Micro-scale modeling of carbon-fiber reinforced thermoplastic materials

A. GHERISSI, F. ABBASSI, A. ZGHAL

URMSSDT- ESST Tunis, 5 Avenue Taha Hussein, BP, 56, Bâb Manara, 1008 Tunisia

abderraouf_gh@yahoo.fr, fethi.abbassi@ipeib.rnu.tn , ali.zghal@esstt.rnu.tn

S. MISTOU and J. ALEXIS

Université de Toulouse ; INP/ENIT ; M2SP-LGP, 47 Avenue d'Azereix; 65016 Tarbes, France

Mistou@enit.fr , Joel.Alexis@enit.fr

Abstract

Thin-walled textile-reinforced composite parts possess excellent properties, including lightweight, high specific strength, internal torque and moment resistance which offer opportunities for applications in mass transit and ground transportation. In particular the composite material is widely used in aerospace and aircraft structure. In order to estimate accurately the parameters of the constitutive law of woven fabric composite, it is recommended to canvass multi-scale modeling approaches: meso, micro and macro. In the present investigation, based on the experimental results established by carrying out observations by Scanning electron microscope (SEM), we developed a micro-scale FEM model of carbon-fiber reinforced thermoplastic using a commercial software ABAQUS. From the SEM cartography, one identified two types of representative volume elementary (RVE): periodic and random distribution of micro-fibers in the yarn. Referring to homogenization method and by applying the limits conditions to the RVE, we have extracted the coefficients of the rigidity matrix of the studied composites. In the last part of this work, we compare the results obtained by random and periodic RVE model of carbon/PPS and we compute the relative error assuming that random model gives the right value.

Introduction

The determination of the mechanical performance of woven fabric composites materials is based on the study of the behavior of the texture and the composite under different solicitations. Currently, the multi scale modeling of composites (figure 1) is one of the most used methods and it was adapted by several researchers. In fact, using this approach, F. Costanzo and L. Gray [1] haves implanted a survey on periodicity and boundary conditions; P. Boisse [2] has raised the constructive equations of the mechanical behavior of the composites woven during the forming; Gilles Hivet [3] has elaborated a mathematical approach to identify the trajectory and the different sections of the yarn in texture, the profiles of the contacts' curves and the contact's sections according to the conic equations; L. Orgéas [4] has studied in meso-scale, the permeability of the reinforcements woven of stratified composites by surveying the velocity in such composites; J. Wang [5] has studied the predictive mechanical behavior modeling in woven composite structure, by analyzing 3D finites elements ; P. Badel and P. Boisse [6,7] have determined fibers orientations, in reinforcements woven during and after composites' formation.

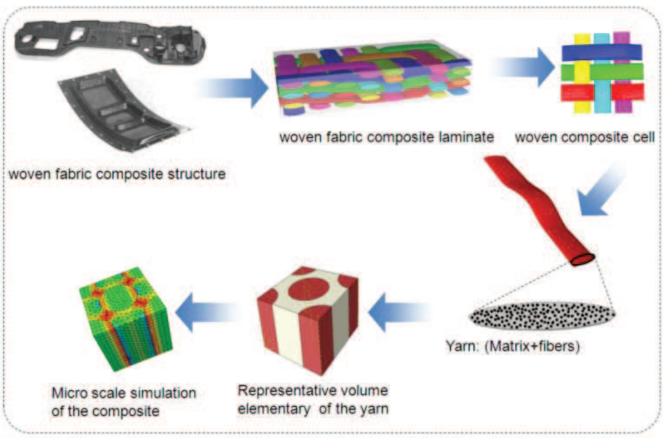


Figure1: Multi-scale modeling techniques in woven fabric composites

In order to identify the behavior of the studied composite using multi-scale approach, we have developed in this paper a simulation of the reinforcement's woven fabric composite (figure 1).

