FiBre MoD
Marie Skłodowska-Curie European Training Network

Benchmarking exercise II for longitudinal strength models of unidirectional composites
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Instructions for participants

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1 Goals

Several models for predicting the tensile response of unidirectional composites are available in the literature. Each of these models is based on a unique set of assumptions, and formulations vary significantly across the different models. The idea of this exercise is to compare the predictions of different models, not only with each other but also with experimental data. This comparison will focus on the tensile strength and accumulation of fibre damage in unidirectional composites.

Since every model has its own drawbacks and advantages, the goal is not to determine which model is the best. Instead, the benchmarking exercise has three goals:

1. To establish benefits and drawbacks of the different approaches.
2. To establish gaps in literature and aspects that should be improved in the future.
3. To provide a platform for researchers in this field to exchange thoughts and concerns.

In the long term, and depending on the outcome of the benchmarking exercise, the goal would be to further develop the models and move towards more practical and complex applications.

2 Modelling requirements

We would like all participants to provide us with the following results:

1. A representative full stress-strain diagram, and for each run as appendix.
2. The failure strain and strength of each run.
3. The average number of fibre breaks/volume as a function of applied strain, and for each run separately as appendix.
4. The average number of i-plets (clusters of size "i") as a function of applied strain, and for each run separately as appendix.
5. The average size of the largest cluster as a function of applied strain (rounded to the nearest integer), and for each run separately as appendix.
6. The average cluster height and average standard deviation of the axial distance of every fibre break from its cluster centre[1] as a function of applied strain, and for each run separately as appendix.
7. The time required to run each simulation, and the specific CPU and memory of the computer that was used.

All of this information should ideally be provided in Excel sheets.

We understand that your model may not be capable of providing all requested results. If so, please provide as much of the requested outputs as possible.

The definition of clusters of fibre breaks should be based on distances, as we cannot base it on stress concentrations in the experiments. All fibre breaks within a centre-to-centre distance of 4 fibre radii and a certain axial distance of another fibre break in the cluster will be considered to be part of the same cluster. The axial distance criterion will be reported separately for each of the four cases.

Some models may not be able to conform exactly to this definition, in which case you should (1) try to get as close as possible and (2) clearly describe how your definition deviates.

[1] Consider a cluster with 4 fibre breaks at z_1, z_2, z_3 and z_4. The height of this cluster would be "max(z_1,z_2,z_3,z_4)-min(z_1,z_2,z_3,z_4)", whereas the standard deviation of this cluster would become STDEV(z_1,z_2,z_3,z_4). If you average this height and standard deviation for all quadruplets at a given strain level, then you have the requested data for the quadruplets. The same procedure should be applied to all other cluster sizes.

We do not consider it practically feasible to run all the models on the same computer. All models should be run on a standard desktop PC or workstation with a maximum of 64 GB RAM. Computing clusters should be avoided to allow for a fair comparison. The reason for this limitation is that we want to get a feeling for the order of magnitude of computational power required by the different models. We will use online benchmarking tools to compare the relative speed of the CPUs.

We require at least 10 and preferably 50 runs of each model, so that the variability of strength can be assessed. We will not compare the variability of strength with experimental data in the exercise. The scatter in failure strain and strength will only be compared between the various models.

3 Model description

Some models will have inherent limitations and assumptions, while others are more flexible to incorporate various aspects. It is important to get a feeling for the benefits, drawbacks and assumptions of the various models, as it will help in interpreting the observed differences. We would therefore like all participants to provide us with a description that describes their modelling approach. An Excel template is provided where you can identify all the relevant aspects. It is important to highlight any possible changes or improvements that have been implemented compared to previously published papers.

4 Virtual comparison

We provide a complete data set, for which the participants have no prior access to the experimental results. These predictions will be 100% virtual and allow us to identify how different the model predictions are. Ideally, it would allow us to identify the causes of these differences.

