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WPC composites, homogenization methods, Digimat software

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INFLUENCE OF HOMOGENIZATION METHODS IN PREDICTION OF STRENGTH PROPERTIES FOR WPC COMPOSITES

Abstract

In order to reduce costs of experimental research, new methods of forecasting material properties are being developed. The current intensive increase in computing power motivates to develop the computer simulations for material properties prediction. This is due to the possibility of using analytical and numerical methods of homogenization. In this work calculations for predicting the properties of WPC composites using analytical homogenization methods, i.e. Mori-Tanaka (first and second order) models, Nemat-Nasser and Hori models and numerical homogenization methods were performed.

1. INTRODUCTION

The common feature of all composite materials is that their micro-scale properties strongly influence on the macro-scale properties of the entire material. The ability to describe microstructural phenomena leads to a better understanding of the macroscopic behavior of the material, but most often the exact microstructural properties are unknown, so it is generally necessary to assume certain assumptions. These properties can be determined by homogenization procedures that are appropriate to averaging the material properties of the analysed area. This sample of material is often referred as a Representative Volume Element (RVE) (Amirmaleki et al., 2016; Soni, Singh, Mitra & Falzon, 2014; Trzepieciński, Ryzińska, Biglar & Gromada, 2017; Frącz & Janowski, 2016).

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Several years ago, calculations about material homogenization could be performed by making appropriate experiments and trials based on existing material sample, or by using analytical methods, which have relatively strong constraints and often fail to provide adequate results. Recently the possibilities of simulating the numerical microstructural behaviors in 3D have been developed in order to obtain more accurate results and consequently, more accurate determination of material properties (Pierard, LLorca, Segurado & Doghri, 2007). These numerical simulations can significantly reduce the number of time consuming and costly experiments with carefully produced samples of material. This should improve the development and design of new materials for modern engineering applications.

Research on the properties of composites based on averaging has been ongoing for many years. Estimates of structural properties have been made based on number of assumptions about internal phenomena in the microstructure of the material. Works of Maxwell (Maxwell, 1867, 1873) and Rayleigh (Rayleigh, 1892) were to describe the general macroscopic properties of materials consisting of a spherical particle reinforced in matrix. As far as Voigt (Voigt, 1889) is concerned, it is one of the precursors of early prediction of the effective mechanical properties of heterogeneous materials. Voigt assumed that the field of deformation in the bulk sample of heterogeneous material was homogeneous, leading to a fairly effective definition of the generalized properties of the material. Over the next decades some important assumptions developing the possibilities of homogenization methods have been developed. The main assumption of the Eshelby (Eshelby, 1957) model is based on the concept of self-deformation, which is used to determine the solution of the single-inclusion problem placed in the infinite matrix of the material under uniform external load. The result of this type of assumption is not largely error-free, however, the difficulty of solving this problem is relatively small and the model itself is easy to use. It was the basis for the development of many approximation methods of homogenization, based on the calculation of the interaction between the inclusion of specific geometry and the matrix.

An example of the most popular model of homogenization is Mori-Tanaka model (Mori & Tanaka, 1973). The general assumption of the model is based on the approximate solution of Eshelby. It has been assumed that the strain concentration tensor relating the volume average of strain over all inclusions to the mean matrix strain is directly the strain concentration tensor of the single inclusion problem. This formulation is presented by:

$$B^{\varepsilon} = H^{\varepsilon}(I, C_0, C_1) \tag{1}$$

where: B^{ε} – strain concentration tensor,
H^{ε} – single inclusion strain concentration tensor,
C_0 – matrix stiffness,
C_1 – inclusion stiffness.

The area is infinite and considered to the average matrix strains in the current RVE as the far field strain. This led Benveniste (Benveniste, 1987) to the advanced interpretation of the Mori-Tanaka model – any inclusion in RVE is interpreted as an individual inclusion in the polymer matrix.

The efficiency of this model is very high in predicting the properties of biphasic material to about 25% of inclusions content (*e-Xstream engineering*, 2016).