We have started by using an experimental characterization of the texture to prepare a geometrical description of fibers' diameters and distributions in the Polyphenylene sulfide (PPS) matrix. Then, we identified two types of RVE (periodic and random one) in order to estimate the errors' values in the results. Then, basing on the homogenization method and after applying the boundary conditions to the RVE, one has extracted the coefficients of the rigidity matrix and the parameters of the yarn composites. Finely, we have identified the able RVE to characterize accurately the yarn of our woven fabric composite.

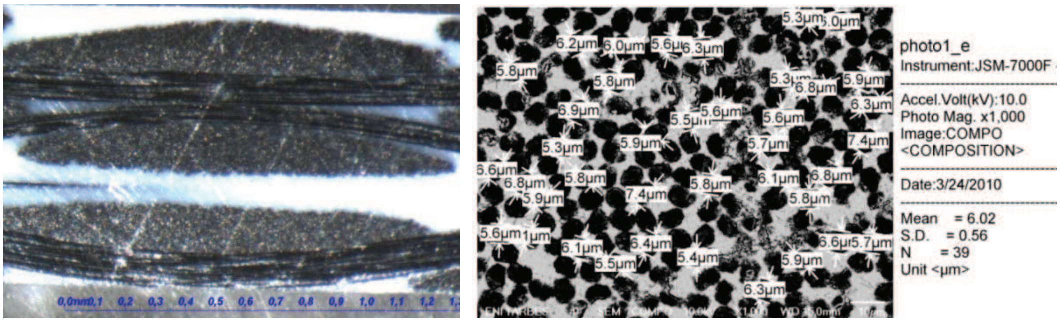
I. Carbon-fiber reinforced thermoplastic materials

The composite texture is consists of a carbon fibers and a PPS matrix and the volumetric fraction of the fibers in the composites is $V_f = 0.5$ .The characteristics of the materials forming the composite are summarized in the following table:

Material	Filament diameter (µm)	Volumetric Mass ρ (kg.m^{-3})	Longitudinal Elasticity module E(Mpa)	Module of Shearing G (Mpa)	Poisson Coefficient υ	Constrained of rupture (traction) MPa	Elongation to The rupture (%)	thermal dilation coefficient °C^{-1}
Carbon Fiber	6.24	1800	390 000	20 000	0.35	2500	0.6	0.08 10^{-5}
PPS		1300	4000			65	100	5 10^{-5}

Table 1: the characteristic of the materials forming the composite

The characterization of the texture of the composite has been carried out throw two main steps. In the first one, we determine the texture's character, the trajectory, and the sections of the yarns (Texture of the composite: satin 4x1 in three layers). Then, in a second step, we find out the micrographic arrangement of the fibers in a yarn (figure 3).



(a) (b)

Figure 2: (a) micrographic of three ply fabric specimens (meso-scale), (b) size and arrangement of the micro fibers in the yarn

The yarn is composed by thousands of small fibers whose diameter in the order of 6.24 µms (figure 2). This value is established by calculating the average of 150 fibers' diameter. The disorganized arrangement of the fibers in the yarn presented in figure3 will produce a variation in the local properties influenced by the distance between these fibers. Then it is necessary to start by characterizing the fibers' arrangement in order to determine the minimal size of the representative volume elementary (RVE) of the yarn. To do so, we can characterize the distribution of the fibers by analyzing the yarn's picture and using the covariance concept adapted already by [8]:

$$C(x, x + h) = P\{x \in d, x + h \in d\} \quad (2)$$

The covariance is defined as the probability of adherence of two points" x "and "x+h" in the same phase d, and it can be valued by carrying out the Fourier's transformed of the figure 2. According to the works of [7] the periodicity of the microstructure is presented by the periodicity of the covariance.

