# PREDICTION OF THE ELASTIC TENSOR OF 3D COMPOSITES BY AN ANALYTICAL MODEL

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**SUMMARY:** The aim of this study is the determination of the overall elastic tensor of two 3D composites. These materials have a multiscale architecture. The representative volume element of the composite architecture (symbolised by a unit-cell) is composed of three bundles in three orthogonal directions and two matrix pockets. Each bundle is a unidirectional composite formed by a juxtaposition of long fibres surrounded by the matrix. Due to their symmetry, the bundles are considered transversally isotropic according to the fibres axis, whereas the pockets are macroscopically isotropic. The analytical computation is produced in two steps. The first step consists of determining the elastic tensor of the bundles. The second step is the calculation of the elastic tensor of the whole composite. The most part of the used equations comes from bibliography, excepted the determination of shear coefficients of the composite. The last part of this study devoted to the influence of material parameters presents the relative role of the fibres, the matrix and their volume fraction.

**KEYWORDS:** 3D composites, homogenisation, mechanical properties, carbon or polymer matrix.

## INTRODUCTION

Numerous high performance applications have led to the development of composite with three-dimensional architecture. These materials named '3D composites' satisfy the requirement of multidirectionnal loading and their high delamination resistance are serviceable. Due to their spatial and inhomogeneous structure, these composites are complex compared to laminated composites. As a result, the application of the classical 2D laminate theory for design and analysis is not possible.

The purpose of this study is the determination of the elastic rigidity tensor [$C_{ij}$] of 3D composites. In order to build a precise relation between the elastic behaviour at the microscale (scale of the fibres and matrix) and at the macroscale (scale of the composite structure) the calculation is performed by an analytical model, also involving the mesoscale of the composite (constitutive yarns, matrix pocket). This model was previously developed on 2D and 3D textile composites in very complex architecture due to yarn waving [1, 2, 3]. 3D composites are periodic architectures which can be modelled from representative volumes elements (RVE) called « the unit cell ». Numerical codes are often used for 3D periodic materials and they require complex refine mesh for an available three dimensionnal stress-strain analysis [4]. The 3D composites possess an orthotropic symmetry. Hence, nine independent elastic coefficients are sufficient to determined the overall elastic tensor. Our objective is to compute the six coefficients in the orthotropic axis called « normal coefficients » by the model of Kuo and Pon [2]. The three shear coefficients were determined by a parallel computation, which constitutes an extension of the previous work. These analytical methods are most convenient at first to guide the choice of the composite architecture and to optimise it. Another advantage of this general analytical approach is that the calculation time is short and so, a parametric study of the reinforcement structure can easily be produced.

This paper starts with a geometrical description and characterisation of the fabric architecture. Then follows the presentation of the analytical model and finally the parametrical study is intended.

## ANALYTICAL METHOD FOR PREDICTION OF THE ELASTIC TENSOR

In this section, the architecture of 3D composites and the two steps of elastic tensor calculation are presented.

### Textile architecture

The 3D composites studied are tri orthogonal materials. The unit cell is described on figure 1.

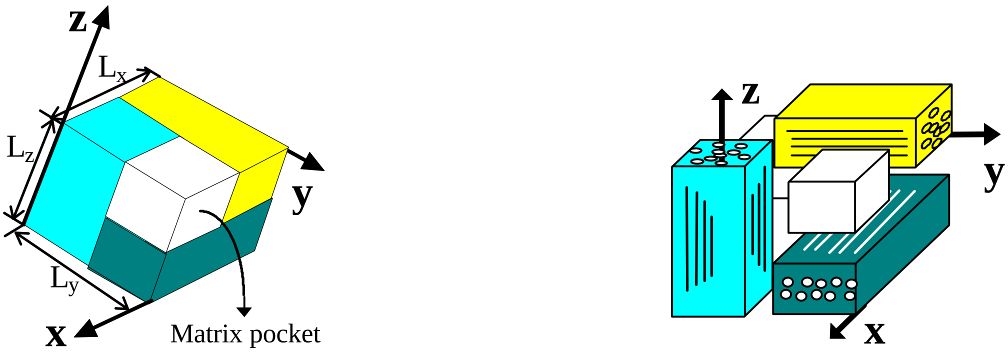



*Fig. 1 : Representative volume element of the 3D composites*
*(Dimensions are depending on the composite considered)*

The unit cell is composed of three bundles, each one is on a main axis of the composite (X, Y and Z). The last constituent is idealised by two matrix pockets. The three bundles can be of different size and their volume fraction can vary from one direction to another. The tri-orthogonal composites are naturally periodic.
In the bundles, the main constituents are the fibres and the matrix. They are of different nature according to the composite considered. That can suggest that the matrix in the bundles and in the pockets could also be different. Practically, it has been observed that for the same chemical constitution, the matrix in the bundles and in the pockets can show different morphological aspects, as different porosity or different properties due to change of matrix texture [5]. These differences experimentally observed in 3D composites can be considered in the model.