4.1 Blind material set 1

The fibre, which is of unknown type, is assumed to be linear elastic and isotropic:

$$\begin{cases} E_f = 200GPa \\ \nu_f = 0.2 \\ R_f = 6\mu m \end{cases}$$

The matrix is assumed to be linear elastic-perfect plastic. That way the different modelling approaches can choose which regime they use. We will make sure to have at least one model that compares the results for both regimes. Interfacial debonding does not occur.

$$\begin{cases} E_m = 1GPa \\ \nu_m = 0.3 \\ \tau_y = 20MPa \end{cases}$$

The Weibull equation for the fibre strength that will be used is:

$$P = 1 - \exp\left(-\frac{L}{L_0} \cdot \left[\frac{\sigma}{\sigma_0} \right]^m \right),$$

With the corresponding parameters being:

$$\begin{cases} \sigma_0 = 4000 MPa \\ m = 4 \\ L_0 = 10 mm \end{cases}$$

The length of the model is 4 mm, with a total of 2000 fibres. For the models where this relevant, we recommend choosing an element length equal to the fibre diameter. For models where this is not possible or not relevant, please choose the element length that suits you. The fibre volume fraction is 50%. The type of fibre packing (hexagonal, square or random) can be chosen freely. Perfect fibre-matrix bonding is assumed and matrix cracks do not occur.

For this material set, the axial distance criterion for cluster calculations should be set to 55 times the fibre radius, which corresponds to 330 µm. If your model has an intrinsic definition of clusters, you can use a different criterion.

Residual stresses are ignored in these predictions.

4.2 Blind material set 2

The second material set used the same fibres and geometric parameters, but a significantly stiffer and stronger matrix. This allows assessing how the matrix properties affect the differences between the models.

$$\begin{cases} E_m = 5 GPa \\ \nu_m = 0.3 \\ \tau_y = 100 MPa \end{cases}$$

For this material set, the axial distance criterion for cluster calculations should be set to 13 times the fibre radius, which corresponds to 78 µm. If your model has an intrinsic definition of clusters, you can use a different criterion.

Residual stresses are ignored in these predictions.

5 Experimental comparison

The purpose of this exercise is again a blind prediction, but this time it is based on existing materials:

- Mitsubishi Grafil 34-700WD carbon fibres inside a NTPT 736LT epoxy matrix.
- Toray T700SC carbon fibres in a Sicomin SiPreg SR8500-KTA315 epoxy matrix

The modelling results will be compared with synchrotron CT data, and measurements on full-size tensile coupons.

5.1 Background information on synchrotron CT measurements

The synchrotron CT measurements were performed on double-notched tensile specimens with nominal dimensions shown in Figure 1. The specimens were cut from the panels using water jetting, which was performed by Cristofoli International Ltd. (Southampton, UK) for 34-700WD/736LT and Safire Waterjet (Southampton, UK) for T700SC/SR8500-KTA315.

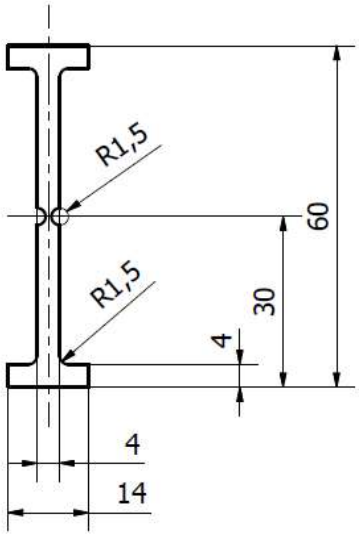

Figure 1: Dimensions of the double-notched tensile specimens for synchrotron CT.

Four aluminium end tabs of 1 mm thickness were used to reinforce the gripping areas. The fully assembled specimen and the dimensions of the end tabs can be seen in Figure 2. The end tabs were joined to the composite specimen using aerospace grade epoxy adhesive 3M Scotch-Weld EC 9323 B/A. The adhesive was cured according to the datasheet using a convection oven exposing the specimens to 100°C for 15 minutes.