II. The micro scale modeling

1. The geometric model of RVE

The choice of the RVE which is a cubic shape was based on several researches works [10, 11, 12 and 13]. This RVE it should have the smallest size which makes it representative of the yarn material. We opted for this step of the simulation for two cubic cells shapes and we considered the fiber has a cylindrical form. The first cell (figure 3-a) is periodic and the second is random (figure 3-b). The volumetric fraction of the reinforcement is calculated by the report between the volume of the fibers and the total volume of the basic cell:

$$V_f = \frac{V_{Fibers}}{V_{Total}} = n\frac{\pi d^2}{4a^2} \quad (3)$$

Where: d is the diameter of the fiber, a is the side of the basis cell, and n: is the number of fibers by cell

(a) (b)

Figure 3: The periodic representative elementary volume of the yarn, number of fiber N = 2 fibers (a) and v_f = 0.505. The random representative elementary volume of the yarn, number of fiber N= 14 fibers and v_f = 0.475 (b)

2. The elastic constructive equations of the yarn's homogenesation

The elastic properties, are calculated by a periodic homogenization via a finite element method developed using ABAQUS software. It will give us the opportunity to study the elastic behavior of the yarn and to calculate the elastic coefficients of the composite material. For 3D RVE (cubic shape), submitted to a volumetric load, its elastic behavior can be presented as follow:

$$\varepsilon = \Phi\sigma \quad (4)$$

Where: ε is the strain tensor, σ is the stress tensor, and Φ: the suppleness Matrix

Then, the stress distribution in the elementary volume can be written as follow:

$$\sigma = C\varepsilon \quad (5)$$

Where $\Phi = C^{-1}$

The mechanical behavior of the yarn is equivalent and it depends on the mechanical and geometric properties of the different constituent: the fiber geometry, behavior, and distribution in the matrix, the matrix behavior and the characteristic of the fiber-matrix interface. The process of homogenization consists in assimilating a material characterized by an important heterogeneity by a homogeneous one. This process was applied to the RVE.

The main step of the homogenization consists in the determination of the stress and displacement fields within the RVE.

The average of the microscopic stress of this RVE can be expressed as follow:

$$\langle\sigma\rangle = \frac{1}{V}\int_{\Omega} \sigma \, dv = \Sigma \quad (6)$$

In the same way, the average of the microscopic strain is give by:

$$\langle\varepsilon\rangle = \frac{1}{V}\int_{\Omega} \varepsilon \, dv = E \quad (7)$$

Where E is the macroscopic strain and $\sum$ is the macroscopic stress

From equation (6) and (7), one can write the Hooke criteria:

$$\langle\sigma : \varepsilon\rangle = \langle\sigma\rangle : \langle\varepsilon\rangle = \Sigma : E \quad (8)$$

➔ The macroscopic stress ($\sum = \langle\sigma\rangle$) is a linear function of the macroscopic strain ($E = \langle\varepsilon\rangle$)

$$\Sigma = C^{hom} E \quad (9)$$

Where C^{hom} represents the macroscopic tensor obtained by the homogenization method.

The calculation of the C_{ijkl}^{hom} coefficients takes place while calculating the stress field that corresponds to an imposed macroscopic displacement. Supposing that the yarn represents a composite with orthotropic characteristic, the macroscopic elasticity relation is expressed as follow:

$$\begin{bmatrix}\Sigma_{11}\\ \Sigma_{22}\\ \Sigma_{33}\\ \Sigma_{23}\\ \Sigma_{13}\\ \Sigma_{12}\end{bmatrix} = \begin{bmatrix} C_{1111}^{hom} & C_{2211}^{hom} & C_{3311}^{hom} & 0 & 0 & 0 \\ C_{1122}^{hom} & C_{2222}^{hom} & C_{3322}^{hom} & 0 & 0 & 0 \\ C_{1133}^{hom} & C_{2233}^{hom} & C_{3333}^{hom} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{2323}^{hom} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{1313}^{hom} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{1212}^{hom} \end{bmatrix} \begin{bmatrix}E_{11}\\ E_{22}\\ E_{33}\\ E_{23}\\ E_{13}\\ E_{12}\end{bmatrix}$$