It was noted that Mori-Tanaka model has additional formulation. For in-elastic composites, e.g., elasto-plastic type the tangent operator for each phase is calculated with the volume average of the strain field in the phase. This received value is described as the first statistical moment of the per-phase strain field. In second-order homogenization not only first but second moment of each phases strain field were used. The second moment is connected to the variance. The latter improves the statistical information in relation to only a simple mean value. Hence it is often expected better predictions value using second-order instead of first-order homogenization.

The second order theory brings some correction when three conditions are received:

- fiber is reinforcement,
- it was established high stiffness contrast between matrix and fibers,
- the elasto-plastic matrix is characterized by small strengthening.

Otherwise, no important differences are received between the predictions of first- and second-order homogenization method (Lagoudas, Gavazzi & Nigam, 1991, Mercier, & Molinari, 2009).

The Double inclusion model was formulated by Nemat-Nasser and Hori (Nemat-Nasser & Hori, 1993) The main premise is that each inclusion (I) (of C_1 stiffness) is surrounded in its close environment (I_o) with matrix (of C_0 stiffness), while outside those place there is a reference medium (of C_r stiffness). Simply put, RVE of composite is swapped with a composite model made of imaginary reference matrix (of C_r stiffness) in which are placed inclusions (of C_1 stiffness) surrounded with a material of matrix (of C_0 stiffness).

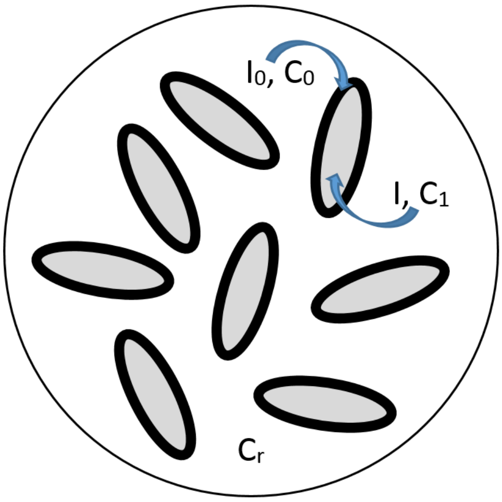

Fig. 1. The idea of Double Inclusion model

Interpolative Double Inclusion model (Lielens, 1999) is determined by the following strain concentration tensor connected with the mean strain over the inclusions to its equivalent over the matrix:

$$B^{\varepsilon} = [(1-\xi(v_1))(B_l^{\varepsilon})^{-1} + \xi(v_1)(B_u^{\varepsilon})^{-1}]^{-1} \tag{2}$$

where: B_l^{ε} – strain concentration tensor for Mori-Tanaka model ($B_l^{\varepsilon} = H^{\varepsilon}(I, C_0, C_1)$)

B_u^{ε} – strain concentration tensor for inverse Mori-Tanaka model ($B_u^{\varepsilon} = H^{\varepsilon}(I, C_1 C_0)$)

$\xi(v_1)$ – interpolation function.

Interpolation function was simplified to quadratic formulation:

$$\xi(v_1) = \frac{1}{2} v_1 (1 + v_1) \tag{3}$$

where: v_1 – volume fraction for inclusion.

For two-phase composites with linear elastic strength characteristic this model usually gives good predictions of the properties, over all ranges of particles volume content, aspect ratios and stiffness contrasts.

The limitations encountered with the use of analytical homogenization methods require additional calculation methods. Therefore, in recent years numerical methods of direct calculation of effective material data have become increasingly numerous and significant (Bendsøe & Kikuchi, 1988). Most of these methods are only developed with respect to the linear strain range – the range of small deformations. Due to the growing calculating power of computers, several methods have been developed to predict the nonlinear behavior of composite material. Numerical calculations can be performed in 2D space, where discretization is most often used to divide the area into triangles. This solution allows to calculate the values that appear in the cross section of material. However, there are some constraints resulting from the specificity of the solution to the problem (e.g. flow direction only penetrating the modeled surface, etc.) (Abdulle, 2013; Bouchart, Brieu, Kondo & Abdelaziz, 2007). Due to the advancement of computer technology in most recent years, more simulation packages are equipped with the ability to solve 3D problems. Discretization usually consists in dividing the area into tetrahedrons finite elements (FE). Such modeling is devoid of the fundamental limitations of 2D technology but is much more demanding in terms of memory and computing power. One of the main types of FE used in microstructural calculations are Voxel finite elements (Doghri & Tinel, 2006). These type of finite elements are regular, incompatible set of brick elements. Each element is assigned to the phase material where its center is located. It is targeted for advanced RVE where discretization is difficult to reproduce the shape of matrix and analyzed inclusions.