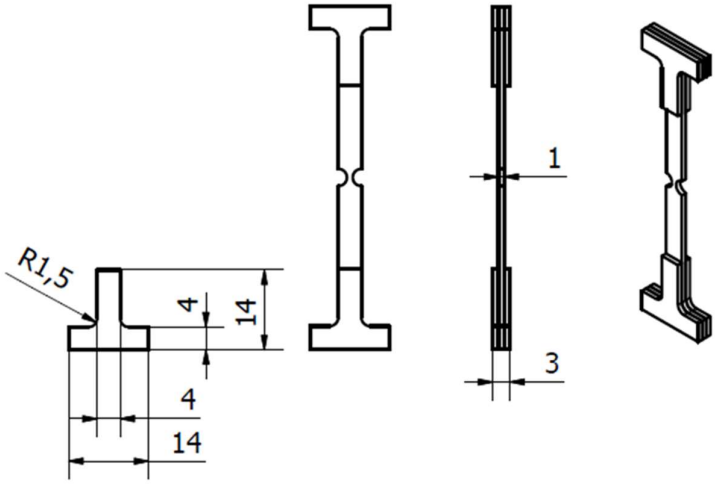

Figure 2: Dimensions of the aluminium end tabs for double-notched tensile specimens for synchrotron CT and view of the fully assembled specimen.

The specimens were not specially conditioned before testing, and the tests were performed at room temperature. The synchrotron specimens were tested on the INSA Lyon loading rig, which measured load and crosshead displacement. The displacement rate was chosen according to Table 1, leading to failure of the specimen in 7-10 min. In this timescale, we aimed to achieve 50-60 CT volumes, although the actual number varies. The actual values are mentioned in Table 1. The pixel size was 0.8 or 1.1 µm.

Table 1: Comparison of test setting for the SRCT specimens

	34-700WD/736LT	T700SC/SR8500-KTA315
Displacement rate [mm/s]	0.0014-0.0016	0.0012-0.0024
Max. Displacement [mm]	0.756-0.864	1.008-1.224
Exposure time [ms]	9	9
Projections	1000	1500
Voxel size [µm]	1.1	0.8
Volumes acquired	60	34-60
Total testing time [min]	9.1-9.3	7.6-8.3

5.2 Experimental material set 1: 34-700WD/736LT

Mitsubishi Grafil 34-700WD-24K carbon fibres with a 1.4%A sizing were used. The 736LT epoxy-based prepregs for this part of the study were provided by North Thin Ply Technology. They also provided the carbon fibre bobbins and neat resin that were used to manufacture the prepregs. The approximately 44 µm thick prepregs had a fibre areal density of approximately 38 g/m².

The prepregs were laminated into a $90°_4/0°_{10}/90°_4$ layup of 300 x 300 mm and cured in KU Leuven's autoclave. The temperature was increased from room temperature to 70°C at 2.8 K/min, after which the temperature was held constant for 60 minutes. The temperature was then increased to 120°C with a temperature ramp of 2 K/min. After 45 minutes at 120°C, the autoclave was cooled at a rate of 1.4 K/min. The autoclave was opened when the temperature had dropped below 40°C. A vacuum pressure of -0.7 bar was applied during the whole cycle. An overpressure of 5 bar was applied once the autoclave reached 70°C and until the end of the autoclave cycle. Figure 3 displays the temperature and pressure cycle. The measured temperature and pressure during the cycle will be provided in a separate Excel sheet. The legend refers to measuring points within the autoclave. Temperature Vent In describes the temperature of the nitrogen that was ventilated into the autoclave. Temperature Tray is measured at the steel tray used to form the composite plates.