For i =j=k=l ; i, j, k, l Є{1,2,3}, the C_{ijkl}^{hom} coefficients, have been determined by imposing a shear loading whose main directions correspond with the symmetry's axes of the cell; that's means:

$$\underline{\underline{E}} = E_{11}\, \underline{e}_1 \otimes \underline{e}_1 + E_{22}\, \underline{e}_2 \otimes \underline{e}_2 + E_{33} \underline{e}_3 \otimes \underline{e}_3 \qquad (10)$$

For i =k and j=l i, k Є {1,2} and j, l Є {2,3}, the coefficients C_{ijkl}^{hom}, have been determined by imposing to the basic cell a macroscopic displacement of type "simple shear" which can be expressed as follow:

$$\underline{\underline{E}} = E_{ij}/2\, (\underline{e}_i \otimes \underline{e}_j + \underline{e}_j \otimes \underline{e}_i) \qquad (11)$$

In the order to have a periodic applied displacement's filed, it is necessary that every cell satisfies the following conditions [10]:

1. The continuity of the vector σ.*n*

2. The compatibility of the strain fields ε; therefore the neighboring should not be separated or superposed.

The periodicity of the passage from a cell to its neighbor is equivalent to pass a face from one face of the cell the cell to the opposite face. The condition (1) becomes: σ.*n* must be on the first opposite to that in the other face. The stress field σ is called periodic on the cell while the field σ.*n* is anti-periodic on its contour.

III. Homogenization of the yarn based on micro scale finite element model

1. The micro scale constructive finite elements models

The adapted method consists in applying three simple traction loads following the three main axes (1, 2 and 3) and three simple shear loads in the directions 2-3, 1-2 and 2-3 (figure 4). In order to applying this method we should be imposed a displacements loading and putting a specific boundary conditions for each load, this method has been adapted by several authors [10, 14].

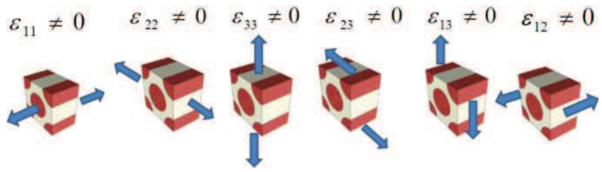


Figure 4: The six different cases to be solved in order to calculate the homogenized elastic properties of the RVE.

The calculation of $\sum_{ij}$ is approximated by the summation of all the volumetric elements of structure already calculated by elementariness integrations throw every finite element. Then we have the following equation:

$$\Sigma_{ij} = \langle \sigma \rangle = \frac{1}{V}\int_{\Omega} \sigma\, dv \cong \frac{\sum_{k=1}^{n} v_k (\sigma_{ij})_k}{\sum_{k=1}^{n} v_k} \qquad (12)$$

Where: $\mathcal{V}_k$ is the volume of the k th element and σ ij is the composing ij of the microscopic constraint of the k th element.

2. Periodic representative elementary volume:

During the simulation, it is necessary to apply the loads as imposed displacements and to impose boundary conditions to the limits for every load. At first, we have supposed that the material is orthotropic. Then, the numeric simulation and the calculations by periodic homogenization gave the rigidity matrix of the yarn:

$$C = \begin{pmatrix} 198953{,}521 & 2916{,}098 & 2915{,}550 & 0 & 0 & 0 \\ 2916{,}099 & 10427{,}265 & 1874{,}303 & 0 & 0 & 0 \\ 2915{,}550 & 1874{,}303 & 10426{,}265 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5820{,}813 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5960{,}149 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5960{,}646 \end{pmatrix}$$

The calculation of the inverse rigidity matrix, will give the values of the suppleness matrix **Φ**, so we can determinate the material parameters. These parameters are summarized, in the following table:

The Young Modules (MPa)	Poisson Coefficients	Shear Modules (MPa)
E_1 = 197570,919 E_2 = 10061,284 E_3 = 10060,343	ν_{23}= 0,176 ν_{13} = 0,237 ν_{12} = 0,237	G_{23}= 5820 G_{13}= 5960 G_{12}= 5960

Table 2: The periodic RVE elastic parameters

➔The yarn's material is unidirectional and the results of the simulation of the periodic RVE using Von Mises constraint are provided in figure 9.

