Determination of the composite’s representative volume for longitudinal tensile test simulations

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Abstract. In this study the proper size of the composite material’s representative volume element is addressed. Longitudinal tensile test simulations are conducted for a range of sizes and several variants of material models for matrix, fibre and interface. It is found, that matrix and interface degradation with prescribed properties do not influence the value of failure engineering stress for the cell in comparison with model, where only fibre damage model is set, and the adequate size of the cell is shown to be 80 µm. In contrast, variant contained stochastic fiber strength distribution shows different value for engineering failure stress and strain and suggests larger size of the material cell for simulations. Received results might be useful for accurate micromechanical modelling of material testing.

1. Introduction
Composite materials go on changing aerospace industry. On the other hand, smart use of the unique properties of the composite materials requires the precise understanding of their behavior in loading conditions, which is traditionally addressed by testing. In material and structures testing routine size of the sample is one of the key factors, that influences a resulting failure mode. Scaling geometrical parameters of the testing specimen in simulations in virtual environment plays the same role. Furthermore, considering the simulations on the micro-scale level, performed within finite element method (FEM), size of the representative volume element (RVE) also impacts objectivity of the results, which means that obtained results for homogenized properties depend on the chosen dimensions of the RVE. For this reason, validating the results of the micro-scale simulations must include checking them for different sizes of RVE and/or ensuring special conditions are met, like well-known Hill’s condition [1].

Field of application of the RVE simulations falls into several most observable categories: analysis of heterogeneous material aimed to define homogenized material properties for upper-level simulations, like transferring from fiber-matrix-interface properties to layer properties; failure analysis of bulk material, outside the stress-concentration effects, with a goal of producing appropriate micro-mechanics based failure criteria for the composite layer; analysis of composite material with minimum of assumptions, e.g. boundary-conditions to provide regular stress-strain state. The latter technique approaches contemplating the damage process on constituents level in particular zones of testing sample, like crack propagation zone in notched specimen. Such zones of interest, like free edges, were studied with micro-mechanical cell, embedded in multidimensional stacking sequence [2]. What more, this type of analysis might be used in simulations of micro specimens testing of composite materials, which to authors view presents a reasonable extension of existing micro-scale methods and supplement to building proper multi-scale approach.
For no doubt, the intrinsic property of all micro-scale modeling is significant numerical resources consumption. That’s why the sufficient size of the RVE for exact case, like applied loads configuration, is of a great deal.

The consistency of chosen RVE should be discussed. There are several developed criteria, with an applicability depending on the type of the task: whether the aim is to calculate the effective properties or recognize the damage patterns on micro-scale. A remarkable effort of examining the dependencies between the RVE size and convergence of different relevant metrics of the received strain-stress state were performed for the case of transverse tension in the work of Trias [3]. Although, the referenced paper considered transverse tension case, the upper boundary of the RVE side was taken from the reported results:

\[ \delta_{\text{max}} = \frac{r_f}{a} = \frac{50}{a_{\text{max}}} = r_f \delta_{\text{max}}. \]  

(1)

In expression (1) \( \delta \) – is a RVE size parameter, introduced by Trias, \( r_f \) – is fiber radius, \( a \) – is a side dimension of the cubic RVE.

In the current study the problem of equivalence of the RVE to the chosen material is solved by certain parameters of the Nearest Neighborhood Algorithm (NNA) and back-calculated properties of fiber modulus and strength from properties of homogenized layer and matrix.

