Micromechanical modeling of CFCs using different pore approximations

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Introduction
Carbon/carbon (C/C) composites fabricated by chemical vapor infiltration (CVI) of carbon fiber preforms have a complicated hierarchical microstructure [1, 2]. In this material carbon fibers are embedded in a matrix of pyrolytic carbon (PyC) which is influenced by the CVI parameters [3]. The microstructural architecture of C/Cs depends on the fibers orientation in the preform (Figure 1) and depending on the infiltration conditions pores with different geometry, size and orientations are formed between fibers with pyrolytic carbon coating.

Accurate estimation of the effective elastic properties of these materials is possible only with consideration and correct modeling of the fibers and pores distributions and approximation of the pores shapes.

One of the goals of the present study is to identify different possibilities of the pores approximations and apply this to microstructure modeling.

Microstructure characterization
The three dimensional distribution of fibers can be determined by micro computer tomographic (µCT) analysis. A cylindrical specimen of the non infiltrated preform was manufactured via water cutting and analyzed in the Desktop CT Scanner (Skyscan 1072). As can be seen in Figure 1 the fiber orientation has been color-coded according to the local direction of the fiber. Therefore, an anisotropic Gaussian filter was applied with pronounced axes evenly distributed on the unit sphere. The voxel was then assigned to the direction with the highest filter response. This allows to create a 3D-Histogramm on the sphere where the fiber-fraction is plotted as intensity and clearly outlines the anisotropy of the material (see Figure 1b).
Porosity characterization, analysis and approximation

Pores approximation through ellipsoids
Porosity is one of the important characteristics of all these materials. Even though the architecture of the fiber preform is the same, different time of the infiltration results in different volume of the pores. In [4], we developed a methodology for description of the porosity using an approximation of the pores by ellipsoids. The 2D-micrograph images, obtained by polarized light microscopy, were used for porosity characterization. The pore contours in the images are replaced by ellipses which are assumed to be the cross-sections of prolate or oblate 3D ellipsoids. Statistical analysis of the orientation and aspect ratios of the ellipses provides the distribution function for the ellipsoidal pores in the composite.

μCT analysis can be used for 3D description of the porosity [5]. For material with layers with mostly unidirectional fibres (UD) orientation the following procedure was carried out (Fig. 2 b):
- Each layer was extracted from the µCT Data and segmented into pores and material with a region growing algorithm:
- The pores were labelled and analyzed in the following procedure (if the pore volume exceeded the minimum volume of 20 voxels):
  1. The pore surface was extracted as a point cloud;
  2. An ellipsoid with the same volume as the pore under consideration was fitted with a principle component analyses;
  3. The Euler angles, principle half axes and the volume of the pore were tabulated.

![Figure 2.](image)

**Figure 2.** a) Polarized light microscopic image of polished section of CFC composite; Approximation of the typical pore contour by an ellipse and determination of the pore orientation angle $\omega$ to the global coordinate system; b) 3D images of the specimen obtained from µCT; 3D images of the single pores; approximation of the pore structure by ellipsoids with the same volume (the principle component analysis was used to fit the ellipsoids).

Using the described procedure, the 3D information about porosity of the material was gathered. All obtained pores were approximated as oblate and prolate spheroids. The distribution of the half-axis ratio of the spheroids and corresponding volume ratio was obtained. The orientation of the spheroid is defined through the orientation of its third semi-diameter, not equal to the two other semi-diameters. Statistical studies show, that in a layer with mostly UD-fibres the volume fraction of the prolate pores is larger than that of the oblate ones and the preferred orientation of these prolate pores coincides with the
preferred orientation of the UD fibers. The oblate pores, which are characterized through the orientation of the short semi-axis, are randomly distributed around the fibres and their discs have orientation coinciding with fibers orientation.

**Extraction of the real shapes of the pores**

Consideration of the real pores shapes is also very interesting for microstructure modeling. We have proposed such a procedure in [6] for 2D problem.

![Figure 3. Extraction of the real pores shapes for 2D microstructure images:](image)

- a) metallographic microstructure image;
- b) processed image with pores contours;
- c) images of the pores shapes and for 3D microstructure images (obtained by µCT analysis);
- d) shape of a single pore;
- e) shape of a single pore incorporated in FE-mesh.

Using this procedure the shapes of the single pores can be extracted from metallographic images (see Figure 3) and directly incorporated in calculation of the tensors, which consider the influence of the pore on the microstructure behaviour. A very similar approach can be applied to 3D case. The shapes of the pores can be extracted from the microstructure using µCT [5] (see Figure 3 d, e) and than used for FE-calculations for studies of the influence of the pore on 3D microstructure. This procedure can be provided for typical pores
shapes and then the effective influence of all possible pores can be calculated.

**Microstructure modeling**

For the prediction of the effective elastic properties of C/C composites we propose the following two-step homogenization scheme:

1. We homogenize the material consisting of the pyrolytic carbon matrix with certainly distributed carbon fibres;
2. We embed the pores in the homogenized material obtained from the previous homogenization step. The pore morphology, i.e., the distribution of the pore size and orientation is taken from µCT or metallographic microstructure studies.