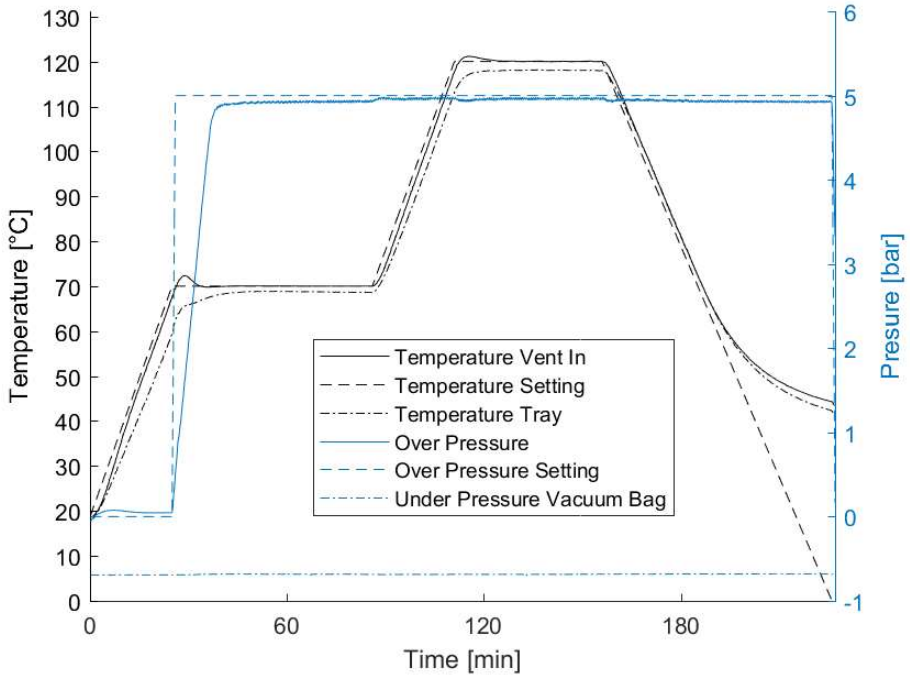

Figure 3: Autoclave curing cycle for 34-700WD/736LT

The carbon fibres are transversely isotropic and the engineering constants are provided below. The longitudinal stiffness is taken from the manufacturers' data sheet, while the other engineering constants were taken from Swolfs et al., *Stress concentrations in an impregnated fibre bundle with random fibre packing*, Composites Science and Technology 74 (2013) p. 113-120, which in turn was based on a combination of Comprehensive Composite Materials (1st edition, 2000) and Searles et al., *Micro- and mesomechanics of 8-harness satin woven fabric composites: I - evaluation of elastic behaviour*, Composites Part A 32 (2001) p. 1627–1655.

$$\begin{cases} E_{11} = 234GPa \\ E_{22} = E_{33} = 15GPa \\ G_{12} = 13.7GPa \\ G_{23} = 6GPa \\ \nu_{12} = 0.25 \\ \nu_{13} = 0.25 \end{cases}$$

The fibres are circular with a diameter of 6.5 µm. Information on the diameter variation is provided in a separate Excel sheet, but it is not expected that you include this in your model.

Many different versions of the Weibull equation exist, and they are crucial in the modelling predictions. Here, we will use the standard, unimodal distribution, as this seemed to fit the experimental data well:

$$P = 1 - \exp\left(-\frac{L}{L_0} \cdot \left[\frac{\sigma}{\sigma_0} \right]^m \right)$$

The entire stress-strain diagram of the matrix will be provided as a separate Excel file. This will contain tensile, compressive and shear stress-strain diagrams. The tensile and compressive diagrams are coming directly from measurements, whereas the shear stress-strain diagrams are derived from a constitutive model based on the tensile and compressive diagrams. The used constitutive model is described in "*X. P. Morelle, J. Chevalier, C. Bailly, T. Pardoen, and F. Lani. Mechanical characterization and modeling of the deformation and failure of the highly crosslinked RTM6 epoxy resin. Mech. Time-Depend. Mater., 21(2):419 – 454, 2017.*" The Poisson's ratio was measured to be 0.39 using 2D digital image correlation. We have calculated two types of yield point in our Excel sheets: 0.2% plastic strain point and the local maximum. For models using perfect plasticity, we suggest to use the local maximum.