In this work calculations for predicting the properties of WPC composites using mainly analytical homogenization methods, i.e. Mori-Tanaka (first and second order) model, Nemat-Nasser and Hori model and the numerical homogenization were performed using Digimat software.

2. EXPERIMENT

The research material was wood-polymer composite (WPC). It consisted of a Moplen HP648T polypropylene as polymer matrix and Lignocel C120 wood fibers (WF), with L/d = 10. The percentage of wood fiber in composite was 10% vol. The composite was extruded using a Zamak EPH-25 single screw extruder (Fig. 2) and then granulated. The resulting granulate was injected into a mold cavity by means of Dr Boy 55E injection molding machine. The specimens for uniaxial tension test, acc. to EN ISO 527-1 were manufactured in this way. The uniaxial tensile test was performed using Zwick Roell Z030 testing machine. Ten specimens were tested at speed of 50 mm/min according to PN-EN ISO 527 standard. The obtained stress-strain characteristic was used as a verification criterion for further numerical analysis.

3. CALCULATIONS

Fig. 2. Manufacturing of WPC composites: 1 – Zamak EPH-25 extruder, 2 – cooling bath, 3 – granulator

The composite properties prediction studies were carried out using DIGIMAT 2017 commercial code. The DIGIMAT MF module of this software was used for calculations using analytical homogenization models. This software allows to make calculations using different models including Mori-Tanaka (first and second order) and Double Inclusion model (Nemat-Nasser and Hori model). For the analysis, data for matrix and fibers have to be introduced. For the proper description of the matrix, experimental data from uniaxial tensile test (Tab. 1, Fig. 3) were introduced and the elasto-plastic model with isotropic symmetry was chosen.

Tab. 1. Chosen properties of the polymer matrix

Property	Value/unit
Density	900 kg/m^3
Young's modulus	1600 MPa
Poisson's ratio	0.39
Yield stress	17
K	19.277
n	0.294

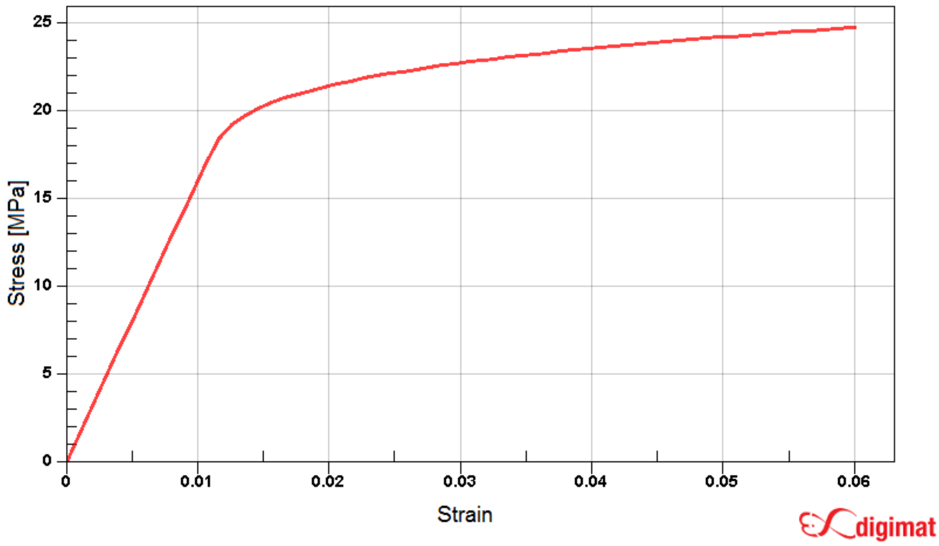

Fig. 3. Stress-strain characteristics for Moplen HP648T polypropylene matrix (elasto-plastic range)

In addition, the data of wood fibers properties – (Tab. 2, Fig. 4) were introduced. They were determined on the basis of literature (Frącz & Janowski, 2016). An elastic mechanical model with transversally isotropic symmetry was selected. In addition, an important step in the preparation of the analysis was to define the geometric parameters of the fibers: the fiber orientation tensor and the l/d ratio. The percentage of wood fiber in polymer matrix was defined as 10%.

