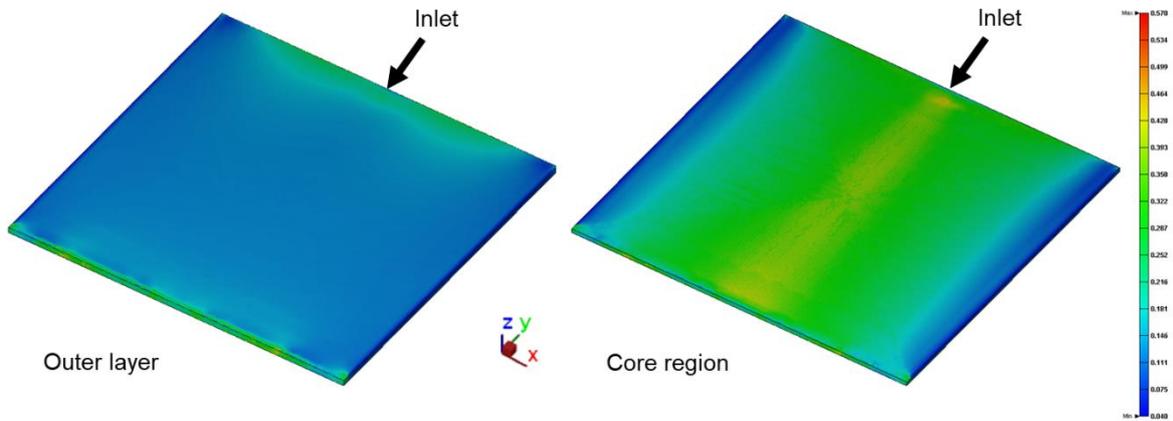
Fig.5: *Degree of fiber orientation in the X direction, cut at 75 % thickness (outer layer) and at 50 % thickness (core region)*
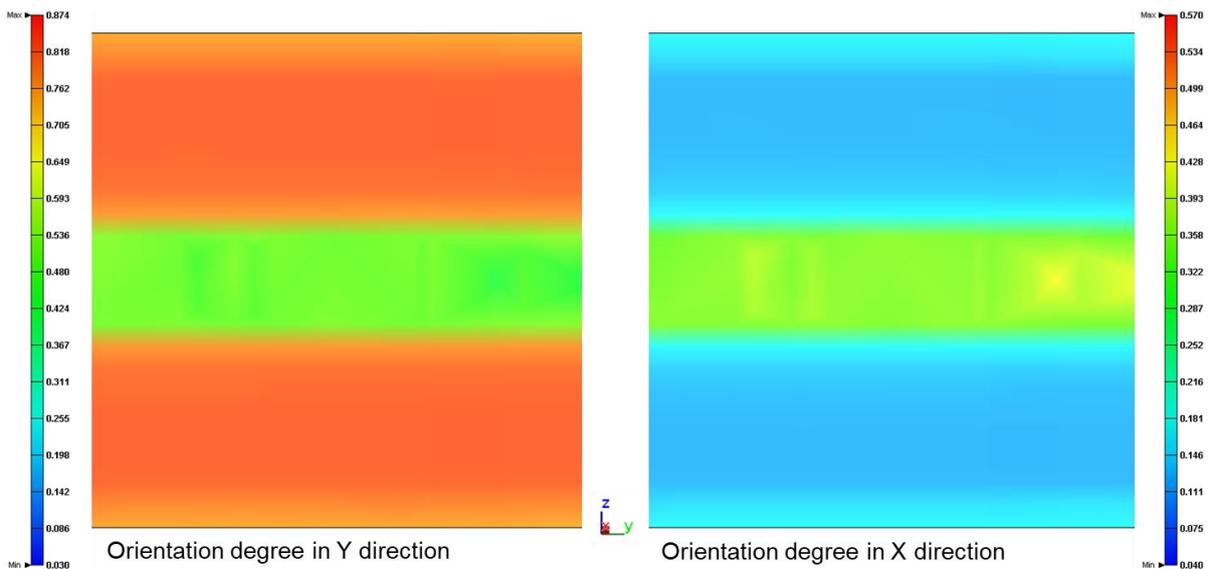
Fig.6: *Degree of fiber orientation through the thickness, cut view is at middle of the plate normal to the X direction*