Consequently, the elastic tensor of composites which have multiscale architecture, will be naturally determined in two steps by the analytical model (Fig. 2). The first step consists of determining the elastic tensor of each bundle from their constituents properties (fibre and matrix). The second one is performed in order to achieve the calculation of the elastic tensor of the 3D composite considering that the three bundles (X, Y and Z) and the matrix pockets are now the basic constituents.

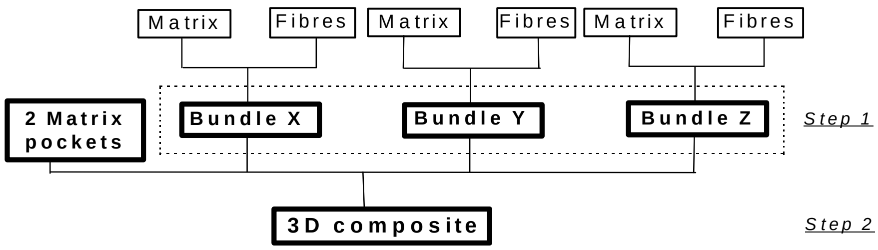



*Fig. 2 : Scheme of the multiscale homogenisation procedure*

**Step 1 - elastic tensor of the bundles**

*Case of straight bundles*

As it was mentioned in the previous section, the elastic tensor of the bundle depends on the geometrical and the mechanical symmetry of its constituents. In this work, simple methods with analytical expression were examined. The Hashin's study [6] based on an analytical periodic approach was considered. Hashin has developed different models for unidirectional composites respectively reinforced by isotropic and transversally isotropic constituents. The effective moduli of the 1D are calculated from a RVE composed of cylindrical fibres randomly dispersed in the cylinder cross section and arranged in regular hexagonal array. This description corresponds to a theoretical periodic 1D structure but constitutes a pertinent assumption for our composites. Assuming that the axis of the transversal isotropy is the fibres axis, the elastic moduli of bundles from the expression of Hashin's bounds[6] were compared to values obtained by the classical rule of mixture approach.
Then, elastic moduli were used to calculate the compliance and stiffness tensors of the bundles. For the transversal isotropy according to the fibres axis, only five independent coefficients are useful to model the elastic behaviour of the bundles.

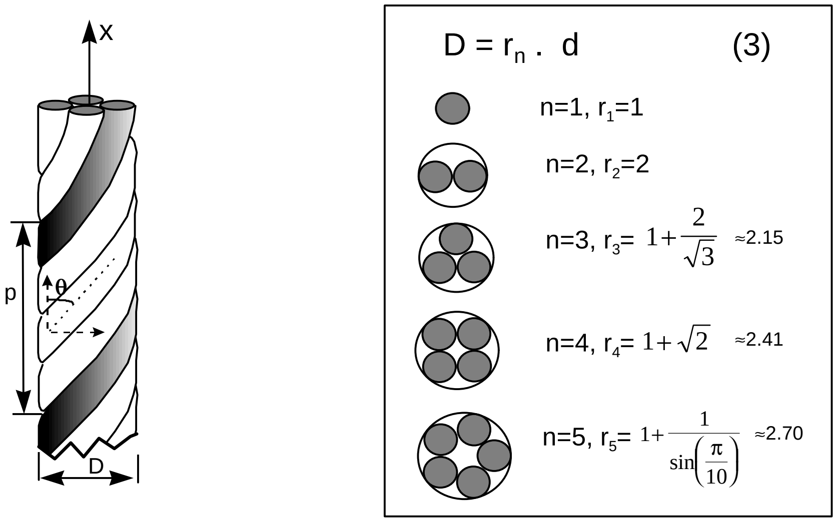
*Case of twisted bundles*

In some case, one or several bundles can be composed of numerous (2, 3 or 4) sub-yarns twisted together. One of the studied material contains this type of bundle. To get the bundles elastic properties, the straight bundle data from Hashin are used as properties of sub bundles and the effect of twisting on elastic property of the bundle is taken into account by a model developed by Byun and Chou [7].
The geometry of the twisted bundles depends on the number of sub bundles twisted together. In the more current case, this number can vary from 2 to 5. The twist angle ($\theta$ see fig.4) is calculated by idealised geometric considerations, where ***p*** is the twist period and ***D*** the overall bundle diameter :

