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COMPUTATIONAL HOMOGENISATION OF A RECYCLED COMPOSITE MATERIAL BASED ON PET AND WOOD PARTICLES

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Abstract. Valorising household solid waste through the creation of new products based on recycled materials is a necessary task to meet new environmental demands. During the last 30 years, wood-plastic composites (WPC) are been used to obtain materials lighter than wood, with mechanical properties higher than plastic and more resistant to moisture and insects. Thus, the recycling of plastic wastes, especially thermoplastics as polyethylene terephthalate (PET) and sawdust - fine particles of wood from woodworking industries - are suited basic materials for WPC. Indeed, to decrease the cost and time of experimental tests to design a new composite made from recycled PET and Chilean Radiate pine's sawdust, this work proposes to study the effective elastic properties (EEP) using a finite element simulation of a representative volume element (RVE) with periodic boundary conditions in the commercial software Digimat-FE. Density, modulus of elasticity (MOE) and Poisson's coefficients are estimated for composite materials made with 0.05 to 0.35 volume ratio of sawdust. The Voigt and Reuss mean-field homogenisation approaches are also given as upper and lower limits.

1 INTRODUCTION

Wood-plastic composite (WPC) refers to a material that contains wood particles and a polymer matrix (thermoset or thermoplastic). Wood is not only used in plastics to decrease the price compared to a solid plastic but because wood has a high strength to weight ratio, has a low density, is easily integrated into existing plastic production lines and is a renewable resource [1]. An up-to-date review of the performance and environmental impacts of wood-plastic composites can be found in [2].

These composites can be further environment-friendly if the matrix and fillers are materials from recycling waste. For this reason, they are usually referred as “green materials” [3] and they can find several industrial applications. In fact, it is certain there is a worldwide increasing interest in developing waste management strategies. For example, extended producer responsibility policies have been widely adopted in most OECD countries [4]; the Chilean government is not the exception and since 2016 is promoting the importance of turning wastes into value-added products [5].

Mechanical properties of WPC mainly depend on the properties of their components: volume fraction, interface strength, particle size and orientation. The particle geometry has been experimentally evaluated in several studies, containing wood flour or short wood fibres. In general, the tensile, compressive and flexural properties as well as the impact strength are higher when increasing the size and the aspect ratio of wood fibers [6–8]. When there are particles with a larger aspect ratio or using additives like coupling agents, there is the potential for more effective load transfer between the matrix and the particles leading to better mechanical properties [8–10].

The plastic industry has been the major producer of WPC due to its prior expertise. These composites are formed into profiles or complicated shapes mostly by extrusion or injection moulding or using a flat press process similar to the industrial particleboard manufacturing systems [10, 11].

Analytic and numerical models have been developed to predict the effective elastic constants and to reduce time and cost needed to develop new composite materials. These approaches are based on micromechanical or continuum models: the first one allows a detailed but expensive description of a heterogeneous medium, while a continuum model is a homogenous equivalent representation which ignores the fact that matter is made of not continuous materials. Homogenisation techniques allow heterogeneous materials to be treated by continuum models by estimating effective properties from the knowledge of the constitutive laws and spatial distribution of the constituents (i.e. from a given micromechanical model) [12].

These analytical models are known as mean field homogenisation schemes and they are based on the solution of Eshelby [13] – the Mori-Tanaka formulation [14], the self-consistent formulations [15], the Hashin-Shtrikman equation [16] among others. In general, they provides reasonable accuracy at modest computational cost, but they are only applicable for reinforcements which can be approximated as ellipsoids.

Alternatively, computational homogenisation has also been developed in recent years [17]. In these approaches, finite element (FE) simulations are used to solve a boundary value problem (BVP) on a representative volume element (RVE) - the smallest volume over which a measurement can be made that yields a representative value of the whole. The basic principle of the method and the scale transitions are highlighted in Fig. 1. The applied strains are then related to the average stresses to generate the equivalent stiffness of the material. Determining a critical size of such RVE is usually difficult and time consuming. Computational homogenisation with periodic boundary conditions is one alternative to reduce the complexity [18].

The chilean project for the regional competitiveness "Valorisation of recycled waste through the creation of new materials for the manufacture of marketable products" aims to design a WPC made from recycled PET and Chilean radiate pine's particles. Pinus radiata D.Don is a native specie from California which has been introduced in Europe, New Zealand, Australia, Chile, Brazil, Colombia and South Africa. The largest plantations are in Chile and New Zealand.