Tab. 2. The selected properties of analysed wood fibers

Property	**Value/unit**
density	2000 kg/m^3
Young's modulus E1	10000 MPa
Young's modulus E2	10000 MPa
Poisson's ratio v12	0.3
Poisson's ratio v21	0.3
Shear modulus	3846 MPa

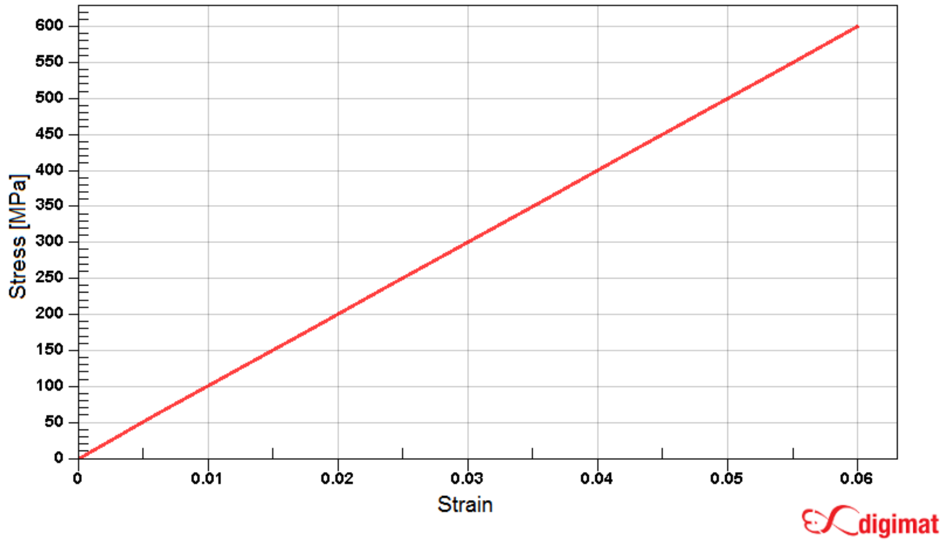

Fig. 4. Stress-strain characteristic for wood fiber (elastic range)

In order to carry out the numerical homogenization using the DIGIMAT FE software, the data about fiber orientation, distribution and geometry in RVE (Tab. 3) were introduced. To describe the adequate shape of the fibers, a curved cylinder geometry was selected which describes well the actual shape of the wood fiber in real conditions. The RVE dimensions were large enough to determine the actual distribution of fibers in the polymer matrix, but also small enough to make good calculations. The RVE with placed fibers in the polymer matrix according to the preset orientation tensor was discretized using 250 thousands finite elements of Voxel type (Tab. 3). The visualization of RVE before and after discretization was shown in Fig. 5.

Tab. 3. The input data for micromechanical analysis using Digimat FE software

Fiber diameter	0.01 mm
Fiber length	0.1 mm
The ratio of length to fiber diameter (L/D)	10
Fiber volume content	0.106445
RVE dimensions	0.2x0.1x0.1 mm
The amount of FE type Voxel in RVE	250 000
The orientation tensor values: a[1,1] a[2,2] a[3,3]	 0.73 0.18 0.09

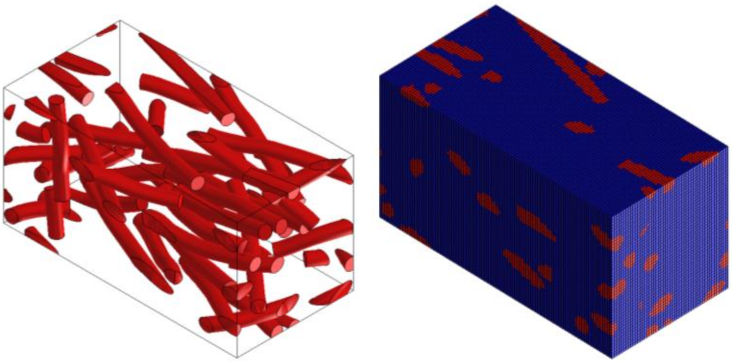

Fig. 5. The visualization of fibers (with curved cylinder geometry) distribution in RVE for defined orientation tensor value: before (left) and after (right) discretization

