STOCHASTIC MULTI-SCALE MODELLING OF SHORT- AND LONG-RANGE EFFECTS IN TEXTILE COMPOSITES BASED ON EXPERIMENTAL DATA

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Keywords: textile composites, variability, multi-scale simulation

Abstract
Realistic virtual textile composites are generated of a carbon-epoxy 2/2 twill woven composite. Each specimen, spanning ten by ten unit cells, possesses the short- and long-range variability characterised from experimental samples in prior work. A stochastic multi-scale modelling approach is presented to simulate many random reinforcements as combination of average trends with zero-mean deviations. Depending on the presence of cross-correlation, either the Monte Carlo Markov Chain method or Series Expansion technique is applied to generate the tow path deviations. Virtual specimens are acquired in the WiseTex format that reproduce the statistical information of the experimental samples on average.

1. Introduction

The internal architecture of textile composites is subjected to a significant amount of variability. A realistic description of the tow reinforcement with corresponding mechanical properties is needed in order to perform reliable numerical analyses of composites structures. Such a representation can only be achieved by [1]: (i) collecting sufficient statistical information of the uncertain tow path parameters on the short- and the long-range by experiments, and (ii) deriving probabilistic information for the macroscopic mechanical properties from the lower scale mechanical characteristics.

This paper presents the general approach and successive steps to build random virtual specimens of a twill 2/2 woven carbon-epoxy composite. The procedure of Vořechovský [2] is applied for generating random fields of the cross-correlated in-plane centroid. The obtained stochastic deviations are combined with the short-range tow path parameters using the Monte Carlo Markov Chain method [3]. The objectives of the paper are to (i) present a stochastic multi-scale modelling approach, (ii) produce the zero-mean deviations using appropriate generator algorithms and (iii) construct a macro-scale random virtual specimen in the WiseTex software.
2. Quantification of the short- and long-range variability

The developed methodology is applicable to any textile composite and is demonstrated for a 2/2 twill woven carbon fabric from Hexcel (G0986) [4]. The dry reinforcement is impregnated with epoxy in a resin transfer moulding (RTM) process. A virtual representation of the unit cell is given in figure 1 with $\lambda_x=11.43$ mm and $\lambda_y=11.43$ mm, respectively the periodic lengths of warp (x-axis) and weft (y-axis) tows.

![WiseTex model of a 2/2 twill woven reinforcement. The x-axis and y-axis of the coordinate system are respectively parallel to the warp and weft direction.](image)

The full tow path is characterised on the short- and long-range for the centroid coordinates and cross-sectional parameters. Considering the production process of the 2/2 twill woven fabric, warp tows can be represented by one representative tow, called genus, and similar for the weft tows. The statistical information is quantified in terms of average trends, standard deviation and correlation information. Correlation is investigated along a single tow, called auto-correlation, and between neighbouring tows of the same genus, named cross-correlation.

Short-range variations are identified in [5] from a seven-ply unit cell sample using micro-CT. The spatial information of each tow parameter is afterwards decomposed in periodic, non-stochastic trends and non-periodic, stochastic deviations. All tow characteristics, with exception of the in-plane centroid, vary within the unit cell dimensions. This is indicated by the correlation length which exceeds the unit cell size for the in-plane position [5]. The in-plane centroid is also subjected to the largest variability with a weak dependency between neighbouring tows, both for the warp and weft genus.

Additional data of the in-plane centroid are collected on larger samples in [6]. The in-plane dimension of two single-ply composite samples, spanning thirteen by thirteen unit cells, is quantified using optical imaging. In-plane positions are derived from the digital images, of which one is shown in figure 2. The in-plane warp and weft undulations are further considered respectively in y- and x-direction, and decomposed in a non-periodic handling trend and zero-mean deviations. A detailed discussion of the procedure and results are given in [6].

The short- and long-range statistics are used as input to generate virtual specimens. All deviations are approximately normal distributed with a summary of the statistical information given in table 2. Only the in-plane centroid is cross-correlated between neighbouring tows.
Figure 2. Digital image of a single ply 2/2 twill woven carbon-epoxy composite. Warp and weft tows are respectively positioned horizontally and vertically. The red square indicates the region where the in-plane position is quantified.