This work is focused on a numerical prediction of the elastic properties of this new WPC, using the software Digimat-FE to generate the RVE and to solve the discretised finite element problem with periodic boundary conditions. The paper has the following outline: Sec. 2 summaries the numerical homogenisation methodology; Sec. 3 compares density, modulus of elasticity (MOE) and Poisson's coefficients for different volume ratios. Finally, conclusions are drawn in Sec. 4.

2 HOMOGENISATION METHODOLOGY

The simplest point of view for homogenisation is that a heterogeneous medium behaves macroscopically in the same way as its constituents, but with different values of the constants of the materials, which we will call Effective Elastic Properties (EEP). In micromechanical analysis, the fields of stresses and deformations in a heterogeneous material are divided into the contributions corresponding to different scales. It is assumed that these scales are sufficiently different, such that:

- The fluctuations of the fields in the microscale have influence at the macroscopic behaviour only through its volumetric average.
- The gradients of the stress and deformation fields at the macroscale are not significant at the micro level, where these fields appear to be constant.

Before obtaining the effective properties of a heterogeneous material, the size of the RVE should be studied because it is necessary to find the appropriate dimensions whose EEP are objective. This RVE must contain enough heterogeneities and its size d must be much larger than the characteristic length l of the microscale. Then, the RVE must be small enough to be assimilated to a point at the macroscopic level. A

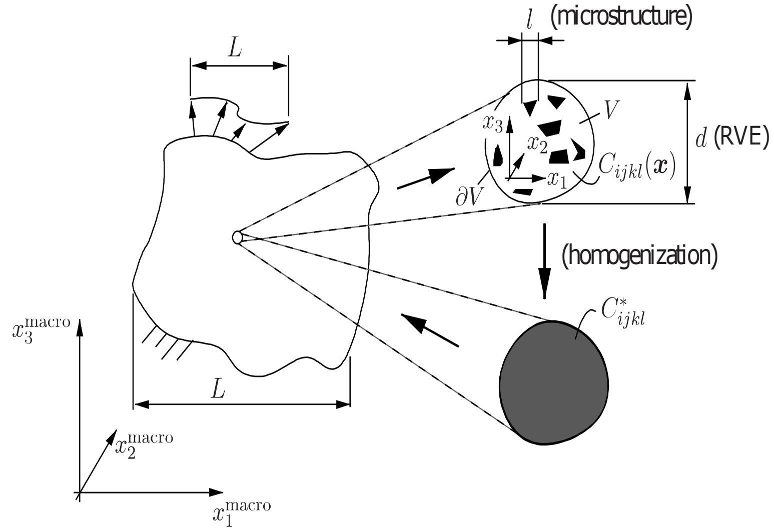


Figure 1: Characteristic scales in a homogenisation schema [19]

characteristic length L at this level can be determined according to the geometry, the spatial variation in the loads or through the strain or stresses fields. Both previous conditions are verified when $l \ll d \ll L$, as schematised in Fig. 1.

The simplest mean-field homogenisation methods are the Voigt [20] and Reuss [21] models. Voigt assumes that the strain field is uniform in the RVE; consequently, the macro stiffness is found to be the volume average of the micro stiffness. In the Reuss model, the stress field is assumed to be uniform in the RVE; the macro compliance is then found to be the volume average of the micro compliances. The EEP calculated are straightforwardly identified as the upper (Voigt) or the lower (Reuss) bound, respectively. These methods are easily implemented but they do not take into account the shape or the orientation of the inclusions.

In this work, we focus our efforts on understanding the mechanisms that dominate the macroscopic properties of the material, but that really arise from its microscopic composition. We propose to generate RVEs as real as possible using the Digimat-FE software. Then, the finite element model is solved by a finite element analysis in the same software. Periodic boundary conditions were imposed on all faces of the RVE through a large set of equations that relate the degrees of freedom of the nodes that are on one face with those of the corresponding nodes that are on the opposite side. Figure 2 illustrates the case of a macroscopic uniaxial deformation ε_{11}.