$$\tan\theta = \frac{\pi.D}{p} \tag{1}$$

Then the ideal circular size of sub bundles depends on their number and on the global diameter of the bundle (***D***) as mentioned in fig. 3. We note that the coefficients $\boldsymbol{r_3}$ and $\boldsymbol{r_4}$ (fig. 3) correct the one given in [7] which were not correct and could have produce anomalous results. Finally, the fraction of fibre in the sub bundles is used to conduct the Hashin approach [9] on the sub bundles. This fraction is called fibre packing fraction (***K***) and is obtained by (Eq. 2) where ***n*** and $\boldsymbol{r_n}$ is given by the geometry (fig. 3), $\lambda$ is linear density of twisted bundle (kg/m) and $\rho$ the fiber density (kg/m$^3$).

$$K = \left(\frac{r_n}{p.\tan\theta}\right)^2 . \frac{4.\pi.\lambda}{\rho.n} \tag{2}$$




a) b)

*Fig. 3 : a) Schematic view of a twisted bundle with 4 sub bundles.*
*b) Idealised geometric parameter for the sub bundles diameter (**d**) function of **n**.*

The model of Buyn and Chou [7] makes the hypothesis of iso-stress in each sub bundle, so the compliance are averaged through one period. The compliance tensor, produced by Hashin approach [6] (fibre fraction taken as ***K)***, is oriented with a first angle equal to $\theta$ between the bundle and sub bundle axis through the classic transformation matrix (Eqn.5 see after). Then, the averaging process consists of calculating the average of the compliance tensor through one turn (the second orientation angle $\Phi$ vary from 0 to $2\pi$).

$$S_{ij}^{\text{twisted.bundle}} = \frac{1}{2\pi}\int_0^{2\pi} S_{ij}^{\text{Hashin/sub.bundles}}.d\Phi \qquad \text{for i,j = 1 to 6} \tag{4}$$

This approach was found to produce good correlation with experimental data [7], and so it will be used in one of the 3D composite model.

**Step 2 - Elastic tensor of the composite**

*Normal coefficients:* $\left[C_{ij}^{c}\right]$ *for i, j = 1,2,3.*

The determination of the elastic tensor of the composite is based on the analytical model reported by Kuo and Pon [2]. The following section is a condensed explanation of this model.
As shown on the figures 1 and 4, the composite coordinates and the bundles coordinates are respectively noted (x,y,z) and (1,2,3). To determine the elastic tensor of the bundles in (x,y,z) we need a three dimensional rotation of the (1,2,3) coordinates. Due to their symmetry, the

bundles are transversally isotropic. Axis 1 being the fibres axis, any rotation with respect to this axis not modifies the properties of these bundles. Accordingly, two angles are sufficient to represent the three dimensional rotation ($\theta$ and $\Phi$ figure 5). As $[C]$ refers to the elastic tensor of the bundles in (1,2,3) system, $[\overline{C}]$ is calculated in (x,y,z) system by the Eqn 5.

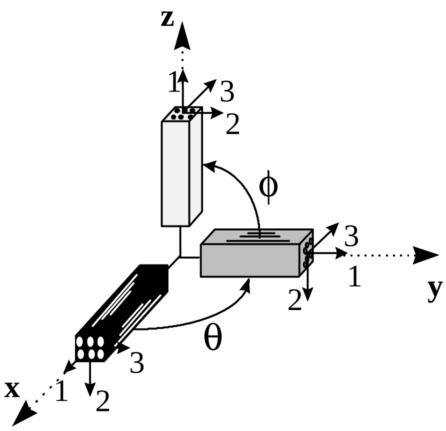



*Fig. 4 : Three dimensional rotation for transformation of coordinates in (1,2,3) to (x,y,z).*

$$[\overline{C}]_{(x,y,z)} = [T]^{-1}.[C]_{(1,2,3)}.[R].[T].[R]^{-1} \tag{5}$$

where [T] is the transformation matrix depending on angles ($\theta$, $\phi$) and [R] is 6-by-6 diagonal matrix with diagonal terms being {1,1,1,2,2,2}.