Fiber orientation for use in subsequent mapping is output through the FEA/Micromechanics interface in Moldex3D, shown in figure 7. The output is the Moldex3D mesh in LS-DYNA keyword format and the fiber orientation in an .o2d-file that defines the orientation tensor for each element in the exported mesh; both are in readable text format. It is also possible to export, for example, weld lines, fiber concentration, stress, and temperature, in similar format as the .o2d.
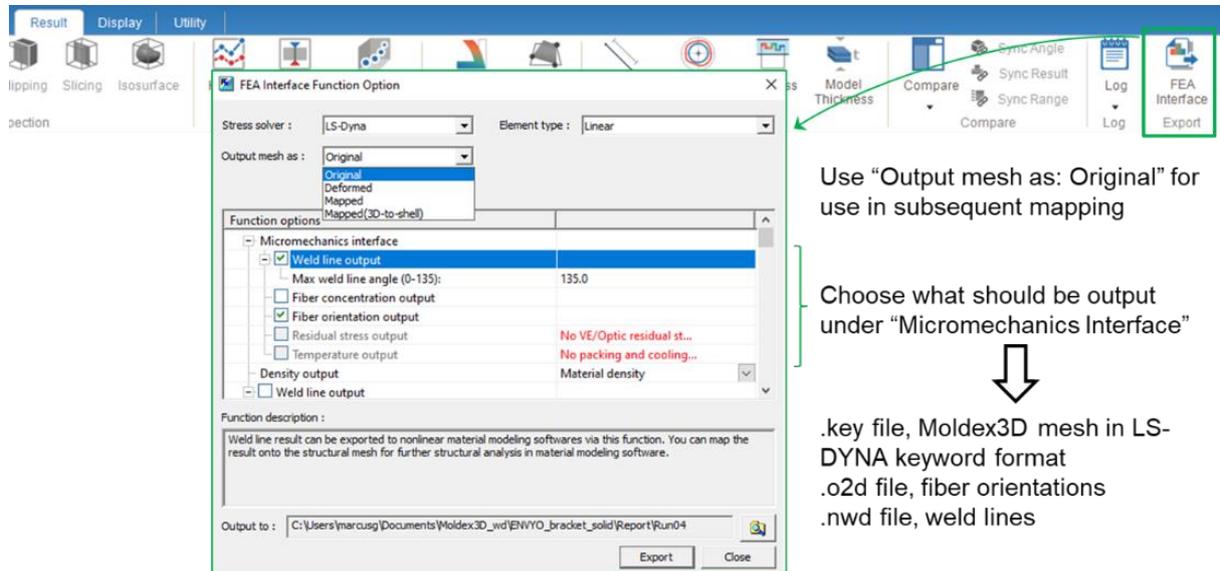
Fig.7: *FEA/Micromechanics interface in Moldex3D*

The fiber orientation results are extracted at the end of the filling phase; one could argue that the packing phase may influence the fiber orientation due to additional displacement of the material. It has been shown that usually the "core region" is thinner at the end of packing than at the end of filling; however, it has also been shown that the effect of packing on fiber orientation is a concern mainly when the injection molded part is relatively large and of complex design, such as having ribs, holes, and changes in thickness [1]. The geometry used in this study is considered to be simple regarding these factors, and for this study, it is sufficient to use the fiber orientation results affected by the filling phase only.

3.2   Mapping with Envyo®

Envyo is a general mapping tool meant for LS-DYNA. It can transfer data between different meshes that have different discretization, element formulations, material models, coming from different software, etc. As Envyo is tailored for LS-DYNA, it can correctly handle material model history variables, node and element numbering and directions, and other definitions specific to LS-DYNA [6].

The process of mapping fiber orientation results to an LS-DYNA model is straightforward. First, the source mesh and fiber orientation tensor files from Moldex3D are needed. In addition to that, a target mesh and name for the mapping result need to be specified. Accompanying the input files are several options that one might need to change depending on, for instance, target mesh element formulation, transformations, change of units, material model and options used in the subsequent LS-DYNA simulation.

As the material model used in this study is ***MAT_215,** the TargetMaterialModel option is set to "215". Note that the only material property that is processed by Envyo is the fiber orientation tensor. Other inputs are made on the material card; read more about this in section 3.4.1. In contrast, if ***MAT_157** were to be used, then all relevant material parameters must be input into Envyo that performs the homogenization. The MapStress option is used as the fiber orientation tensor should be prescribed via ***INITIAL_STRESS_SOLID**. Further, the target mesh consists of 1-point tetrahedron type 13 elements using invariant node numbering, INN = 4 on ***CONTROL_ACCURACY**; it is important that the settings in Envyo are consistent with the target LS-DYNA model. Consult the manual for correct settings regarding these aspects [6]. Transformations are used to position the source mesh such that it corresponds to the selected specimen cut out.