The Von Mises constraint in the RVE structure is

$$\bar{\sigma} = \sqrt{\frac{3}{2}\sum_{ij} S_{ij}S_{ij}} = \sqrt{\frac{3}{2}\sum_{ij} \sigma_{ij}\sigma_{ij-\frac{1}{2}}\left(\sum_k \sigma_{kk}\right)^2} \qquad (13)$$

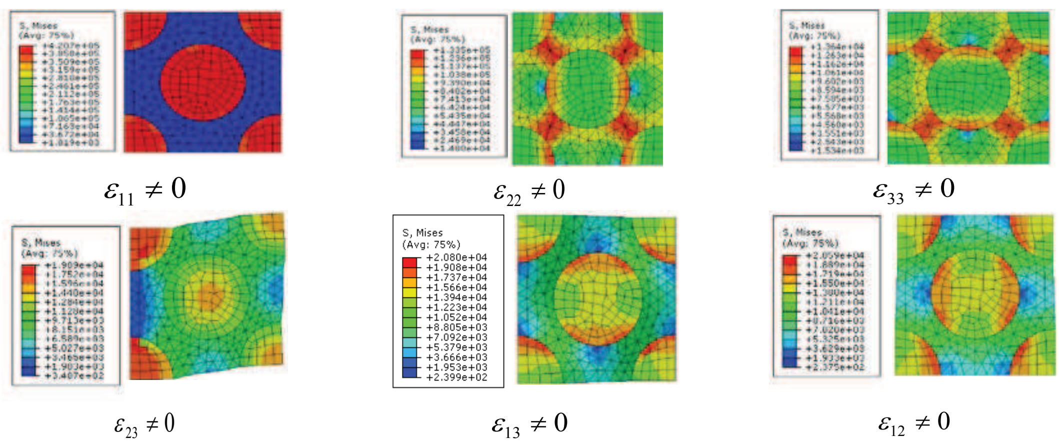


Figure 5: Results of simulation of the RVE, Von Mises constraint in the different loads (plan y z),

3. Random representative elementary volume

By one applying the same boundary conditions and the same loads on the random cell, we can determine the constants of the rigidity matrix C of the yarn and the suppleness matrix Φ, and consequently we can determinate the material random parameters which are shown in the following table:

The Young Modules (MPa)	Poisson Coefficients	Shear Modules (MPa)
E_1 = 183019,394 E_2 = 11588,548 E_3 = 9951,280	ν_{23}= 0,093 ν_{13} = 0,222 ν_{12} = 0,243	G_{23}=4498 G_{13}= 5354 G_{12}= 5369

Table 3: The random RVE elastic parameters

The results of the simulation of the random RVE using Von Mises constraint are provided in figure 11