Periodic boundary conditions generally lead to the best predictions when compared to the Dirichlet, Neumann or mixed edge condition type. It also shows a faster convergence speed as the size of the RVE increases, but at the expense of greater

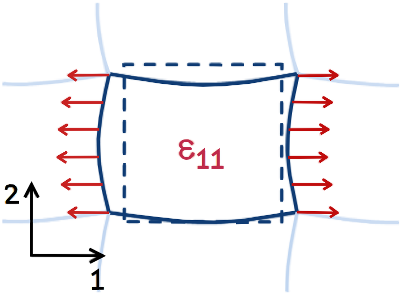


Figure 2: Periodic boundary condition type [22]

CPU time and memory requirements due to the large set of constraint equations that must be imposed [22].

The micro constituents under analysis are defined in Tab. 1. The chosen polymer matrix was PET and its isotropic properties, as a first approach, were provided by the American Industry Professional Plastics [23]. The elastic properties of the sawdust particles were taken into account from mechanical tests performed on Pinus radiata D.Don specimens from the Chilean Company Arauco, containing 12% moisture [24]. To assimilate wood particles with ellipsoidal shape, we assume a transversally isotropic material.

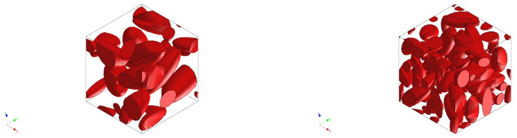
Table 1: Properties of Pinus radiata D.Don and PET [23, 24]

material	axial elastic modulus [GPa]	in-plane elastic modulus [GPa]	in-plane Poisson's ratio [-]	transversal Poisson's ratio [-]	transversal shear modulus [GPa]	density $[kg/m^3]$
Pinus radiata	10.048	1.091	0.4	0.3	1.217	442
PET	3	3	0.41	0.41	1.064	1370

In this study, the dimensions for the sawdust particles are established according to Table 2, where the size ranges of the particles are identified. For the aspect ratio (length-to-diameter ratio) of the sawdust we have chosen 2.5 in concordance with aspect ratio of wood flour particles in [25]. Orientation has a great influence on the maximum volume fraction that can be reached. The more random the orientation, the smaller the fraction of maximum volume which can be reached. This effect becomes stronger when the aspect ratio is high [22].

Table 2: Composition of sawdust by size range [26]

Size [mm]	<0.25	>0.25; <0.425	>0.425 <1.00	>1.00; <1.40	>1.40; <2.00	>2.00; <2.80	>2.80; <3.35	>3.35; <4.75	>4.75
	2.64	6.06	25.56	18.13	18.03	12.33	4.06	6.31	6.89



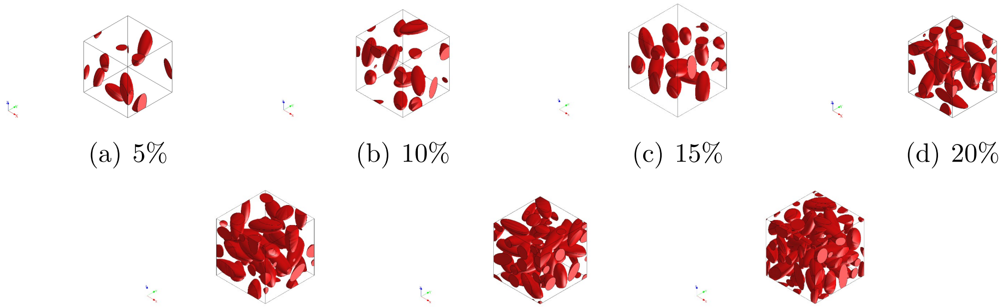
(a) side = 1.0 [mm] (b) side = 1.5 [mm]

Figure 3: Side length for cubic RVEs with 35% sawdust

Two cubic RVE are proposed to verify the size's influence on the EEP. The first one is 1.0 [mm] on a side and the second is 1.5 [mm], as shown in Fig. 3 for a content of 35% of sawdust. The distribution of the particles is fully 3D random as illustrated in Figure 4, while Fig. 5 shows their meshes.