In case you need them, we have estimated the coefficients of thermal expansion to be:

$$\begin{cases} CTE_m = 62,5 \cdot 10^6 \, / \, ^\circ C \\ CTE_{f,long} = -0,56 \cdot 10^6 \, / \, ^\circ C \\ CTE_{f,\text{trans}} = 5,6 \cdot 10^6 \, / \, ^\circ C \end{cases}$$

We suggest to model a 0° ply with a length of 1.2 mm and a total of 5850 fibres. This corresponds to a rectangular cross-section of 0.913 by 0.44 mm. For the models where this is relevant, we recommend choosing an element length equal to the fibre diameter. The fibre volume fraction is $48.32 \pm 0.44\%$. You are also welcome to model the entire specimen, including the 90° plies and notch geometry, but we do not expect you to do so. The cross-

section is nominally rectangular, but due water jetting some degree of tapering occurred. If needed, we can provide more information on the shape.

For this material set, the axial distance criterion for cluster calculations should be set to 15 times the fibre diameter, which corresponds to 97.5 µm. If your model has an intrinsic definition of clusters, you can use a different criterion.

5.3 Experimental material set 2: T700SC/SR8500-KTA315

The format of the data for the second material combination will be the same. The fibre is a T700SC-12K-50C carbon fibre from Toray Industries with 1%A sizing. The pre-pregging resin was supplied by Sicomin, specifically the SiPreg SR8500 KTA315 system was used. The prepreg was produced in house on a drum winding machine at KU Leuven. The prepregs had a fibre areal density of approximately 172 g/m², corresponding to a cured ply thickness of approximately 165 µm.

The prepregs were laminated into a $90°/0°_2/90°$ layup of 300 x 300 mm at KU Leuven and cured in KU Leuven's autoclave. The temperature was increased from room temperature to 70°C at 2.8 K/min, after which the temperature was held constant for 60 minutes. The temperature was then increased to 120°C with a temperature ramp of 2 K/min. After 90 minutes at 120°C, the autoclave was cooled at a rate of 1.4 K/min. The autoclave was opened when the temperature had dropped below 40°C. A vacuum pressure of -0.7 bar was applied during the whole cycle. An overpressure of 5 bar was applied once the autoclave reached 70°C and until the end of the autoclave cycle. An overview of the curing cycle can be seen in Figure 4. The measured temperature and pressure during the cycle will be provided in a separate Excel sheet.