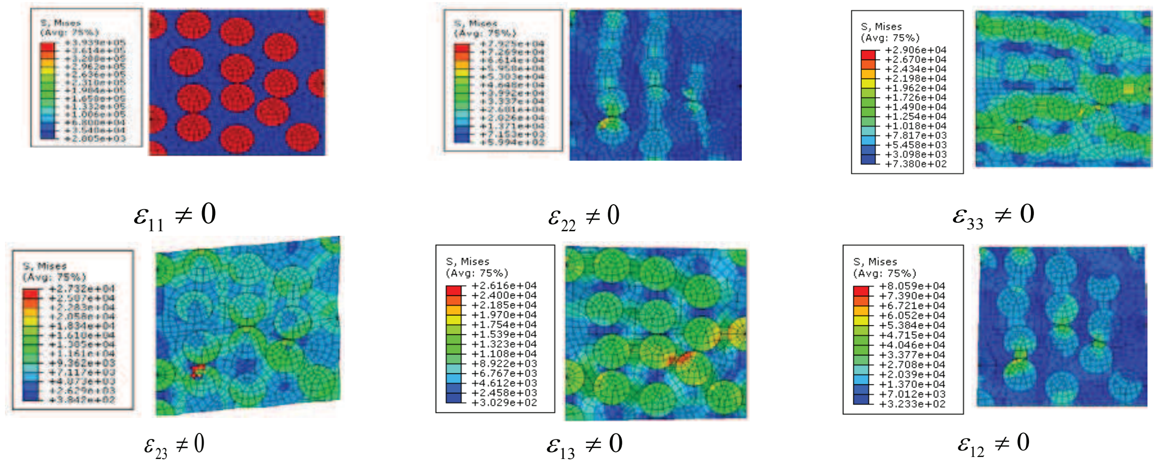


Figure 6: The results of simulation of the RVE, Von Mises constraint in the different loads (plan y z),

4. Comparisons between periodic and random model

The results gotten for the periodic and random model are reported in table 4. We can identify a fluctuation in the Young modules and the Poisson coefficients among the two models: the relative error for E_2 reaches 13% and, for the Poisson coefficients $\nu_{12}$and ν_{13} it is respectively 2, 47% and 6.76% .These results converge with the 2D studies in simple traction following the (OY) axis achieved by D.Trias [13], where the Young module present a differentiation of 12% and 6% for the Poisson coefficient.

Variables	Young Module			The share Modeling			The poisons coefficients		
	E_1	E_2	E_3	G_{23}	G_{13}	G_{12}	ν_{23}	ν_{13}	ν_{12}
Periodic RVE	197570,919	10061,284	10060,343	5820	5960	5960	0,176	0,237	0,237
Random RVE	183019,394	11588,548	9951,280	4498	5354	5369	0,093	0,222	0,243
Relative error (%)	7,95	13,18	1,096	29,39	11,32	11,01	89,25	6,76	2,47

Table 4: Computation of effective properties for the periodic and random model of the yarn

Our survey in 3D simulation will give some results more advanced than [13]. The difference between the random and the periodic RVE in Shear Modules G_{13} and G_{12} is roughly 11% and 29.39% for $G_{23.}$ Concerning the Poisson coefficient ν_{23} the relative error between the two models is around 89%.

In the numerical results, for the periodic REV, we observe a like value of YOUNG modules E2 and E3 (E2=10061, 284 MPa and E3=10060,343 MPa) and a regular behavior in the tow transverse directions. But for the random model, a small difference between the value of the two YOUNG modules (E2=11588, 548 MPa and E3=9951,280 MPa), this difference is generally due to the proposed arrangement of fibers and the irregular distances inter-fibers in the REV (see figure 3a-b). Also a variation of the value of E2 of 13% and the value of G23 of 29,39 % has been observed in the two cases random and periodic REV. This deference is due to the closeness between fibers in the random REV who will give a more resistance.

The results of the distribution using Von Mises constraint in the matrix and the fibers (figure 5 and 6) present a huge difference between the two types of RVE. Indeed, the random model gives a more real response than the periodic model.

5. Analytic results

In order to validate the numerical results presented in the previous section, a simplest theoretical approaches. These theoretical models are able to predict the composites parameters'. The Voigt model and the Reuss model are expressed by [16 and 17]:

Reuss model (transverse model):

$$E_t = [V_f/E_f + V_m/E_m]^{-1} \quad (14)$$

The Voigt model (longitudinal model):

$$E_l = E_f . V_f + E_m . V_m \qquad (15)$$

Shear Module and poisons coefficient are calculated by the mixtures law as follow:

$$\upsilon_{lt} = \upsilon_f . V_f + \upsilon_m . V_m \qquad (16)$$

$$G_{lt} = [V_f / G_f \ + V_m / G_m \ ]^{-1} \qquad (17)$$

The analytical results bases in Reuss and Voigt approaches are:

E_l = 197000 MPa ; $E_2 = E_3$ = 7918.718 MPa ; υ = 0,175

Particularly, the analytic results prove the numerical prediction in periodic model of E_1, poisons coefficient ν_{23}, but we observe a small variation of the values of E_2, E_3, ν_{12} and ν_{13}, this difference is due to the no into account the morphology of the composite material in the used theoretical models.

