Polish Society of Composite Materials
Polskie Towarzystwo Materiałów Kompozytowych

19: 2 (2019) 50-55

COMPOSITES THEORY AND PRACTICE
ISSN: 2084-6096
ISSN (online): 2299-128X

Wiesław Frącz[1]*, Grzegorz Janowski[2]

[1] Rzeszow University of Technology, Faculty of Mechanics and Technology, Department of Integrated Design and Tribology Systems al. Kwiatkowskiego 4, 37-450 Stalowa Wola, Poland
[2] Rzeszow University of Technology, Faculty of Mechanical Engineering and Aeronautics, Department of Materials Forming and Processing al. Powstańców Warszawy 8, 35-959 Rzeszów, Poland
**Corresponding author. E-mail: wf@prz.edu.pl*

Received (Otrzymano) 15.05.2019

FIBER SHAPE SELECTION PROBLEMS IN MATERIAL MODELS USED IN NUMERICAL STRENGTH ANALYSIS OF WOOD-POLYMER COMPOSITES

The paper presents the problems in selecting the fiber shape in numerical strength analysis for wood-polymer composites. For this purpose numerical analysis of the uniaxial tensile test for the wood-polymer composite sample was performed. Variable geometry of the fiber model was used. The fiber orientation data were obtained using Autodesk Moldflow Insight 2016 software. Micromechanical calculations based on homogenization methods were performed using Digimat FE commercial code. The results of the numerical simulations were compared with the experiment ones. To manufacture the WP composite, Moplen HP 648T polypropylene (PP) from Basell Orlen Polyolefins was used as the polymer matrix. As the filler 10 vol.% Lignocel C120 wood fiber manufactured by JRS - J. RETTENMAIER & Söhne Company was used. Adhesion promoter P613 by Dupont was used as well. A Dr Boy 55E injection molding machine was used to produce the test specimens. It was noted that the selection of the fiber shape has a significant impact on the consistency of the obtained results and consequently on compliance with the experiment ones. Fiber location calculations were performed for each geometry type available in the Digimat software. The most consistent results for numerical homogenization (Digimat FE) are associated with the choice of a curved cylinder shape of fiber. This may be due to the greatest convergence of the orientation tensor value received from the numerical simulation of the injection molding process during its transformations to the representative volume element model. In addition, this result may be due to the fact that the curved cylinder type of geometry is characterized by the most variable shape due to the degree of curvature. This reflects the real, non-standard problems to determine the shape of the wood fiber in the polymer matrix.

Keywords: **wood-polymer composites, homogenization methods, micromechanical analysis, numerical simulations, filler shape model, injection molding process**

PROBLEMATYKA WYBORU GEOMETRII WŁÓKIEN W MODELACH MATERIAŁOWYCH STOSOWANYCH W NUMERYCZNYCH ANALIZACH WYTRZYMAŁOŚCIOWYCH KOMPOZYTÓW TYPU DREWNO-POLIMER

Przedstawiono problematykę wyboru geometrii włókna w numerycznej analizie wytrzymałościowej kompozytu typu drewno-polimer. W tym celu przeprowadzono symulację próby jednoosiowego rozciągania dla próbek wykonanych z kompozytu polimerowo-drzewnego. Badano zmienną geometrię włókna, gdzie dane dotyczące orientacji włókien otrzymano z użyciem programu Autodesk Moldflow Insight 2016. Obliczenia mikromechaniczne opierające się na metodach homogenizacji przeprowadzono z użyciem programu Digimat FE. Wyniki otrzymane w symulacjach numerycznych porównano z eksperymentem. Stwierdzono, że dobór geometrii włókna w analizach numerycznych ma istotny wpływ na otrzymane wyniki, a w konsekwencji zgodność z eksperymentem.

Słowa kluczowe: **kompozyty typu drewno-polimer, metody homogenizacji, analizy mikromechaniczne, symulacje numeryczne, model kształtu wypełniacza, formowanie wtryskowe**

INTRODUCTION

Wood is a material that consists of natural polymers such as: lignin, cellulose and hemicellulose. These polymers have different properties compared to synthetic polymers. The structure and composition of wood makes it rigid, durable, relatively light and exhibits a high water absorption capacity. The low costs of this type of material and its availability have made it a useful building material for thousands years. Thanks to the above advantages, wood has a positive effect as a filler or reinforcement in plastics. In turn, the hydrophilic nature of natural fibers is a significant problem for use in polymer composites [1, 2].

As with most natural materials, the wood structure is complex - it is porous, fibrous and anisotropic. In principle, wood can be divided into two groups: coniferous and deciduous. It is generally classified not according to the strength properties criterion, but according to its botanical characteristics and structure. Coniferous wood comes from such trees as pine, fir, spruce, cedar, etc. In turn, deciduous wood represents, for example, oak, maple, ash [1, 3].