3. RESULTS ANALYSIS

One of the most important results is the stiffness matrix. It can be noted that the obtained stiffness matrix using the Mori-Tanaka homogenization model has the same value for the first and second order models (Fig. 6). Furthermore, in the case of stiffness matrix using a numerical model, the matrix was filled in all cells, indicating a slight numerical error.

a)

	11	22	33	12	23	13
11	3755.2	2317.2	2290.5	0	0	0
22	2317.2	3584.1	2270	0	0	0
33	2290.5	2270	3558.8	0	0	0
12	0	0	0	644.4	0	0
23	0	0	0	0	647.49	0
13	0	0	0	0	0	628.5

b)

	11	22	33	12	23	13
11	3755.2	2317.2	2290.5	0	0	0
22	2317.2	3584.1	2270	0	0	0
33	2290.5	2270	3558.8	0	0	0
12	0	0	0	644.4	0	0
23	0	0	0	0	647.49	0
13	0	0	0	0	0	628.5

c)

	11	22	33	12	23	13
11	3771.1	2328.1	2301.2	0	0	0
22	2328.1	3597.2	2281.2	0	0	0
33	2301.2	2281.2	3571.5	0	0	0
12	0	0	0	645.62	0	0
23	0	0	0	0	648.24	0
13	0	0	0	0	0	629.27

d)

	11	22	33	12	23	13
11	3851.07	2378.55	2320.42	18.6963	3.56373	4.72553
22	2378.41	3648.28	2288.18	27.4198	9.20855	15.4909
33	2318.58	2287.02	3672.57	18.3458	2.55344	-1.79352
12	1.7039	1.67646	2.73226	661.937	12.3035	-2.06523
23	-1.04414	-0.60794	-0.590882	10.7581	665.909	2.7773
13	6.43266	9.87309	6.18807	-1.23184	2.7086	619.035

Fig. 6. Stiffness matrices for WPC composite with 10% WF: a) Mori-Tanaka homogenization model (1st order), b) Mori-Tanaka homogenization model (2nd order), c) Nemat-Nasser Hori homogenization model, d) numerical homogenization

In addition, composite strength data were obtained after homogenization in the elastic range (Tab. 4). It was noted that the Mori-Tanaka models of first and second order give the same results. Very good compatibility was obtained in results of all analytical homogenization methods. The results of calculations using numerical homogenization method are quite different from them.

Tab. 4. Received data (in elastic range) for variable type of homogenization

	Mori-Tanaka (1st order)	Mori-Tanaka (2nd order)	Nemat-Nasser and Hori	Numerical homogenization
Density	1001 kg/m^3	1001 kg/m^3	1001 kg/m^3	1006 kg/m^3
Young's modulus E1	1937.7 MPa	1937.7 MPa	1944.1 MPa	1994.0 MPa
Young's modulus E2	1814.8 MPa	1814.8 MPa	1818.2 MPa	1857.9 MPa
Young's modulus E3	1821.1 MPa	1821.1 MPa	1824.4 MPa	1940.1 MPa
Poisson's ratio v12	0.4008	0.4008	0.40105	0.41989
Poisson's ratio v21	0.37358	0.37358	0.37507	0.39134
Poisson's ratio v13	0.38797	0.38797	0.38817	0.37021
Poisson's ratio v31	0.36462	0.36462	0.36426	0.35976
Poisson's ratio v23	0.39624	0.39624	0.39841	0.37574
Poisson's ratio v32	0.39761	0.39761	0.39841	0.39237
Shear modulus G12	644.4 MPa	644.4 MPa	645.6 MPa	661.7 MPa
Shear modulus G23	628.5 MPa	628.5 MPa	629.3 MPa	665.7 MPa
Shear modulus G13	647.5 MPa	647.5 MPa	648.2 MPa	618.9 MPa