The three dimensional elastic law is written in Eqn 6. The Poisson's effects are taken into account in an average manner and the normal-shear coupling is neglected [2].

$$\begin{aligned}
\sigma^k_{xx}(x) &= \overline{C^k_{11}}\varepsilon_x(x) + \overline{C^k_{12}}.\overline{\varepsilon_y} + \overline{C^k_{13}}.\overline{\varepsilon_z} \\
\sigma^k_{yy}(y) &= \overline{C^k_{21}}.\overline{\varepsilon_x} + \overline{C^k_{22}}\varepsilon_y(y) + \overline{C^k_{23}}.\overline{\varepsilon_z} \\
\sigma^k_{zz}(z) &= \overline{C^k_{31}}.\overline{\varepsilon_x} + \overline{C^k_{32}}.\overline{\varepsilon_y} + \overline{C^k_{33}}\varepsilon_z(z)
\end{aligned} \tag{6}$$

where (k) is an index for the composite constituents (x, y and z bundles plus matrix pockets). The $\left[\overline{C}^k_{ij}\right]$ are the rigidity tensor of the k[th] constituents in the (x,y,z) co-ordinates. The barred strains are the average values of strains.

Combining the relation between the local stress in each constituent element to the externally applied stress at far-field, the detailed expression for coefficient in x direction given in [2] is written as follow :

$$C^c_{1j} = \int_0^{L_x} \frac{\sum_k A^k_x(x).\overline{C^k_{1j}}}{\sum_k A^k_x(x).\overline{C^k_{11}}}.dx.\left[\int_0^{L_x} \frac{L_y L_z}{\sum_k A^k_x(x).\overline{C^k_{11}}}.dx\right]^{-1} \tag{7}$$

where the superscripts (c) stands for composite, (j) is an index ranging from 1 to 3 and $A_x^k(x)$ is the area of the $k^{th}$ constituent normal to the x direction.

The $C_{2j}^c$ and $C_{3j}^c$ coefficients are determined by Eqn 7 in changing respectively in $\overline{C}_{1j}^k$ and $\overline{C}_{11}^k$ the superscript (1) by (2) and (3), in changing respectively in $A_x^k(x)$ and $L_x$ the superscript (x) by (y) and (z) and in exchanging respectively the product ($L_y$ $L_z$) with ($L_x$ $L_y$) and ($L_x$ $L_z$).

*Shear coefficients:* $\left[C_{ii}^c\right]$ *for i = 4, 5, 6.*

To complete the elastic tensor with the shear coefficients, we offer to decompose the unit cell in small components. The case of a shear load in the plane (y, z) is detailed here after. The two other shear cases are similar and the shear coefficients are obtained by index permutation.

To calculate $G_{yz} = \left[C_{44i}^c\right]$, we suppose that the cell is fixed at his lower side and loaded by a shear force in the y axis (Fy see fig. 5).