Wood consists mainly of elongated spindle cells that are parallel to each other along the stalk. The length of wood fibers (WF) is varied, and is about 1 mm for conifers and 3÷8 mm for deciduous trees. The aspect ratio, i.e. the length (l) to diameter (d) ratio, is a very important parameter directly influencing the mechanical properties of wood-polymer composites (WPC) [4].

Due to the natural origin of wood fibers, it is problematic to determine the shape of a single fiber. Producers of this type of fiber in their material data card give average values or ranges of length and diameter. For fibers used as fillers in a polymer matrix, it is difficult to characterize the shape under a microscope (Fig. 1). This is due to the different geometry of each fiber. This problem directly affects prediction of the orientation of the fibers in the polymer matrix, as well as the results from microstructural analysis [5-7].

Fig. 1. Molded piece sample made of wood-polymer composite with enlarged area showing variable shape of wood fibers

Rys. 1. Wypraska wykonana z kompozytu drewno-polimer (WPC) - powiększony obszar przedstawia widoczne rozmieszczenie włókien drzewnych

Homogenization methods allow one to predict the mechanical properties of composites, including their complex structure. Both analitycal and numerical homogenisation methods are used. Analytical methods are most often used for this. Their limitations require additional calculation methods. Therefore, in recent years numerical methods of directly calculating effective material data have become increasingly numerous and significant [8]. Most of these methods are only developed with respect to the range of small deformations. Due to the growing computing power of computers, several methods have been developed to predict the nonlinear behavior of composite materials. Calculations are performed in 2D space. This method allows the values that appear in the cross section of material to be calculated. There are many restrictions resulting from the specificity of the solution to the problem (e.g. flow direction only penetrating the modeled surface, etc.) [9, 10]. In most recent years, increasingly more software is equipped with the ability to solve 3D problems. The discretization process usually consists in dividing the area of the model into tetrahedral finite elements (FE). Such modeling is deprived of the fundamental limitations of 2D technology, but it is much more demanding in terms of computing power. One of the main types of finite elements used in these calculations is Voxel FE. Each Voxel FE is assigned to the phase material where its center is located. It is intended for an advanced representative volume element (RVE), in which discretization is difficult to reproduce the matrix shape and analyze the inclusions [11].

One of the software packages that uses homogenization methods is Digimat software. Digimat is nonlinear, large-scale software for modeling materials and structures. This software consists of several modules, among which there is the Digimat FE module, which uses the numerical homogenization method.

The aim of the study was to analyze the effect of the selected fiber shape used in microstructural analysis on the stress-strain characteristics, referring directly to the experimental results. For this purpose, experimental research was carried out consisting of the following steps: producing the composite, manufacturing the specimen, and performing the strength test (uniaxial tensile test). In the next step, numerical analysis of composite injection molding and microstructural studies for various fiber shapes using the numerical method of homogenization were conducted. This allowed the authors to directly verify the results of the experiment and to evaluate the impact of the selected fiber shape used in the microstructural analysis on the stress-strain characteristics.

EXPERIMENTAL PART

Materials

To manufacture the WPC composite, Moplen HP 648T polypropylene (PP) from Basell Orlen Polyolefins was used as the polymer matrix. As the filler 10 vol.% Lignocel C120 wood fiber, manufactured by JRS - J. RETTENMAIER & Söhne Company was used. Adhesion promoter P613 by Dupont with MFR = = 49 g/10 min was used as well. The bulk density of the composite components was as follows: wood fibers - 167 kg/m^3, PP - 565 kg/m^3.

Composite manufacturing

The WPC composite was manufactured by the extrusion process using a single screw extruder machine (Zamak EHP 25E), equipped with a cooling bath and a granulator. During extrusion the following parameters were used: plasticizing unit temperature zones: 180, 175, 170 and 140°C, screw rotation - 10 rpm. The wood fibers were dried in a dryer at 100°C for about 4 hours before being extruded.

A Dr Boy 55E injection molding machine (Fig. 2) was used to produce the test specimens (Fig. 3). The processing parameters of injection molding during manufacturing of the uniaxial tensile samples are summarized in Table 1.

Fig. 2. Dr Boy 55E injection molding machine used in the research

Rys. 2. Wtryskarka Dr Boy 55E stosowana w badaniach

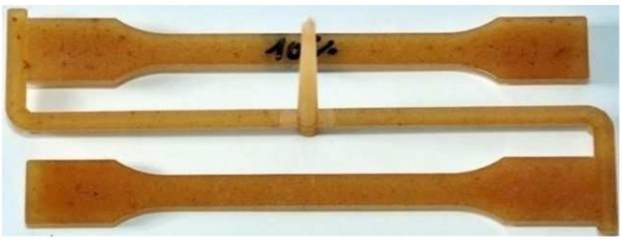


Fig. 3. Injection molded piece made of WPC (10 vol.% WF)

Rys. 3. Wypraska wytworzona z kompozytu WPC (dla 10% obj. włókien drzewnych (WD))

TABLE 1. **Processing parameters of injection molding for uniaxial tensile test samples**

TABELA 1. **Parametry technologiczne procesu wtryskiwania próbek do badań dla próby jednoosiowego rozciągania**

Parameter	Unit	Value
Mold temperature	[°C]	40
Melt temperature	[°C]	190
Flow rate	[cm^3/s]	20
Cooling time	[s]	35
Packing time	[s]	20
Packing pressure	[MPa]	30

Testing methods

The uniaxial tensile test was performed using a Zwick Roell Z030 testing machine (Fig. 4). Ten specimens were tested at the speed of 50 mm/min according to the PN-EN ISO 527 standard. The obtained stress-strain characteristics were used as a verification criterion for further numerical analysis. This representative stress-strain curve was determined for the series of tests including 7 samples.