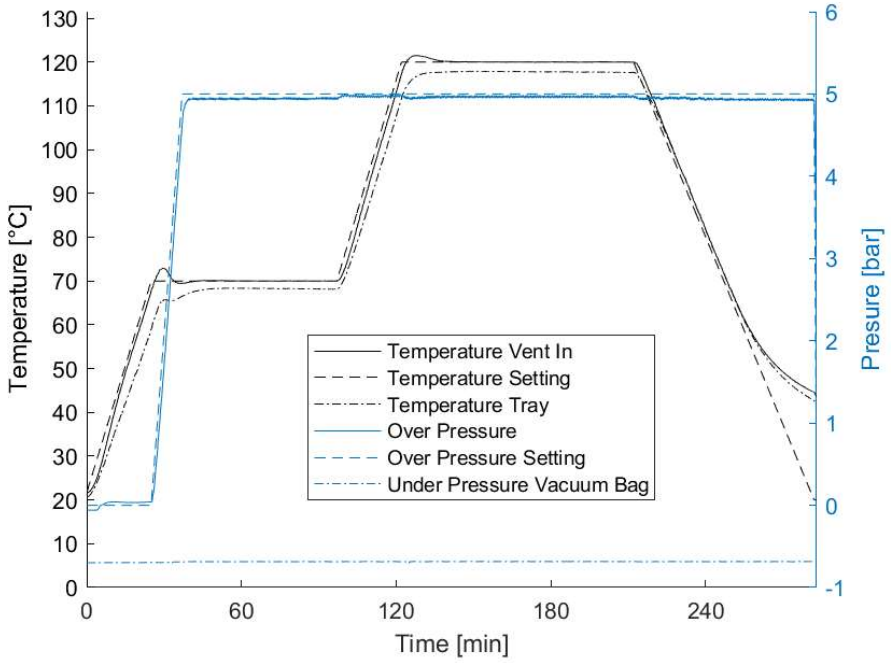

Figure 4: Autoclave curing cycle for T700SC/SR8500-KTA315

Given the similarities between T700SC and 34-700WD, we will assume they have the same off-axis moduli, Poisson's ratio and coefficients of thermal expansion. The longitudinal

modulus of T700SC, however, is a bit lower: 230 GPa (versus 234 GPa for the 34-700WD carbon fibres). The fibre diameter is 6.8 µm.

SiPreg SR8500-KTA315 is an epoxy resin from Sicomin. It is highly cross-linked, and relatively similar to 736LT. This resin will also be fully characterised in the same manner as the 736LT resin. The Poisson's ratio was measured to be 0.42 using 3D digital image correlation. We have calculated two types of yield point in our Excel sheets: 0.2% plastic strain point and the local maximum. For models using perfect plasticity, we suggest to use the local maximum.

We suggest to model a 0° ply with a length of 1.2 mm and a total of 4430 fibres. This corresponds to a rectangular cross-section of 0.74 by 0.376 mm. For the models where this relevant, we recommend choosing an element length equal to the fibre diameter. The fibre volume fraction is 57.9 $\pm$ 0.7%.

For this material set, the axial distance criterion for cluster calculations should be set to 15 times the fibre diameter, which corresponds to 102 µm. If your model has an intrinsic definition of clusters, you can use a different criterion.

6 Size scaling

Size scaling is an important feature of the models, as the model size is often many orders of magnitude smaller than the test coupons or components. We therefore would like to compare the size scaling effects in all participating models, both for cross-sectional scaling and length scaling. For this study, we will use the material input from section "5.2 Experimental material set 1", although we will not compare against experimental data for this case. You should aim to model at least 4 different sizes and run enough models per size to allow reliable determination of trendlines through your data.

For length scaling, we will fix the number of fibres to 1000. We suggest to start at gauge lengths of 0.5 mm, and then go as large as your model allows.

For cross-sectional scaling, we will fix the gauge length to 5 mm. We suggest to start with as few fibres as your model allows and go up to as many as possible.

7 Future work

We would like to explicitly highlight some areas where the benchmarking exercise could benefit from further elaboration in a second stage. These areas can be further explored by interested participants at a later stage, either on an individual, bilateral or even broader scale. Where possible, we are already trying to provide all the necessary data to all participants. These areas will be discussed in detail at the meeting that we will organise in 2019 to discuss the outcome of the exercise.

Here are a few areas that we see as potentially useful to explore:

- We ask participants to use a unimodal distribution for fibre strength, even though other options are possible. We will provide all individual measurements so participants can also fit other distributions through this for follow-up studies.
- There are many different ways to characterise cluster development. We chose a criterion that is not too difficult to implement, so the definitions are as consistently as possible for all models and the experiments. However, we recognise that any cluster criterion is going to be arbitrary or subjective to some extent. We suggest that a statistical cluster

analysis (see https://en.wikipedia.org/wiki/Cluster_analysis) is performed afterwards to analyse this in more detail. We will aim to provide all xyz locations for all fibre breaks in the experiments to facilitate such studies.

- We gathered experimental time-temperature dependency for the matrix systems, and this can be subject of more detailed comparisons. However, as most models cannot include this, we decided not to make it part of the core of the exercise.
- We measured the matrix properties on large scale specimens, even though we realise that the microscale properties may be significantly different. Other measurement techniques, such as nano-indentation or microscale epoxy fibres, could be explored to achieve more representative matrix properties.