One of the most important results of strength data is the stress-strain characteristic from uniaxial tensile test. The characteristics obtained from the experiment stress-strain were compared with the results of the homogenization calculations. It was noted that the worst compatibility with the experiment gives the characteristic calculated using numerical homogenization (Fig. 7, Tab. 5). Analytical methods of homogenization give much more compatibility of results. For the analyzed value of 0.1 strain, the greatest compatibility of the stress-strain results was found for the numerical homogenization model (12.5% of the relative error). Such a high relative error value (relative to the experiment) is due to an assumed elastic-plastic model for the polymer matrix which does not fully reflect the viscoelastic nature of the polymer. It should be noted, however, that the scope of the analysis concerns very small values of the strain. A more significant and interesting result is the relative error of stress values for the strain of 0.3 and 0.5. For the value of 0.3, the lowest relative error value for the Nemat-Nasser and Hori model was obtained (relative error was 1.08%). Moreover, for strain 0.05, the highest compatibility of the stress values with the experiment was obtained for the Mori-Tanaka (second order) homogenization model (relative error value was only 0.27%). It should be noted that the Mori-Tanaka homogenization models of first and second order definitely gives different results in calculating the stress-strain characteristics above 0.01 strain. This is due to the fact that these calculations were in elastic-plastic range.

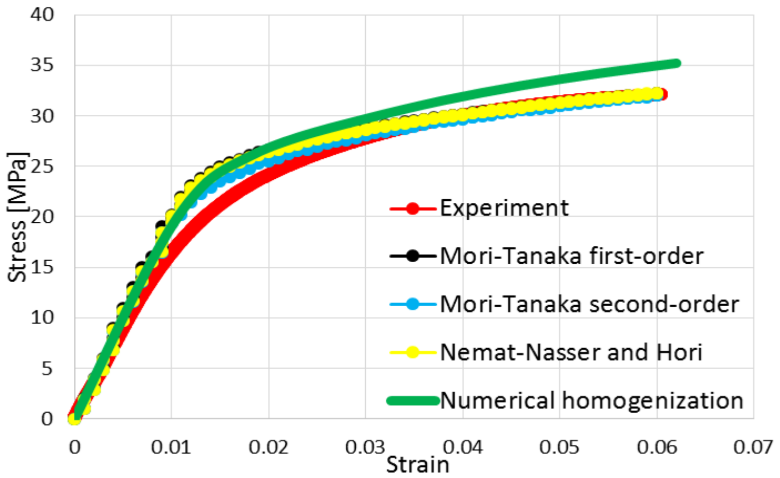

Fig. 7. Stress-strain characteristic for WPC composite with 10% WF for different homogenization models

Tab. 5. Relative errors calculated for individual homogenization methods at fixed strain value

Strain	Homogenization methods (relative to the experiment)			
	Mori-Tanaka (1st order)	Mori-Tanaka (2nd order)	Nemat-Nasser and Hori	Numerical homogenization
0.01	17.73%	21.23%	17.22%	12.50%
0.03	2.88%	3.15%	1.08%	6.84%
0.05	0.28%	0.27%	1.28%	6.98%

4. CONCLUSIONS

1. WPC composite properties were predicted using analytical and numerical homogenization methods. For this purpose, it was important to introduce the strength and geometry data of the fiber and matrix.
2. In the case of numerical homogenization, an additional significant step was the design of RVE that reflected the heterogeneous structure of the composite.
3. It was noted that the stiffness matrix calculated using the numerical model of homogenization was filled in all cells, indicating that occurred small numerical errors.
4. It can be noted that the results of calculations based on the first and second order Mori-Tanaka models are very similar up approx. 0.01 strain. Only in the case of the obtained stress-strain characteristics the results are different. This is most probably due to the fact that at this stage the analysis was considered in the area of larger deformations (elasto-plastic range).

5. For all types of analytical homogenization, there is a relatively good agreement between the results of the calculations and the experimental results. It is most likely caused that the analyzed composite contained only 10% vol. of inclusions. With such a fiber content in the polymer matrix, analytical models such as the Mori-Tanaka model gives a high degree of compatibility between the results of the calculation and the experiment.

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