In this case, the OUTPUT_OPTION = INITIAL_STRESS_ONLY option is used, which makes Envyo output only the ***INITIAL_STRESS_SOLID** keyword containing fiber orientation tensor expressed relative to the target mesh specified but without any ***NODE** or ***ELEMENT** keywords. This makes it easy to use a particular orientation and position in a simulation by simply swapping out the included mapping results to what is otherwise the same model. Another helpful option is TransformedMesh which outputs the transformed source mesh so that the transformation can be verified.

Envyo can handle weld line mapping as well. The part is then divided into separate subparts consisting of elements that are near a weld line specified in the .nwd-file from Moldex3D. These subparts can then have a reduced strength assigned to them. For a more extensive description of all the options and procedures in Envyo, see the manual [6]. The Envyo graphic interface is shown for Moldex3D solid to solid mesh mapping in figure 8, and an example of the resulting fiber orientations viewed LS-PrePost in figure 9.
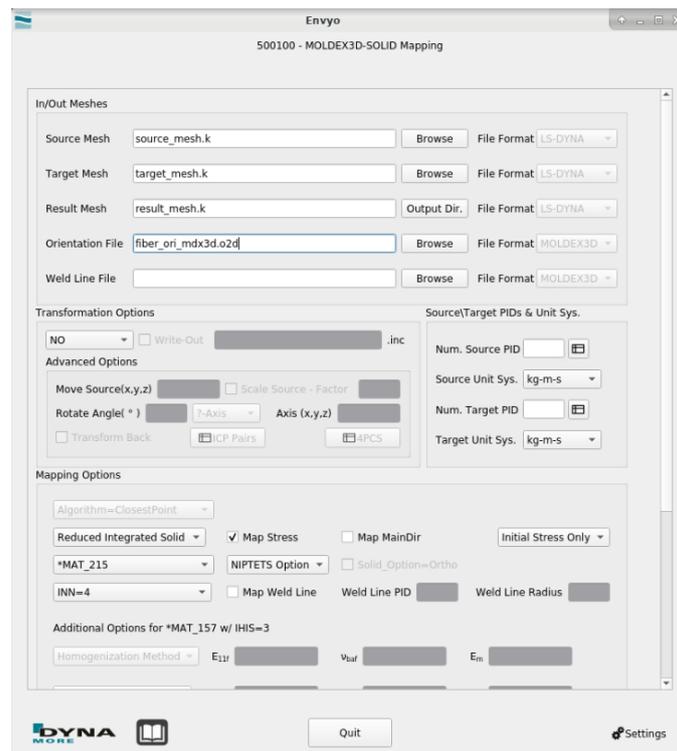
Fig.8:   *Envyo GUI för Moldex3D to solid element mapping*
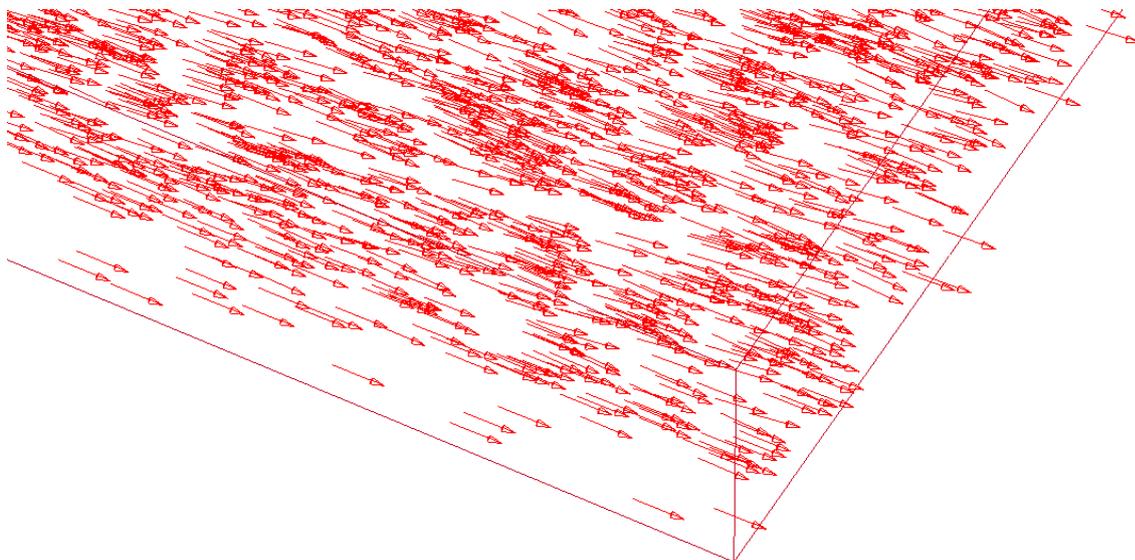
Fig.9:   *Sample of mapped fiber result in viewed LS-PrePost for the 0° specimen*