Longitudinal tensile failure generally can be thought as ultimate failure of ply and overall laminate. The most straightforward way to obtain lamina tensile strength is to perform a longitudinal tensile test like ASTM D3039 procedure [4]. Size effect was widely studied for direct tension test [5]. Experiments showed significant size effect when Weibull module is in the range 13-29 [5]. Analysis techniques are widely developed in different frames like continuum damage mechanics [6], based on classical but still effective fiber-bundle models [7-9]. Permanent experimental and numerical effort is maintained [10] Finite element based numerical approaches, primarily concern ply level and a number of comprehensive efforts exist [11]. There is a justified tendency to study the damage state of the material on micro-level [12,13]. One of the common lines in conclusions of referenced studies is the contribution of weak interface to the evolution of damage in composite material, then accounting for this phase becomes a must in any failure modeling of multiphase systems. Recently, the augmented finite element techniques have been introduced in the micro-scale failure domain [12,13]. Unfortunately, to author’s knowledge, just a limited number of studies are devoted to the problem of longitudinal tensile failure on micro-scale level. The detailed analysis was conducted by Mishnaevsky [14,15], where the effects of random fiber-strength distribution, viscosity of matrix, matrix cracking, interface defects on damage state of the model were studied. Unfortunately, the simulations were conducted on relatively small RVE, containing 20 fibers, and the influence of the RVE size has not been estimated.

This research studies the influence of RVE size for longitudinal tensile failure modeling. The hypothesis taken is that failure tensile stress will converge to a certain value with rising the dimensions of testing volume of the material. Thus, the size, starting from which the failure stress becomes nearly constant will be decided as minimum necessary for simulations of longitudinal tension. The influence of fiber strength distribution is also considered by drawing the certain value of tensile strength with known from literature parameters of Weibull law [16].

2. Methods and materials

In this paper we conduct virtual tensile test on the RVE of different sizes. The starting range of sizes for the side of cubic RVE was between 20 \( \mu \)m and 175 \( \mu \)m and additional simulations would be performed in the ranges of interest, observed from the results of first series of simulations for starting range.

For each of the RVE size in the range several variants of models were prepared in Abaqus/CAE [17] to estimate influence of certain parameters on the magnitude of the failure load along fiber direction (table 1).
Table 1. Model variants.

| Feature                        | Variant 1 | Variant 2 | Variant 3 |
|--------------------------------|-----------|-----------|-----------|
| Random fiber distribution      | yes       | yes       | yes       |
| Stochastic fiber strength      | no        | no        | yes       |
| Fiber damage                  | yes       | yes       | yes       |
| Matrix and interface damage    | no        | yes       | yes       |

2.1. Ply material
Material used is representative of advanced polymers reinforced with continuous carbon fibers. Fiber volume fracture is around 59% and this value is slightly adjusted due to the limitations of RVE generation algorithm [18]. Properties of virtual unidirectional ply are presented in table 2.

Table 2. Composite ply material properties.

| Property               | Designation, units | Value    |
|------------------------|--------------------|----------|
| Fiber volume fracture  | \(V_f\), %         | \(\approx 59.5\) |
| Tensile strength       | \(F_{tt}\), MPa    | 2200     |

2.2. Fibres
High-strength carbon fibres common to T300 are used. The angle of misalignment is not considered in this study, so all of the fibres are modelled as straight cylindrical bodies. Due to the lack of information about fibre strength properties, the following procedure was made to deliver values to material model of fibre. First, fibre strength is back-calculated from ply strength with rule of mixture (ROM) formula (2) [19]:

\[
F_{tt} = \left[ V_f + \frac{E_m}{E_f} (1 - V_f) \right] \rightarrow F_f = \frac{F_{tt}}{V_f + \frac{E_m}{E_f} (1 - V_f)}
\]  

(2)

Obtained value of fibre strength is assumed to equal to average fibre strength and prescribed as fibre strength in simulations for model variant 1 and model variant 2. So that mechanical properties of fibre and received fibre tensile strength are close to T300 carbon fibre, for model variant 3 it was decided to use stochastic fibre strength properties, calculated for Weibull modulus \(m\) and guage length \(L_0\) of T300 fibres. For all sizes of the cell in the range, scale parameter of Weibull distribution \(\sigma_0\) corresponds to gage length \(L_n = 1\) mm. The expressions (3-4) were used [11,15]:

\[
\sigma_0' = \frac{\sigma_0}{\Gamma \left(1 + \frac{1}{m} \right)}
\]  