3 RESULTS

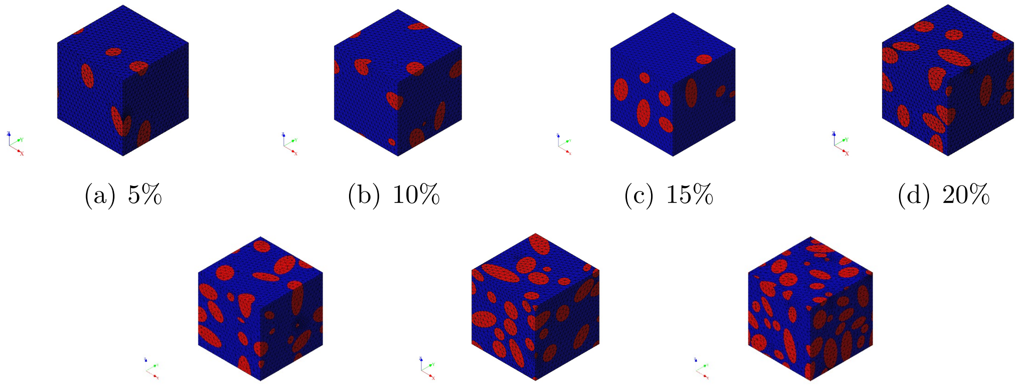
After computing the numerical periodic homogenisation with Digimat-FE, the obtained EEP – Young modulus, Poisson ratios and shear modulus – are summarised in Figures 6(a)-6(f) for 0.05 to 0.35 volume ratio of sawdust and considering the two RVE sizes. Because there is not a significant difference between the 1 [mm] (blue



(a) 5% (b) 10% (c) 15% (d) 20%

(e) 25% (f) 30% (g) 35%

Figure 4: Geometrie for different sawdust volume ratio (RVE 1.5 [mm])



(a) 5% (b) 10% (c) 15% (d) 20%

(e) 25% (f) 30% (g) 35%

Figure 5: Finite element mesh for different volume ratio (RVE 1.5 [mm])

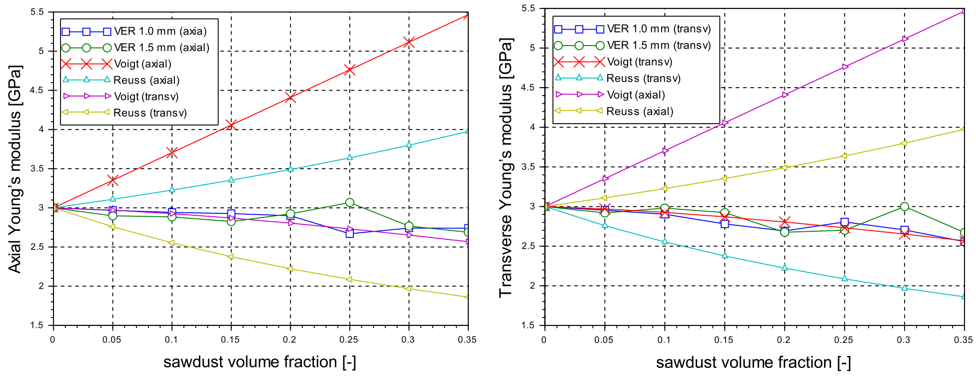
line) and 1.5 [mm] (green line) RVE's, we considere the smallest one for the following.

The periodic EEP are always contained into the Voigt and Reuss bounds (except for some Poisson's ratios), but considering both transversal and in-plane bounds are crossed. This is expectable due to the random spatial distribution of the wood particles which are not considered by Voigt and Reuss models. The six EEP shown in Figures 6(a)-6(f) decrease when increasing the sawdust volume but remain close to the PET properties. Indeed, due to the random spatial distribution of the wood particles, the homogenised constants are highly independent of the direction in space, enabling to produce a quasi isotropic composite material – even the relation $G = E/2(\nu + 1)$ is near to be verified – as highlighted in Tab. 3.

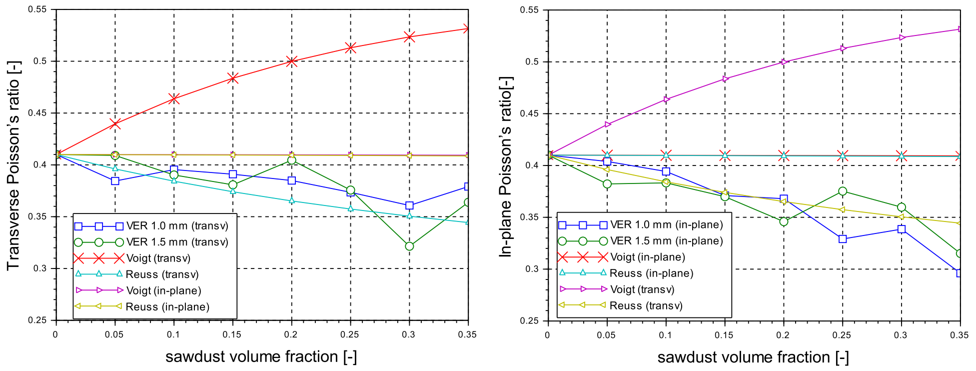
Fig. 7 shows that the density decreases as the volume of sawdust increases due to the fact that the wood's density is almost three times lower than PET.