3.3 Testing

Test specimen were cut out from the plates with 0°, 45° and 90° angles with respect to the flow direction, using a specimen geometry according to ISO 527-2-1B. To get more samples, as well as study the variation within each plate, five specimens were cut from each plate in the 0° and 90° directions and three in the 45° direction, as shown in figure 10. This allowed studying both variations within the plate as well as checking the symmetry of the plate.
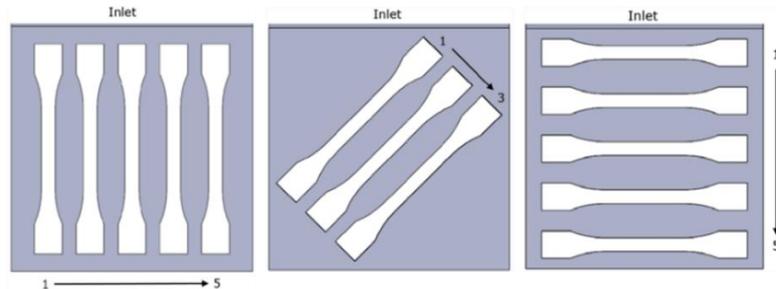
Fig.10: *Specimen cut out for 0°, 45°, and 90°*

Before any mechanical testing was performed, the specimen had to be conditioned to the right humidity level. This was ensured by placing them in a climate chamber at 60°C and 65RH until they showed less than 0.1 weight difference over three separate measurements. This setting is according to ISO 1110.

The mechanical properties were extracted through tensile tests according to ISO 527-1. The velocity was set to 1mm/min up to 0.3 global engineering strain (taken between the grips) then increased to 50mm/min until fracture. A Digital Image Correlation (DIC) equipment was used to measure the displacement, thereby reducing any effect of mechanical extensometers and enabling an unlimited number of extensometers in the post-processing. The nominal length of the extensometer was set to 75mm in accordance with iso 527-1, while the tensile modulus and the Poisson's ratio were measured through the use of a region measurement (75mm x 10mm). The reason why these two different methods were used, is that the region calculates a mean value of the distances and updates the region if the area comes out of frame or gets lost. This is acceptable for small deformations, thereby acceptable for the evaluation of tensile modulus and Poisson's ratio.

The final results in figure 11 are a subset of all experiments, i.e each curve represents one unique and representative test specimen. The specimens used in the calibration were selected, one for each direction, based on which specimens were the most generic, i.e. force-displacement response closest to the mean response.

The noise seen at the beginning of each curve might depend on several factors. First, a high sample rate is used in this area to catch the tensile modulus and Poisson's ratio. Second, the settling of the specimen in the grips might also contribute to initial noise. Third, electrical disturbance might also contribute to noise, since the global force and displacement measures from the testing machine include a scaling of current, and at small displacements it will be more pronounced.
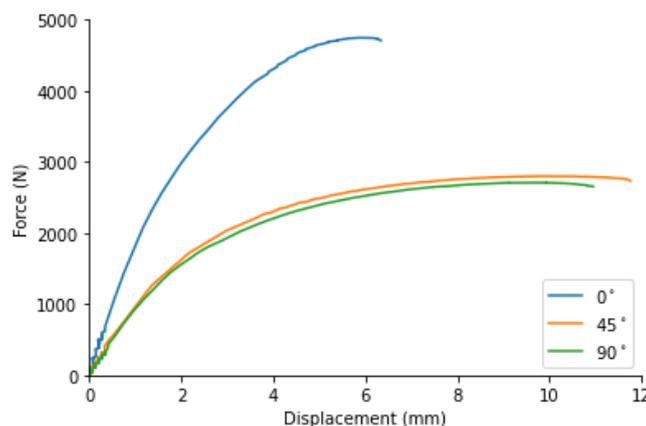
Fig.11: *Force vs. displacement for 0°, 45°, and 90° oriented tensile specimens*

3.4 Calibration for `*MAT_215` using LS-OPT®

3.4.1 Material Model *MAT_215*

`*MAT_4A_MICROMEC/*MAT_215` is a micromechanical material model that separates the input for matrix and fibers properties. This and the many options tailored for fiber reinforced plastics makes `*MAT_215` a particularly suitable choice due to its ease of use. The matrix is assumed to be isotropically elasto-viscoplastic while the fibers are assumed to be elastic only with transverse isotropy, these separate properties are then homogenized by the material model, sources on the homogenization techniques used by `*MAT_215` can be found in LS-DYNA's documentation and other publications [7, 8]. In comparison, for `*MAT_ANISOTROPIC_ELASTIC_PLASTIC/*MAT_157`, which is another suitable alternative for SFRP materials, the material properties have to be homogenized prior to input.