(3)

\[
\sigma_{av} = \sigma_0' \left( \frac{L_n}{L_0} \right)^{-\frac{1}{m}}
\]  

(4)

\(\sigma_{av} = F_{tt}\) – average fiber strength used for model variant 1 and model variant 2; \(\sigma_0'\) – Weibull scale parameter for \(L_0\) gage length, \(\sigma_0'\) – Weibull scale parameter for \(L_n = 1\) mm gage length, \(m\) – is a Weibull shape parameter of T300 carbon fiber, \(\Gamma\) – is gamma function. Fibre radius \(r_f\) is taken to be 3.5 µm. Properties of the fibers are presented in table 3.
Table 3. Fiber material properties.

| Property         | Designation, units | Value |
|------------------|--------------------|-------|
| Young’s moduli   | $E_f$, GPa         | 230   |
| Poisson’s ratio  | $\mu_f$           | 0.2   |
| Tensile strength | $F_{ft}$, MPa      | 3665  |
| Fracture energy  | $G_f$, N/m         | 5     |
| Density          | $\rho_f$, g/cm³    | 1.75  |

2.3. Matrix

Typical elastic properties of epoxy resin from literature [20] were input for simulations. Failure of matrix is modelled using Von Mises plasticity, which is attainable, when primary loading is tension. Material properties of matrix are presented in table 4.

Table 4. Matrix material properties.

| Property         | Designation, units | Value |
|------------------|--------------------|-------|
| Young’s moduli   | $E_m$, GPa         | 3.1   |
| Poisson’s ratio  | $\mu_m$           | 0.38  |
| Tensile strength | $F_{mt}$, MPa      | 80    |
| Fracture energy  | $G_m$, N/m         | 5     |
| Density          | $\rho_m$, g/cm³    | 1.2   |

2.4. Interface

The interface between matrix and fibre was given a built-in cohesive contact behaviour [17], which consists of three parts. Initial constitutive behaviour is related to uncoupled linear traction-separation law, i.e. total stress depends on the total displacement jump across interface. In this part each component of total stress depends linearly on respective displacement jump with penalty stiffness $K$ in equation (5), which is expressed by:

$$
\begin{bmatrix}
t_n \\
t_s \\
t_t
\end{bmatrix} = 
\begin{bmatrix}
K_{nn} & 0 & 0 \\
0 & K_{ss} & 0 \\
0 & 0 & K_{tt}
\end{bmatrix}
\begin{bmatrix}
\delta_n \\
\delta_s \\
\delta_t
\end{bmatrix} = K \delta
$$

(5)

$t$ – a traction vector, $K$ – contact penalty stiffness matrix, $\delta$ – separation vector. Damage process in contact starts after meeting the quadratic stress criterion, described by equation (6):

$$
\left(\frac{t_n}{t_n^0}\right)^2 + \left(\frac{t_s}{t_s^0}\right)^2 + \left(\frac{t_t}{t_t^0}\right)^2 = 1
$$

(6)

$t_n^0$, $t_s^0$, $t_t^0$ – nominal normal and two shear components of traction. Damage process itself is described in energy terms, that are collected in Benzeggagh-Kenane [17] criterion with exponent $\eta = 1.2$. Prescribed properties of the interface are shown in table 5.

Table 5. Interface cohesive contact properties.

| Property                  | Designation, units | Value |
|---------------------------|--------------------|-------|
| Maximum normal traction   | $t_n^0$, MPa       | 42    |
| Maximum shear traction    | $t_s^0 = t_t^0$, MPa | 63    |
| Normal fracture energy    | $G_n^s$, N/m       | 2     |
| Tangential fracture energy| $G_s^c = G_t^c$, N/m | 30    |
| Benzeggagh-Kenane exponent| $\eta$            | 1.2   |
2.5. Model
Pre-processing of the model was made in Abaqus/CAE and by means of the Python code, which consisted of the following:

- Database of varied mechanical properties and RVE sizes (Excel spread-sheet);
- Fibres spatial arrangement generator;
- Abaqus script for building RVE assembly, meshing, properties assignment and analysis job submission.