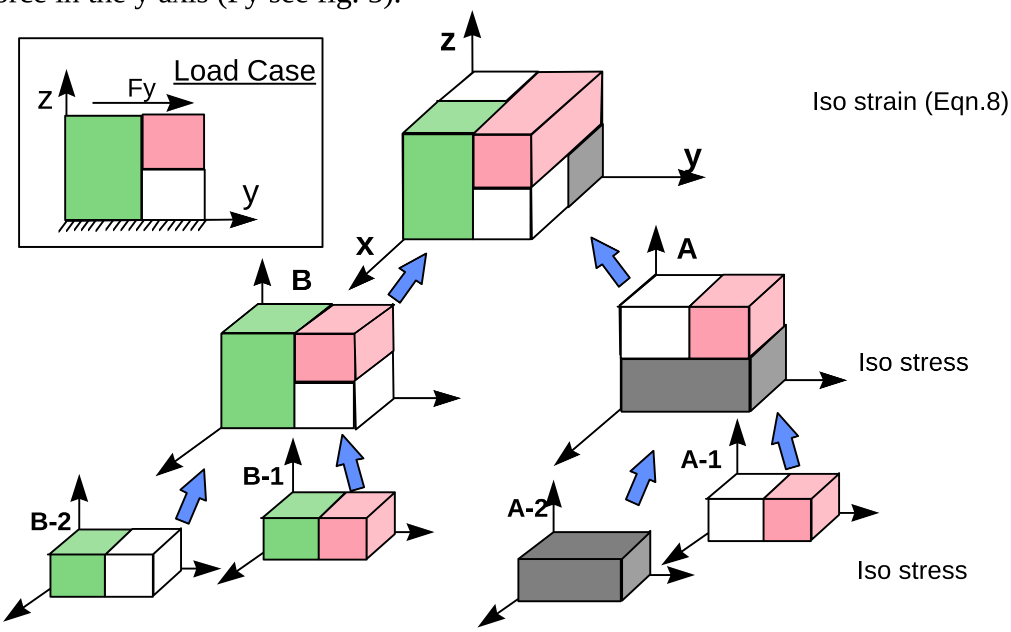



*Fig. 5 : Schematic view of the load case used to determine $G_{yz}$ and decomposition of the unit cell.*

The cell is divided in half-cells (A and B see fig. 5). We suppose that the shear strain (γ) is the same on these two half cells, then the global load applied (Fy) is the sum of the load applied on the two half cells A and B. These half cells are divided to produce quarter cells noted A-1, A-2, B-1 and B-2 (fig.5). All these parts contain a maximum of two materials and it is possible to calculate their shear modulus with the iso-stress assumption. Hence the same assumption is made to predict the A and B parts shear modulus.

Finally, the global shear modulus can be obtain by summing the A and B parts. Considering the iso strain assumption, we obtain the Eqn 8 where $V^A$ and $V^B$ are the volume fraction of the two half cells (fig. 6).

$$G_{yz} = G_{yz}^A . V^A + G_{yz}^B V^B \qquad (8)$$

## MATERIALS AND EXPERIMENTS

In this section, we give a short description of the two composites studied and of the characterisation methods used to produce experimental elastic tensor of two materials called M1 and M2. The constituents (fibre and matrix) and the volume fraction of each bundles is presented in table 1.

*Table 1 : Description of materials M1 and M2.*

| | | | Volume fraction in each bundle (%) | | |
|---|---|---|---|---|---|
| Material ref. | Fibres | Matrix | X | Y | Z |
| M1 | silica | Polymeric resin | 22 *(straight)* | 22 *(straight)* | 6 *(twisted)* |
| M2 | carbon | carbon | 16 *(straight)* | 16 *(straight)* | 16 *(straight)* |

The experimental data are produce by classic tensile or compressive mechanical tests and by ultrasonic wave velocity measurements [8]. The scattering of the experimental results is about 10 to 20 percents.

## RESULTS AND DISCUSSION

### Correlation experimental and model

The description of the structure and the properties of the basic constituents are used to implement the model described above. The computation of *step1* (fig. 2) provides the elastic tensor for each bundle (straight or twisted). Due to the Hashin's relations [6], the result is an interval with two limits called « + » for the superior and « - » for the inferior. Hence the *step2* calculation is completed two times, once for the « + data » and once for the « - data » to finally produce the limits on the 3D composite (table 2). The *step1* results are not presented because of the lack of experimental data on the bundles.

*Table 2 :Theoretical bounds for elastic tensor of composites M1 and M2 compared to experimental results*

| $C_{ij}$ (Gpa) | $C_{11}$ | $C_{22}$ | $C_{33}$ | $C_{44}$ | $C_{55}$ | $C_{66}$ | $C_{12}$ | $C_{13}$ | $C_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| **M1 +** | 29.6 | 28.7 | 18.8 | 3.71 | 3.69 | 3.57 | 4.7 | 5.9 | 5.7 |
| **M1 -** | 27.3 | 26.4 | 15.0 | 3.59 | 3.57 | 3.52 | 3.1 | 3.5 | 3.4 |
| **M1 exp.** | **28.2** | **23.3** | **19.9** | **4.3** | **4.3** | **5.3** | **4.8** | **6.8** | **6.5** |
| **M2 +** | 109.4 | 109.4 | 109.4 | 3.38 | 3.38 | 3.38 | 7.3 | 7.3 | 7.3 |
| **M2 -** | 108.8 | 108.8 | 108.8 | 3.36 | 3.36 | 3.36 | 6.9 | 6.9 | 6.9 |
| **M2 exp.** | **100** | **100** | **100** | **2.25** | **2.25** | **2.75** | **5.3** | **5.3** | **5.3** |