Conclusions:

The micro scale modeling adopted in this work has permitted to extract the elastic features of the composite yarn and the simulation of the periodic and random RVE gave that the yarn material is unidirectional. According to the works of D.Trias [13] where two types of 2D representative models (random and periodic) were compared, we can conclude that the periodic models could be used in some cases when the observed error is considered like negligible and no assessment for the material's security. But this type of model cannot be adopted to calculate accurately the material properties. The uses of periodic models could cause misjudge estimation (crack in the matrix and initiation of the damages), contrarily to the random models which can provide useful information for reliability analysis not achieved with periodic models. We have confirmed the numerical simulation by classical analytic models (Reuss and Voigt) but it is recommended to develop an appropriate law for our composite yarn. The results gotten using the random RVE will be implanted shortly in the meso-scale modeling of our woven fabric composite. This study is promoter and it requires an advance model in damage and the rupture problems and to define the constitutive law of the yarn.

References:

[1] F. Costanzo and L. Gray; Multiscale Modeling and Simulation of Composite Materials andStructures: Chapter 5: A Micromechanics-Based Notion of Stress for Use in the Determination of Continuum-Level Mechanical Properties via Molecular Dynamics; Springer Science (2008)

[2] P. Boisse and Gilles Hivet: Consistent mesoscopic mechanical behaviour model for woven composite reinforcements in biaxial tension Composites: Part B 39 (2008) 345–361

[3] Gilles Hivet, Consistent 3d geometrical model of fabric elementary cell. application to a meshing preprocessor for 3d finite element analysis, Finite Elements in Analysis and Design 42 (2005) 25–49

[4] L. Orgéas: Woven fabric permeability: From textile deformation to fluid flow mesoscale simulations, Composites Science and Technology 68 (2008) 1624–1630.

[5] Jinhuo Wang: Predictive Modeling and Experimental Measurement of Composite Forming Behavior: Thesis submitted to The University of Nottingham for the degree of Doctor of Philosophy; (2008)

[6] P. Boisse: Computational determination of in-plane shear mechanical behavior of textile composite reinforcements, Computational Materials Science 40 (2007) 439–448

[7] P. Badel, S. Gauthier, E. Vidal-Sallé, P. Boisse: Rate constitutive equations for computational analyses of textile composite reinforcement mechanical behaviour during forming; Composites: Part A 40 (2009) 997–1007

[8] Guillaume COUÉGNAT : Approche multiéchelle du comportement mécanique de matériaux composites à renfort tissé, thèse Université de Bordeaux 1- (2008)

[9] J. Molimard : Mécanique des Matériaux composites, EMSE Version 2 (2004).

[10] Faiza Ben Abdallah-Maamoun : Elaboration, caracterisation et modelisation d'un materiau composite à base d'une matrice thermoplastique renforcee par du liege, thèse ENIT (2009)

[11] A. Alzina: Multiscale modelling of thermal conductivity in composite materials for cryogenic structures, Composite Structures 74 (2006) 175–185

[12] Jayesh R. Jain and Somnath Ghosh: Damage Evolution in Composites with a Homogenization-based Continuum Damage Mechanics Model; International Journal of Damage Mechanics (2009)

[13] D. Trias: Random models versus periodic models for fibre reinforced composites, Computational Materials Science 38 (2006) 316–324

[14] B.Van Den Broucke: Determination of the mechanical propreties of textile-reinforced composites taking into account textile forming parameters; Springer/ESAFORM (2010)

[15] Moran Wang, Ning Pan: Elastic property of multiphase composites with random microstructures; Journal of Computational Physics 228 (2009) 5978–5988

[16] W. Voigt, **Ü**ber die Beziehung zwischen den beiden Elastizitätskonstanten isotroper Körper, Wied. Ann. 38 (1889) 573–587.

[17] A. Reuss, Berechnung der Fliessgrenz von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle, Z. Angew. Math. Mech. 9 (1929)