<table>
<thead>
<tr>
<th></th>
<th>x [mm]</th>
<th>y [mm]</th>
<th>z [mm]</th>
<th>AR [-]</th>
<th>A [mm²]</th>
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<tbody>
<tr>
<td>$σ_{warp}$ [mm]</td>
<td>-</td>
<td>0.106</td>
<td>0.014</td>
<td>1.774</td>
<td>0.023</td>
</tr>
<tr>
<td>$ξ_{auto}$ [mm]</td>
<td>-</td>
<td>114.89</td>
<td>1.78</td>
<td>7.26</td>
<td>2.53</td>
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<tr>
<td>$ξ_{cross}$ [mm]</td>
<td>-</td>
<td>4.49</td>
<td>-</td>
<td>-</td>
<td>-</td>
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<tr>
<td>$σ_{weft}$ [mm]</td>
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<td>-</td>
<td>0.015</td>
<td>1.440</td>
<td>0.024</td>
</tr>
<tr>
<td>$ξ_{auto}$ [mm]</td>
<td>52.89</td>
<td>-</td>
<td>1.62</td>
<td>5.48</td>
<td>1.01</td>
</tr>
<tr>
<td>$ξ_{cross}$ [mm]</td>
<td>13.16</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 1. Standard deviation, auto- and cross-correlation length of the tow path parameters.

3. Stochastic multi-scale modelling

Virtual textile specimens, spanning a region of ten by ten unit cells, are generated that are representative for a ply within a laminate. The approach is presented in figure 3. First, a two-dimensional lattice is constructed with rows representing warp tows and columns representing weft tows. The grid length in x- and y-direction is equal to the experimentally derived unit cell dimensions. Next, the reinforcement of each specimen is built by combining the systematic and handling trends with zero-mean deviations. While the systematic and handling trends are taken from the experimental data, stochastic deviations are generated using different generator techniques. Tow path parameters which vary within the unit cell size (out-of-plane centroid, tow area and tow aspect ratio) with no cross-correlation are generated using a Monte Carlo Markov Chain algorithm for textile structures [3]. Cross-correlated in-plane centroid deviations are produced as Gaussian random fields using a methodology described by Vořechovský [2]. A virtual model of the textile composite is obtained in the WiseTex format [7] by overwriting the original tow path information of a nominal WiseTex representation.
3.1. Generation of short-range parameters

The zero-mean deviations of the out-of-plane centroid, area and aspect ratio are generated using the Markov Chain algorithm for textile structures [3]. Deviations are produced (i) independently for each tow parameter at the same grid location and (ii) also independently from any parameter value at neighbouring tows. This method is thoroughly discussed in [8] for the generation of random unit cell structures. When using this approach for the simulation of larger samples, a larger grid is considered that spans the length of ten unit cells. Smoothing is applied using information of ±2 neighbouring grid points to remove the unphysical low-amplitude short-range spikes present in the discretized tow path. A representation of the random out-of-plane centroid for one unit cell is given in figure 4.

![Figure 4. The warp out-of-plane tow centroid for a single unit cell, generated using the Markov Chain procedure. The smoothing operation removes the unphysical spikes present in the path.](image)

The standard deviations and auto-correlation lengths of single unit cells, corresponding to the thousand generated specimens, are centered around the experimental target values. Smoothing has limited effect on the standard deviation, while the correlation lengths are slightly shifted to higher values. This is demonstrated for the z-centroid of the warp tows in figure 5. Similar conclusions are made for the other tow parameters and the weft tows.

3.2. Generation of the long-range in-plane centroids

The in-plane centroid deviations must be produced simultaneously for all tows of the same genus in order to model the cross-correlation correctly. A methodology proposed by Vőrechovský [2] is applied where series expansion methods based on Karhunen-Loève decomposition produce cross-correlated Gaussian random fields. Within a virtual specimen, in-plane positions
of each tow are modelled as Gaussian random fields \( H_i \). Tows belonging to the same genus possess an identical auto-correlation structure and are at the same time cross-correlated with neighbouring tows of the same type by introducing cross-correlated random variables:

\[
H_i(x, \theta) = \sum_{j=1}^{N_i} \lambda_{ij} \chi_{D,i,j}(x)
\]

with \( \lambda_i \) and \( \phi_i \) the eigenvalues and eigenvectors of the auto-correlation structure and \( \chi_{D,i,j} \) the cross-correlated random variables belonging to field \( H_i \). Random fields of the in-plane centroids of warp and weft tows are simulated using a truncated series. Only the largest eigenvalues and corresponding eigenvectors are considered in the procedure. The error introduced by the reduction is fixed to maximum 0.9975, meaning that 99.75% of the variability is captured.

\[
\sigma_{\text{comb}} < \sigma_{\text{spec}} > \xi_{\text{auto}} \xi_{\text{comb}} \xi_{\text{spec}} < \xi_{\text{cross}} \xi_{\text{comb}} \xi_{\text{spec}}
\]