2.5.1. Input database. A range of material failure properties was combined with a range of RVE sizes to acquire representative set of analysis models.

2.5.2. Fibres spatial arrangement. The microscopic digital image analysis data presented in [21] was used to extract fibre diameters and x,y coordinates of each fibre centre. The data extracted was used to generate statistical functions that characterise the morphology of the CFRP (carbon fibre reinforced plastic) microstructure. There exist a number of algorithmic implementations to build the fibre distributions, among them: nearest neighbour algorithm (NNA, [18]), second-order intensity and radial distribution functions. The NNA was used to generate high-volume fraction fibre distributions that are statistically equivalent to the CFRP microstructure.

2.5.3. Abaqus script for building RVE. With the extensive use of Abaqus embedded Python scripting capabilities [17], a fully automated tool for generating RVE models was developed.

2.6. Finite element model
Three model variants of the model were assessed. Basic one included a single part, which had merged bodies of fibres and matrix. This way, the perfect interface was assumed. In the second variant, RVE had separate parts for fibres and matrix, while interface was defined within cohesive surfaces method. Strength of fibre, which drives tension performance in longitudinal direction, is modelled by prescribing artificial yield stress equal to back-calculated fibre-strength and nearly zero plastic strain at damage initiation point. After this point, the fibre material state follows energy-based damage evolution law, defined within Ductile Damage properties in Abaqus [17]. Fracture toughness value choice is explained by two reasons: first, to overcome the instantaneous failure of material that might cause numerical problems, and second – not to change the brittle type of failure, natural to CFRP. Third variant of the model considered different strength of fibres, with accordance to single shape Weibull distribution.

Boundary conditions mimicked the uniaxial stress loading along fibre direction, parallel to global Z axis. Motivation for used boundary conditions configuration can be found in [22]. Fixed sides of the cell were restrained to have displacements in the direction, perpendicular to the orientation of the respective side, namely: bottom face had U2=0, right side had U1=0, back side had U3=0. Displacement equivalent to the longitudinal strain $\varepsilon_Z = 5\%$ was applied to the front side of the cell in Z global direction via Coupling type constraint [17], and it was found to be representative value for displacement to observe both stress-strain state and damage state. Layout of model with notation is presented on the figure 1, boundary conditions are collected in table 6.

|                | U1 | U2 | U3 |
|----------------|----|----|----|
| Front          | -  | -  | $\varepsilon_Z \cdot a$ |
| Back           | -  | -  | 0  |
| Right          | 0  | -  | -  |
| bottom         | -  | 0  | -  |

*Traction-free sides are denoted with ‘-’.*
Figure 1. RVE representation and notation.

Mesh assignment was chosen to follow structured technique with universal length of the quad element, which equals 1 µm. Although this resulted in satisfactory quality of the elements, model consists of significant number of elements, namely 10,940 for 20×20 cell and 7,845,075 for 175×175 cell.

After setting the model, the simulation was carried on in Abaqus/Explicit, mainly for coping with convergence difficulties and also to control rate of strains more obviously, with above mentioned strain and 1 second time of simulation the strain rate 0.05 sec\(^{-1}\) was held constant for all sizes and variants of the RVE.