Table 3: Homogenised elastic properties (RVE 1.0 [mm])

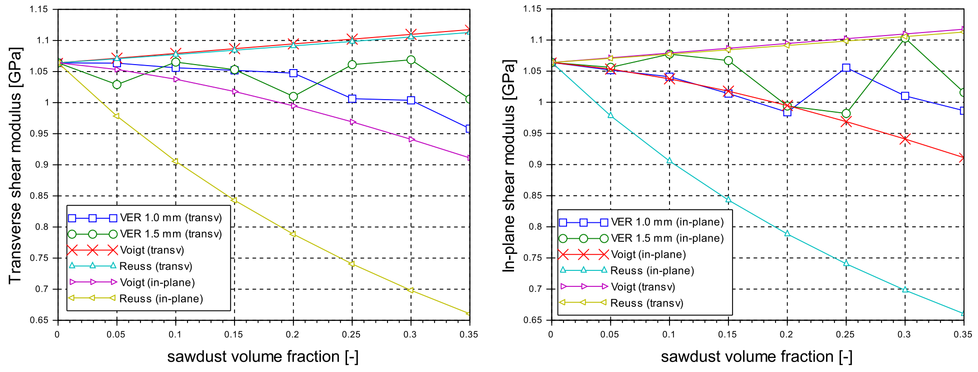
f [-]	0.05	0.1	0.15	0.2	0.25	0.3	0.35
E_{axial} [GPa]	2.9677	2.9418	2.9270	2.8993	2.6693	2.7414	2.7404
E_{transv} [GPa]	2.9532	2.9030	2.7806	2.6924	2.8061	2.7047	2.5572
υ_{axial}	0.3844	0.3954	0.3910	0.3849	0.3735	0.3608	0.3791
$\upsilon_{in-plane}$	0.4039	0.3942	0.3710	0.3680	0.3291	0.3386	0.2961
G_{transv}[GPa]	1.0635	1.0561	1.0520	1.0474	1.0064	1.0038	0.9582
$G_{in-plane}$[GPa]	1.0518	1.0411	1.0141	0.9841	1.0556	1.0103	0.9865
ρ $[kg/m^3]$	1323.6	1277.2	1230.8	1184.4	1138.0	1091.6	1045.2



(a) Axial Young modulus (b) Transverse Young modulus



(c) Transverse Poisson ratio (d) In-plane Poisson ratio



(e) Transversal shear modulus (f) In-plane shear modulus

Figure 6: Voigt, Reuss and periodic EEP for different sawdust volume fraction

4 CONCLUSIONS

The computational periodic homogenisation which has been implemented using Digimat-FE is suitable for working with composite materials whose inclusions are

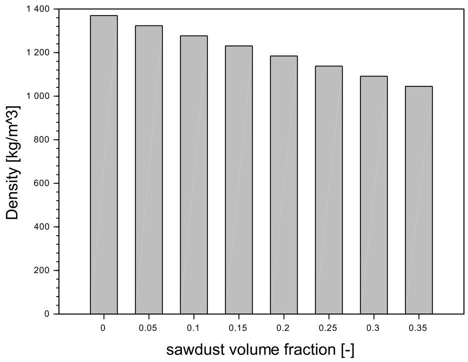


Figure 7: Density for different sawdust volume fraction

randomly distributed in space. The classic Voigt and Reuss models, those that ignore the effects of size, geometry, number of inclusions and their distribution, are not accurate enough to predict the EEP, but they are necessary to discuss a range of properties.

The effect of considering the wood particles oriented in 3D and randomly distributed in the space helps to achieve a quasi isotropic material with effective elastic properties close to the PET ones.

Next work will study the effect of increasing overall size of the particles and their aspect ratio, because orienting them, due to the manufacturing methodology, will not be possible. A further step will consider an experimental comparison of the results.

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