<table>
<thead>
<tr>
<th></th>
<th>( \sigma_{\text{comb}} )</th>
<th>( &lt; \sigma_{\text{spec}} &gt; )</th>
<th>( \xi_{\text{auto}} )</th>
<th>( &lt; \xi_{\text{auto}} &gt; )</th>
<th>( \xi_{\text{comb}} )</th>
<th>( &lt; \xi_{\text{comb}} &gt; )</th>
<th>( \xi_{\text{spec}} )</th>
<th>( &lt; \xi_{\text{spec}} &gt; )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Warp tows [mm]</td>
<td>0.106</td>
<td>0.103</td>
<td>115.81</td>
<td>114.00</td>
<td>4.54</td>
<td>4.42</td>
<td></td>
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</tr>
<tr>
<td>( \Delta_{\text{warp}} ) [-]</td>
<td>0.09%</td>
<td>3.48%</td>
<td>0.80%</td>
<td>0.78%</td>
<td>1.03%</td>
<td>1.72%</td>
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<tr>
<td>Weft tows [mm]</td>
<td>0.613</td>
<td>0.570</td>
<td>52.95</td>
<td>52.76</td>
<td>13.10</td>
<td>13.05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \Delta_{\text{weft}} ) [-]</td>
<td>0.28%</td>
<td>7.38%</td>
<td>0.12%</td>
<td>0.25%</td>
<td>0.45%</td>
<td>0.87%</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Standard deviation and correlation lengths of the in-plane deviations for the combined data set and average values for the individual specimens.

The generated deviation trends demonstrate good agreement with the experimental in-plane deviations as shown in figure 6. The short wavelength of the experimental warp fluctuations and long wavelength of the measured weft deviations are reproduced without an additional smoothing operation. The statistical information of the in-plane tow positions are verified for the combined data set and the individual specimens. The normalised difference \( \Delta \) from the experimental values in table 2 is defined as \( \Delta = \frac{|\epsilon_{\text{exp}} - \epsilon_{\text{sim}}|}{\epsilon_{\text{exp}}} \cdot 100 \), with \( \epsilon \) equal to the standard deviation, auto-correlation length or cross-correlation length. An overview of the produced statistics is given in table 3.2. The standard deviation \( \sigma \) and correlation lengths of the combined data set demonstrate that the series expansion method reproduces the experimental data within \( \Delta=1\% \) difference of the target data. The statistics of the individual specimens show good agreement with the experimental values. In figure 7, the histogram is shown of all simulated auto- and cross-correlation lengths for the warp tows. The mean of the generated correlation lengths has a normalised error \( \Delta \) which is less than 7.4\% for the standard deviation and maximum 1.72\% for the correlation lengths.
When considering the statistical information of individual tows, significant differences are present between simulations and experiments. However, produced correlation lengths of the 1-D random fields are of the same order of magnitude. This discrepancy is expected to originate from the normality assumption of the distribution and the fitted input correlation functions which only approximate the real correlation trend.

3.3. Virtual specimens in the WiseTex format

Descriptions of the random tow reinforcement are obtained as combination of the systematic and handling trends with the zero-mean deviations. Each tow is constructed by defining the path length and the orientation vectors that fix each cross-section in space [8, 9].
of the tow parameters is accompanied by a recalculation of the final unit cell dimensions and properties. A stochastic representation in the WiseTex software [7] is acquired using the XML-structure. The nominal tow paths and unit cell properties are overwritten in the original WiseTex XML-file by the updated information of the random tow paths. An arbitrary virtual 2/2 twill woven composite is shown in figure 8. Due to the independent generation of the tow width from the in-plane position, limited interpenetration is present between neighbouring tows of the same genus. Small adaptations are thus required when transforming to a finite element model.

![Virtual specimen in the WiseTex format. The in-plane dimension and a single unit cell is presented to demonstrate the short- and long-range variability.](image)

**Figure 8.** Virtual specimen in the WiseTex format. The in-plane dimension and a single unit cell is presented to demonstrate the short- and long-range variability.

### 4. Conclusions

Virtual specimens are generated of a carbon-epoxy 2/2 twill woven composite that span a region of ten by ten unit cells. In a first step, experimental data of the centroid locations and cross-sectional shape are collected on the short- and long-range. Except for the in-plane centroid, all tow path parameters vary within unit cell dimensions. Next, virtual specimens are constructed as mean patterns combined with zero-mean deviations possessing the target statistics. The tow parameters without cross-correlation are generated with a Monte Carlo Markov Chain, while the cross-correlated in-plane centroid is produced based on Karhunen-Loève expansions. All simulated tow deviations achieve the target statistics. Virtual models are introduced in the WiseTex format that can subsequently be used for application of structural, forming or impregnation analysis.

### Acknowledgements

This study is supported by the Flemish Government through the Agency for Innovation by Science and Technology in Flanders (IWT) and FWO-Vlaanderen.
References