Post-processing involved transforming gained relationship between reaction force \(RF_3\) and displacement \(U_3\) into the form of engineering stress and strain. In equations (7) and (8), the recalculation for stresses was made both with respect to full cross-section area and fibers cross section areas respectively, i.e.:

\[
\sigma_z^F = \frac{(RF_3)}{n_f \pi r_f^2} \tag{7}
\]

\(\sigma_z^F\) – is a stress value calculated using fibers area; \(RF_3\) – reaction force, tracked during simulation, \(n_f\) – number of fibers in the simulation, \(r_f\) – radius of fiber

\[
\sigma_z = \frac{(RF_3)}{a^2} \tag{8}
\]

\(\sigma_z\) – is engineering stress recalculated using full cross-section, \(a\) – side of the cubic RVE cell.

Results of simulations and calculations are collected in the following section.

3. Results and discussion

3.1. Model-1 variant

At first simulations were conducted for the variant of cell with perfect and tough interface, elastic and damage-free matrix, so that the only possibility of collapse was fiber tensile failure. Moreover, the tensile strength of fiber was equal among all fibers. The minimum size in the range under consideration was 20 µm and maximum was 175 µm. The results are captured in the table 7 and figure 2.

On the picture of the damaged state (figure 3, half of the cell) of the model initiation of failure occurs in the regions, nearest to the load application zone and support region. Before the final failure, there is still a load transfer through the matrix, with failure regions occurring in closer to the middle of the cell in the Z direction.

For better illustrating the convergences of strength values the plot of failure stresses against cell size was built and presented on figure 4.
Table 7. Model variant 1 results.

| Cell side, μm | Number of fibers | Number of elements | Failure strain | Strength by section area, MPa | Strength by fiber section area, MPa |
|---------------|------------------|--------------------|----------------|-------------------------------|-----------------------------------|
| 175           | 500              | 7,855,050          | 1.425          | 1756.03                       | 2794.808                          |
| 150           | 365              | 4,887,300          | 1.525          | 1833.027                      | 2936.11                           |
| 120           | 236              | 2,533,320          | 1.55           | 1820.286                      | 2886.052                          |
| 100           | 159              | 1,452,000          | 1.55           | 1832.96                       | 2995.50                           |
| 80            | 103              | 748,000            | 1.57           | 1860.610                      | 3004.08                           |
| 50            | 34               | 178,700            | 1.6            | 1670.577                      | 3100.64                           |
| 20            | 4                | 10,940             | 1.6            | 1214.75                       | 3156                              |

Figure 2. Model variant 1 convergence of failure stresses for sizes in range.

Figure 3. Damage state of the model variant 1.

Figure 4. Model variant 1 convergence of failure stresses for sizes in range.

Figure 5. Model variant 1 strength difference for sizes in convergence range.
The values of basic ply longitudinal tensile strength and back-calculated strength of fiber with rule-of-mixtures formula (ROM) are set with horizontal dashed lines. From this perspective, one can see that there is a significant difference between average fiber tensile strength and prescribed fiber strength as well as between cell engineering tensile strength and ply tensile strength. The largest difference for ply and cell engineering strength is 985 MPa, received for the smallest cell of 20 µm. As to fiber strength – it has a nearly constant and slow increasing rate of difference with respect to the calculated value of strength using ROM.

To advocate the choice of the micro-mechanical cell for longitudinal tension simulations, the difference in percents for each cell size between the engineering strength for considered cell and following cells in the range was calculated. The results are shown on figure 5.

So that for practical reasons the smallest proper size must be chosen, 80 µm of the side appears to be quite justified with maximum ≈6% of difference with respect to the larger cells.

3.2. Model-2 variant

For estimation of the influence of damage in matrix and interface, simulations of appropriate variant were conducted, where the size range and arrangement of fibers remained the same as in first model. The resulted are collected in table 8 and figure 6.

The results show, that stress-strain state doesn’t differ from previous variant in general. This point might be a contribution to the statement of fiber dominant properties which control the failure no matter if matrix and interface are also prescribed for damage.

Figure 6. Model variant 2 convergence of failure stresses for sizes in range.