As the fibers inclusions themself can be oriented in an arbitrary manner in the matrix, the composite material can have arbitrary anisotropy throughout the part. A local fiber orientation tensor can be prescribed to element integration points via the `*INITIAL_STRESS_SOLID` keyword. These are written to history variables 9 – 16 and overrides principal fiber orientations input on the material card.

Density and stiffness data are input both for the matrix and the fiber. The matrix plastic hardening properties can also be specified. For the fiber, one can specify ultimate tensile strength as well as fiber-volume-fraction (FVF) and fiber length (FL). FVF and FL can also be input as non-uniform in the same way as the fiber orientation tensor, however, they are assumed constant in this study. `*MAT_215` also includes a ductile failure model for the matrix (or composite) and a stress-based failure criterion for the fibers. However, failure has not been considered in this study. It is important to note if the fiber fraction input is defined by weight or volume, as the density of the fiber usually is significantly higher than of the matrix. The material in this study has a fiber volume fraction of 30 %. Default input for *MAT_215 is fiber volume fraction, a negative input is interpreted as fiber weight fraction [7].

Fiber properties from a datasheet are commonly used, as in this study where the data is obtained through the Moldex3D material database, where it is provided by the manufacturer. The same goes for the matrix Young's modulus and density.

3.4.2 Setup

For the calibration of the material model, three quasi-static tensile tests were used. The tests have been cut out from an injected plate such that the majority of the fibers are aligned with the specimen (0°), diagonally aligned (45°), or transversely aligned (90°).

This study only considers the hardening of the matrix material in the calibration of this material model. All other components of the model, i.e. the fiber properties and the elastic modulus of the matrix material, are retrieved from a datasheet. This is motivated by the fact that without manipulating these data, and simply map the fiber directions from the injection molding simulation, a good agreement with the elastic properties of the tensile specimens is already achieved. Strain-rate dependent properties have not been considered.

To enable a calibration using LS-OPT, it is necessary to parameterize the hardening in some way. Here, the hardening is assumed to follow the Hocket-Sherby equation

$$\sigma = A - Be^{-C\varepsilon_p^H} \tag{1}$$

where A can be expressed in terms of the yield strength σ_Y as

$$A = \sigma_Y + B \tag{2}$$

The calibration utilizes the curve matching composites in LS-OPT, in which extracted force-displacement curves from the simulations are paired with the corresponding experimental curves. The setup of this in LS-OPT is very simple, see figure 12. It consists of a pairwise selection of a simulation curve and an experimental curve, and a choice of error type calculation for the mismatch between the selected curves. This study uses a mean squared error (MSE) calculated at 50 equidistant points along each experimental curve.
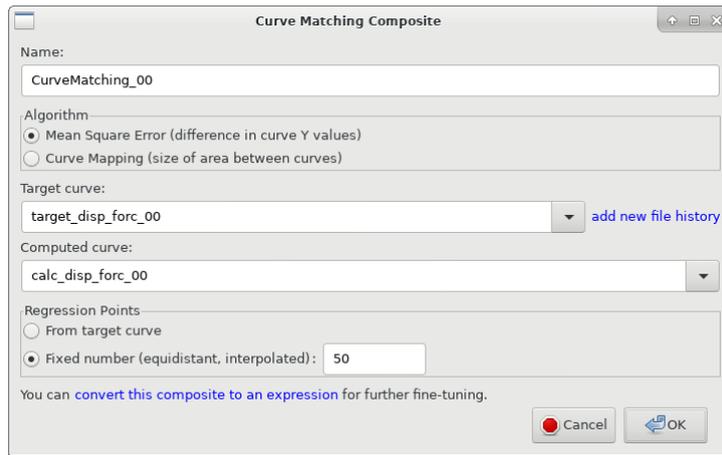
Fig.12: *Setup of curve matching composite in LS-OPT.*