The general bounds are closer for the material M2 than for M1. For M2 material, this observation for $C_{ii}$ coefficients (i = 1,2,3) is due to the extreme closeness of bundles Young's modulus to the rule of mixture. Another explanation lies in the close values of transverse elastic properties of carbon fibres and carbon matrix, leading to a very small difference between the « + » and « - » bounds of bundles transverse properties. In the case of M1 material the deviation of the bundles transverse properties produces the bounds observed (table 2). For the shear elastic data ($C_{ii}$ i=4,5,6), we note that the experimental data are above the model for M1 and below for M2. This effect is probably due in the case of M2 to the imperfection of interfaces between bundles not considered in the model.

The experimental and model data comparison is relevant as regards to experimental scattering. All the experimental data are not strictly included into the model bounds which could be an effect of the bad knowledge of the basic constituents elastic properties. In the model, the matrix pockets are idealised as continuum material which is not the case in the two materials studied because of the presence of large porosity.

In spite of the sensibility of theoretical results to constituent properties introduce in the model, we still propose a parametric study in order to exhibit the relative weight of both parameter.

**Parametric study**

The parametric study is based on M2 material because of equivalence between the three orthotropic axis that reduces the number of data to be presented. The engineer data Young's modulus ($E_X$) and shear modulus ($G_{XY}$) of the composite are used to present the effect of three parameters. These variable parameters are chosen to observe the effect of the impregnation process and of the damage accumulation.

- the 1st parameter, is the volume fraction of fibres in each bundle.
- the 2nd, related to the infiltration of the matrix, is the volume fraction of the porosity in the pockets.
- the 3rd is affiliated to transverse damage in the Y and Z directions when the material is loaded in the X direction. In this last case, the symmetry of the material is affected and the data presented are only valid for the X direction.

The evolution of composite moduli ($E_X$ , $G_{XY}$) are computed using the « + » bound of the model and normalised with the M2 properties. The arbitrary choice of the « + » bounds is efficient due to the very close bounds observed in table 2. The effects of these three parameters are presented in fig. 6 and discussed here after.

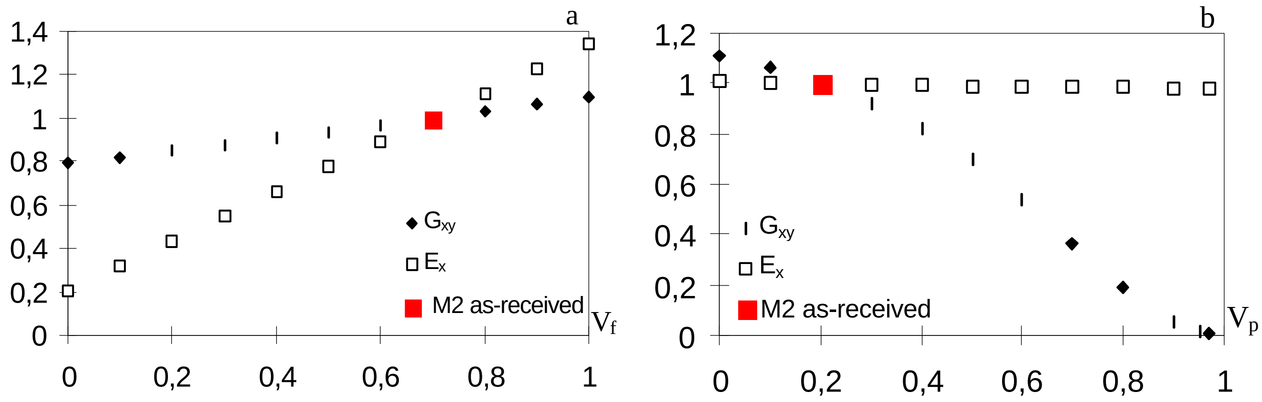



*Fig. 6 : Evolution of $E_x$ and $G_{XY}$ as a function of different parameters : a) the volume fraction of fibres ($V_f$); b) the volume fraction of porosity in the matrix pockets ($V_p$)*