Meantime on the figure it is seen, that within considered strain right after reaching failure load, matrix is mostly degraded as well as interface (figure 7, half of the cell)

It was previously studied by some authors, that matrix properties are suspected to provide failure of the material at higher engineering strain levels [23], although in the current study matrix is prescribed to have reasonable strength and fracture strain under tension, and therefore statement is better to be proved qualitatively, e.g. how much increase in matrix properties is needed to achieve significantly higher failure load for the composite. Moreover, the results reported in [23] mainly relate to cross-ply laminates, but not the unidirectional material.

The convergence of failure stress value with enlargement of cell size is shown on figure 8. The convergence of strength value and difference of strength value has very similar appearance to the variant with the variant 1 of analyses (figure 9).
3.3. Model-3 variant
In third variant we estimated the influence of the stochastic representation of fiber strength in the RVE section. Results follow in table 8 and figure 10.

Table 8. Model variant 3 results.

| Cell side,  | Number of | Number of | Failure | Strength by | Strength by |
| µm          | fibers | elements | strain | section area, | fiber section area, |
|             |        |          |        | MPa         | MPa          |
| 175         | 500    | 7,855,050| 1.65   | 1795        | 2856.876    |
| 150         | 365    | 4,887,300| 1.77   | 1820.431    | 2915.935    |
| 120         | 236    | 2,533,320| 1.77   | 1923.235    | 3049.27     |
| 100         | 159    | 1,452,000| 1.737  | 1863.16     | 3044.87     |
| 80          | 103    | 748,000  | 1.77   | 1870.610    | 3020.23     |
| 50          | 34     | 178,700  | 1.7    | 1762.5      | 3271.26     |
| 20          | 4      | 10,940   | 1.79   | 1385        | 3599.8      |

To compare the damage state the distribution of stresses is shown on the half of the cell in figure 11. The convergence of failure stress value with enlargement of cell size is shown on figure 12.
It is well observed (figure 13), that stress is redistributed from broken on the intact fibres with higher strength, mean while there is observable stress relief in the broken fibres on some distance from the fracture. Another detail is matrix degradation localization, which occur in the region of broken fibre and even more probably in the branch of weak broken (which are recognized by stress free areas). The failure of material cell happened with accumulation of fibre-bundles failures, until the number of the latter reached certain critical values. This results are comparable with experimentally observed [24].

Figure 12. Model variant 3 convergence of failure stresses for sizes in range.  
Figure 13. Model variant 3 strength difference for sizes in convergence range.

The convergence of strength value and difference of strength for variant number 3 is adequate starting from 50 µm (figure 13).

For comparison purpose the size value of 80 µm remains the first candidate for minimum adequate dimension for simulations. The failure stress curve tells that this time it is even deeper drop in strength of tensile strength observed between small and intermediate size. Finally, results for adequate cell sizes for 3 variants of model are summarized in table 9.

|                          | Variant 1 | Variant 2 | Variant 3 |
|--------------------------|-----------|-----------|-----------|
| Proposed size of cell side, µm | 80        | 80        | 80        |
| Mean, MPa                | 1820      | 1805      | 1854      |
| Standard deviation, MPa  | 34.86     | 43.89     | 44.1      |

4. Conclusion and future works
In the current research the minimum size of RVE for carbon-fiber-reinforced composite material, necessary for practical modeling of composites on the micro-scale, was investigated and the value of 80 µm was delivered. The presence of damage properties of matrix and interface hasn’t shown the significant influence on the failure process of the virtual sample and on the characteristic size of the RVE as well. The new evidence was put in the topic of mismatching the experimental and informed by micro-scale simulations properties of the layer and constituents. Here, the most remarkable difference was met between prescribed and averaged fiber strength.

However, there are many fields, where received results must be proved and complemented. Suggested problems include simulations for other stress-states, proportions of the RVE and variable properties of matrix and interface. Another question to be tested would be the influence of the anisotropic properties of carbon fibers and some works report this influence to significant in terms of stress concentration factor and ineffective length.
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