The objective for the simulation was set to the sum of the three errors calculated from the curve matching composites, and the SRSM strategy was chosen for the optimization, LS-OPT setup shown in figure 13.
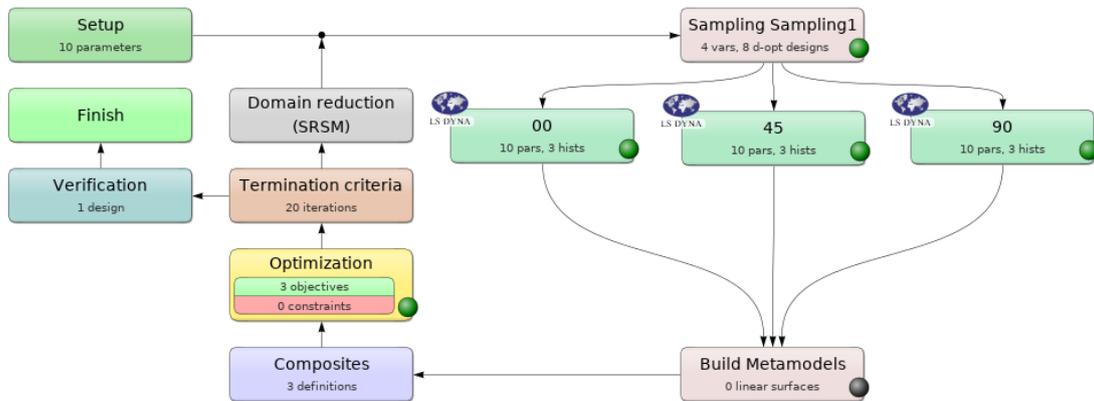
Fig.13: *LS-OPT setup of the hardening calibration.*

3.4.3 Calibration Results

The optimization was run for 20 iterations, and the yield stress σ_Y and the B-parameter converged to optimum values. The C- and H-parameters, on the other hand, continued to increase over the last iterations, creating a more and more linear hardening approximation, see figure 14. This behavior is a consequence of the definition of the objective. As the residuals are squared and summed, the optimizer tries to minimize the largest residuals in order to make the total error smaller. From this point of view, it is beneficial to minimize the residuals at the end of the 0°-curve, which explains why the almost linear hardening produces a lower objective function value.
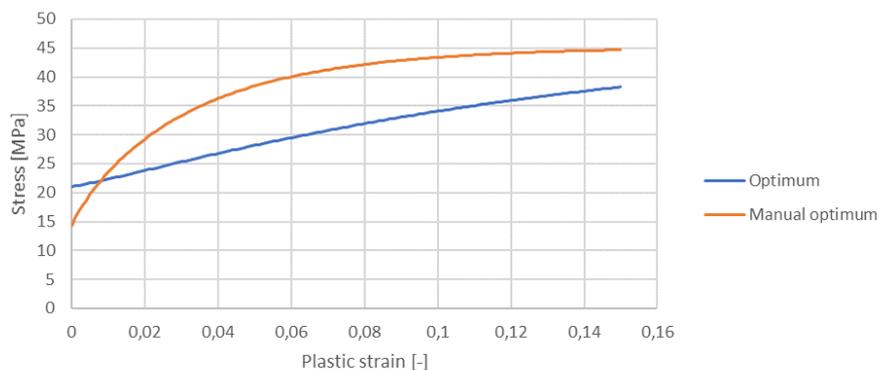
Fig.14: *Hardening curves retrieved by the optimization and the manual calibration using the approximate histories function, respectively.*