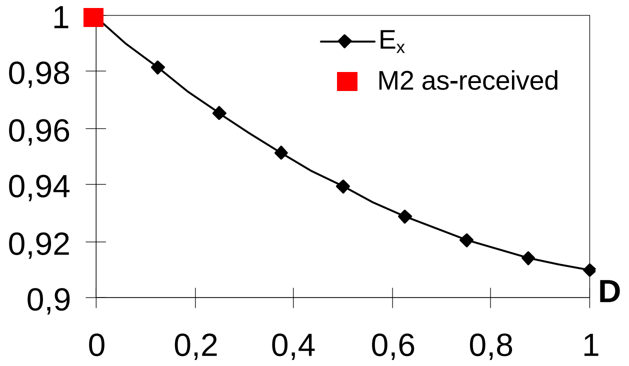



*Fig. 7 : Evolution of $E_x$ as a function of a damage parameters (D).*

*Effect of fibre volume fraction*

As it could be expected, the volume fraction of fibres in the bundles greatly influences the Young's modulus (fig. 6-a). As regards to the composite architecture, increasing $V_f$ up to 100% in the bundles implies a maximum increase of 38% of $E_X$. Decreasing $V_f$ down to 0 implies a decrease of $E_X$ of 80%. So, $E_X$ is equal to the matrix modulus.

In addition, for the same variation of $V_f$, the evolution of $G_{XY}$ is less prominent. It follows an increase of about 5% and a decrease of about 20%. This less sensibility on the shear modulus is due to the very close shear elastic properties of the fibres and the matrix. These variations imply that, even in a 3D tri-orthogonal composite, the property $E_X$ and $G_{XY}$, are respectively controlled by the fibres and the matrix.

*Effect of the porosity in the matrix pockets*

The above conclusion is confirmed by the effect of the porosity in the matrix pockets (fig. 6-b). Indeed, the normal modulus is not really affected by the increase of porosity in the matrix pockets whereas the shear modulus extremely decreases. Consequently, a special attention has to be paid to the matrix pockets porosity if shear rigidity is specified. There is a way to highly improve or decrease the shear rigidity by the impregnation process.

*Effect of the transverse cracks :transverse damage accumulation in bundles*

A transverse damage law was included in the Y and Z bundles to artificially produce a decrease of transverse modulus of these bundles. The relation used to link the bundle transverse modulus ($E_2$=$E_3$) to damage parameter (D) is the one studied by Lebon [4]. This type of transverse damage (Y and Z bundles) can occur when the composite is loaded in the X direction. Because we are not able to model the effect of this kind of damage on the shear properties, only the Young modulus ($E_x$) is studied.

As shown by fig. 7, the evolution exhibits a light decrease of Young's modulus ($E_X$) when the damage increases. The value of $E_X$ only decreases to 90% of its initial value when the Y and Z directions are totally cracked (D=1). This small decrease in the Young modulus of the X direction, indicates the very light influence of transverse cracks in the Y and Z bundles.

Because they need Y and Z bundles completely cracked to see a decrease of 10% on the X direction modulus, the 3D tri-orthogonal composites can be considered as nearly insensitive to transverse cracking. More critical damage, like interfacial debonding at bundle/bundle interfaces could produce dramatic effect on elastic properties.

## CONLUSION

This paper intends to calculate the elastic tensor of 3D composites. The analytical model developed for this purpose is based on Kuo and Pon works [2] for the $C_{ij}$ with i,j=1, 2, 3 and an extension to the shear coefficients is offered here. The model respects the multi-scale geometry of the 3D tri-orthogonal composites by processing in two steps. The first one deals with the basic constituents to produce straight or twisted bundles and the second one builds the 3D composite with the bundles and matrix pockets properties. This analytical approach is very easy to implement and produces good correlation between model and experimental data for two very different 3D composites (carbon/carbon and silica/polymeric). Some imperfections are mainly due to the lack of knowledge of the basic constituents properties and to the cracked bundle/bundle interfaces which are not considered in the model.
The parametric study shows that even in 3D composites the normal elastic properties are governed by the fibres content and the shear one by the matrix. We also note that the increase of porosity in the matrix pockets only influences the shear properties in an important amount and that the 3D composites have small sensibility to transverse cracking. Thus, other parametric studies can be produced to optimise the definition of this kind of composites materials, to improve their properties in regards to process adjustable parameters or to evaluate their sensibility to damage growth in the material. This model is a tool for material and processing engineering of 3D composites.

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