In the *first homogenization step* we homogenize material consisting of PyC matrix and carbon fibres. For this homogenizations step, carbon fibres are approximated as needle-shaped inclusions. We obtain the distribution function of the fibres from microstructure characterization and it can be described by the following function as in Schjødt-Thomsen and Pyrz [7]:

$$g(\theta) = \frac{\sin(\theta)^{2P-1} \cos(\theta)^{2Q-1}}{\int_{\theta_1}^{\theta_2} \sin(\theta)^{2P-1} \cos(\theta)^{2Q-1} d\theta}$$  \hspace{1cm}(1)

and for different values of $P$, $Q$ different fiber architectures can be obtained.

Then for the Mori-Tanaka model [7], the approximation of the compliance (or elasticity) tensor of the material is given by:

$$\mathbf{D}^{MT} = \mathbf{D}^{PyC} + f_f \{ (\mathbf{D}^{F} - \mathbf{D}^{PyC}) \mathbf{T} \} ((1 - f_f) \mathbf{I} + f_f \{ \mathbf{T} \})^{-1}$$  \hspace{1cm}(2)

Where $\mathbf{D}^{PyC}$ is the compliance (or elasticity) tensor of the pyrolytic carbon matrix and $\mathbf{D}^{F}$ is the compliance (or stiffness) tensor of all fibers, curly brackets denote averaging over all possible directions.

$$\mathbf{T} = \left( \mathbf{I} + \mathbf{S}(\mathbf{D}^{PyC})^{-1} (\mathbf{D}^{F} - \mathbf{D}^{PyC}) \right)^{-1}$$  \hspace{1cm}(3)

and $\mathbf{S}$ is the Eshelby tensor of the circular cylinder.

In the *second homogenization step* we embedded pores in effective material with effective compliance $\mathbf{D}^{MT}$ from the last step (2). For simplicity and in consideration, that we have small volume fracture of the pores, for calculation of the influence of porosity we use following formulae:

$$\mathbf{D}^{eff} = \mathbf{D}^{MT} + \mathbf{H}^{Pores}.$$  \hspace{1cm}(4)
with \( H_{\text{pores}} \) being the contribution in the compliance tensor of all pores. It can be calculated using non-interacting model and it consists of the sum of the contribution tensors of the single pores weighted by the effective volume fraction of the single pore.

For different methods of the pore approximations different formulae for \( H \)-tensor of the single pore can be used (see [4, 6, 8]): it can be presented using the Eshelby tensor of the ellipses, which were used for approximation of the irregular shape of the pore or using holes shape factors of typical 2D-pores, or calculated from six-loading cases using FE-calculation of the 3D pores-shapes extracted using \( \mu \)CT.

**Numerical results**

As input values for our calculations we use the measured transversal isotropic material properties of the PyC [9]. Firstly, the material properties of the infiltrated felt were calculated. For this case the distribution of the fibers is random and pores were calculated as ellipsoids. The shape approximation was provided as described for pores approximation trough ellipsoids. The effective Young's modulus obtained was compared to the experimentally obtained ones. Three infiltrated felt materials with different porosity were tested (porosities see Table 1): one of these materials (Felt1) by the tensile, and two others (Felt2 and Felt3) by four points bending tests. The results of these measurements of the mean values of Young’s modulus, as well as the numerical results are presented in Table 1. Analyzing these results, we can conclude that the calculated material properties show good correspondence with the experimental data.

Secondly, the material properties of the laminate with UD layers in one preferred orientation separated through thin felt layers were calculated (Table 1 results for Laminate).

**Table 1.** Calculated and experimental values of Young’s modulus of felt and material with mainly UD fibers orientation.

<table>
<thead>
<tr>
<th>Volume</th>
<th>Volume</th>
<th>Calculated</th>
<th>Measured</th>
</tr>
</thead>
<tbody>
<tr>
<td>fibers</td>
<td>pores</td>
<td>( E ) [GPa]</td>
<td>( E ) [GPa]</td>
</tr>
<tr>
<td>(%)</td>
<td>(%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Felt 1</td>
<td>12</td>
<td>7.3</td>
<td>18.18</td>
</tr>
<tr>
<td>Felt 2</td>
<td>12</td>
<td>15</td>
<td>16.43</td>
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<tr>
<td>Felt 3</td>
<td>12</td>
<td>48</td>
<td>13.07</td>
</tr>
<tr>
<td>Laminate</td>
<td>23 in UD</td>
<td>9 in UD</td>
<td>49.94</td>
</tr>
</tbody>
</table>
Conclusions
The characterization, modeling and experimental verification procedure is presented for the calculation of effective material properties of C/Cs composites. This procedure consists of fibres and pores distributions characterization using metallographic studies or µCT, followed by consequential steps of the microstructure homogenization.

For porosity description different methods are proposed including the approximation of the pores through ellipsoids and consideration of the exact shapes of the pores.

The homogenization procedure consists of two steps in which firstly the effective material properties of the fibres and PyC-matrix are calculated, and secondly the pores are embedded in effective material from the first homogenization step.

The verification of the numerical modeling is provided using experimental methods. The comparison shows that using the proposed homogenization procedure, it is possible to provide a good prediction of the overall material properties of the composite.

The proposed method provides a methodology to predict the effective material properties of C/C materials based on the information on their microstructure and volume fractions of the micro constituents. The utilization of this method allows to reduce the volume of experimental mechanical tests, and also opens a perspective to provide numerical optimization of C/C composites to obtain the required material behaviour.

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References