Using the approximate histories functionality in LS-OPT on the first iterations in the optimization, a manually identified optimum could also be found, displayed in figure 14. The simulation results of both the optimum and the manually found optimum can be seen in figures 15 and 16.
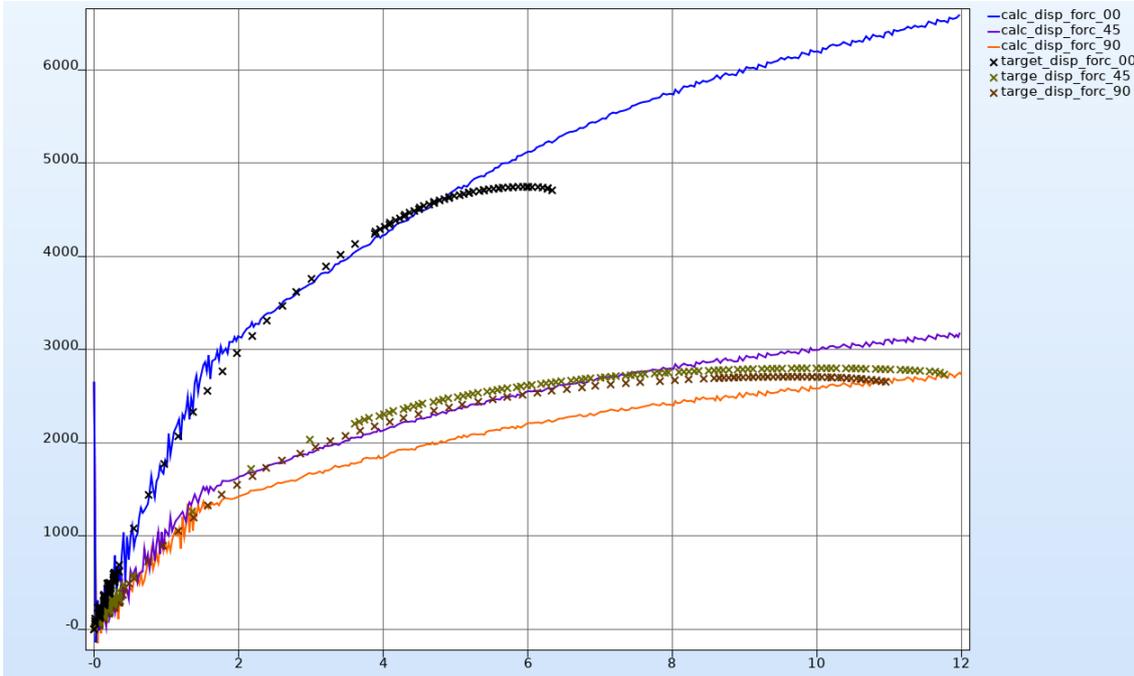
Fig.15: *Comparison of simulation and experimental results using the optimum hardening.*
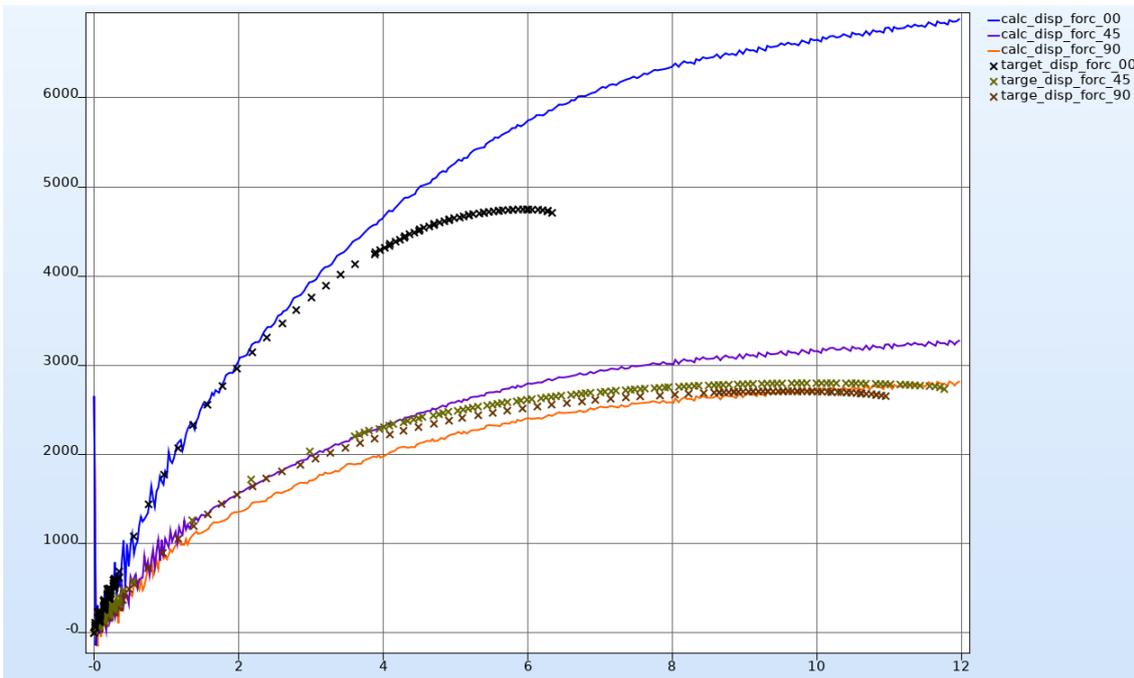
Fig.16: *Comparison of simulation and experimental results using the manually found optimum hardening.*

In the end, it was decided to use the manually identified optimum. It gives a better prediction for lower strains and provides a better compromise between the over-prediction of the 0° curve and the under-prediction of the 90° curve. It would probably have been possible to achieve a better fit in LS-OPT by adding more flexibility to the shape of the hardening curve by e.g., using a spline function parameterization instead, and possibly also shorten the experimental curve for the 0° direction or add a damage and failure model. However, the retrieved fit was considered adequate for the purposes of this study.

As can be seen in figure 17, the 0° specimen have significantly higher stress levels on the outer top layers than in the core region, both the 45° and 90° specimens have in principle the opposite characteristics. For the 45° specimen, a skewed stress field due to the unsymmetric fiber orientation bias is observed.
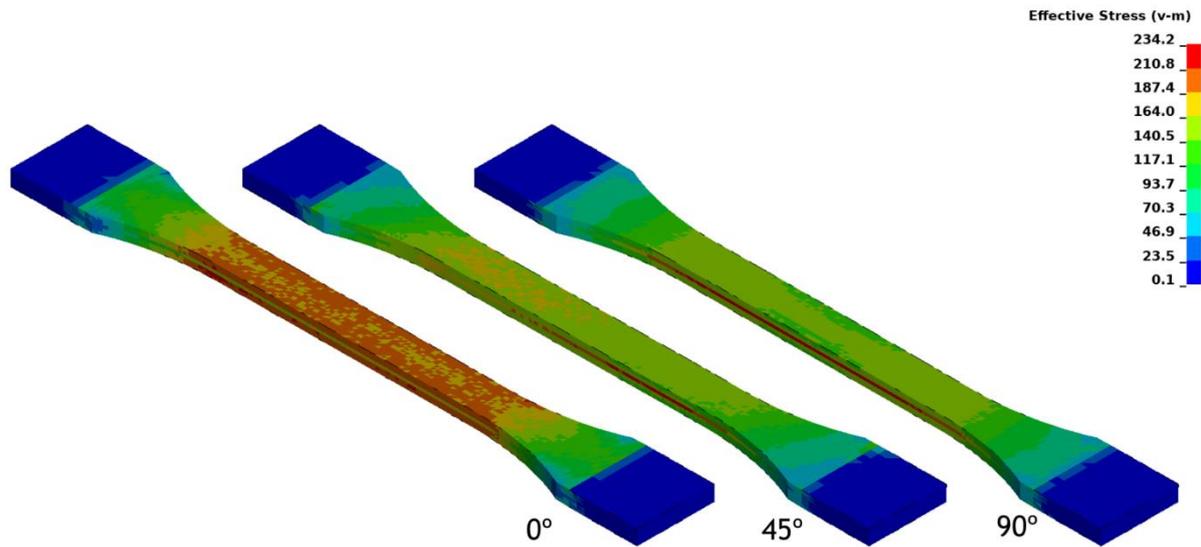
Fig.17: *Stress for the camibrated specimens*

4 Summary & Discussion

The procedure as shown can capture the anisotropy found in SFRP samples, and does so by only having different fiber orientations assigned to what is otherwise the same model and material card. It would have been possible to achieve a better fit in LS-OPT by adding more flexibility to the shape of the hardening curve by e.g., using a spline. However, the retrieved fit was considered adequate for the purposes of this study. The stresses are overpredicted at higher strains, which is consistent with the final matrix hardening input and not including any failure or damage.

The study focused on the practical aspects, in the future there might be more work done on how to capture the properties of SFRP with more accuracy, such as including failure and damage as well as including other material parameters or experiments in the calibration.

There are numerous paths and CAE tools that can produce and transfer information about fiber orientation for use in LS-DYNA simulations. Nevertheless, the principle of the methodology shown regarding transferring fiber orientations to LS-DYNA should essentially be the same for most compatible CAE software, or other testing methods for that matter.

5 Literature

[1]   Tseng, H.-C., et al.: Effect of the packing stage on fiber orientation for injection molding simulation of fiber-reinforced composites, Journal of Thermoplastic Composite Materials, 31, 2018, 1204 – 1218

[2]   Kagan, V: Optimized Mechanical Performance of Welded and Molded Butt Joints: Part II - Weld and Knit Lines Integrity, Journal of Reinforced Plastics and Composites, 22, 2003, 867 – 879

[3]   Moldex3D® Complete Brochure, Molding Innovation, www.moldex3d.com/products/product-documentation/, CoreTechSystem Co., Ltd, 2021

[4]   Tseng, H.-C., et al.: Method and Computer Readable Media for Determining Orientation of Fibers in a Fluid, U.S. Patent Pending in USPTO with Publication Application Number of US-2012/0330627-A1, 2012

[5]   Moldex3D® Material Hub Cloud, www.moldex3dmaterial.com, CoreTechSystem Co., Ltd, 2021

[6]   Envyo® User's Manual, DYNAmore GmbH, February, 2021, 90 – 98

[7]   LS-DYNA® Keyword User's Manual – VOLUME II – Material Models, LIVERMORE SOFTWARE TECHNOLOGY (LST) – AN ANSYS COMPANY, Draft (r:13775), 2021, 867 – 879

[8]   Reithofer, P., et al.: *MAT 4A MICROMEC - Theory and Application Notes, International LS-DYNA Users Conference 2018 volume 15th, 2018