Fig. 4. Zwick Roell Z030 materials testing machine used in uniaxial tensile test

Rys. 4. Maszyna wytrzymałościowa Zwick Roell Z030 stosowana w próbie jednoosiowego rozciągania

NUMERICAL ANALYSIS

Injection molding process

The numerical analysis was performed for an identical material composition as in the experimental research and with identical processing parameters of the injection molding process. The simulation of the injection molding process was performed using Autodesk Moldflow Insight ver. 2016 commercial code. The numerical simulations of WP composite injection molding included the following steps: designing the 3D geometrical model of the molded piece using NX9 software, model discretization by means of tetrahedral finite elements (FE), setting the initial and boundary conditions, numerical simulations and results interpretation. The main condition for performing a correct numerical simulation was to introduce the WP composite properties to the software material database taking into account the rheological, PVT and thermodynamic properties.

In order to take into consideration the fiber orientation in micromechanical analysis, the simulation results of the injection molding process were used. The fiber orientation analysis was performed on the basis of the filling phases of the injection molding and the flow vectors. In the calculations, based on microscopic measurements, a fiber l/d ratio of 10 was assumed. The Tucker-Folgar model was used to determine the fiber orientation [12]. The numerical procedure was used to calculate the interaction coefficient of the fibers and the polymer matrix. The elastic properties were calculated based on the Halpin-Tsai micromechanical model [13]. The properties of the polymer matrix and fibers, as well as the fiber content were also taken into account. The coefficients of thermal expansion were estimated using the Rosen-Hashin model [14]. As a result of the calculations, among others, the fiber probability distribution in the polymer matrix, described by the orientation tensor, was obtained (Fig. 5). The tensor components are interpreted as the probability of fiber arrangement in the main directions, i.e. along the flow direction of the composite, transverse to the flow direction and in the thickness of the mold cavity. A fiber orientation tensor value of about 1 determines the high probability of fiber orientation in a given direction [15].

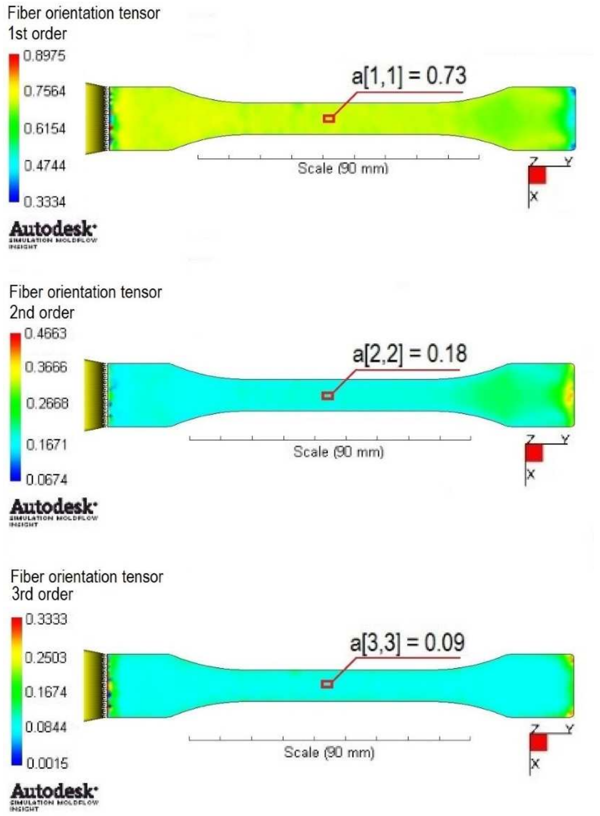


Fig. 5. Calculated fiber orientation tensor values (1-, 2-, 3-order) in chosen areas of specimen (10% WF)

Rys. 5. Obliczone wartości tensora orientacji włókien (1, 2, 3 rzędu) w wybranych obszarach próbki (dla 10% WD)

Micromechanical analysis

The heterogeneity of the composite structure is not only a processing and structural problem, but also a computational one. One of the solutions to this problem is micromechanical modeling, which provides the possibility of predicting the interaction between the micro- and macrostructures of materials [16, 17]. Micromechanical modeling can be performed presently by means of Digimat commercial code. Digimat software is a nonlinear, large-scale platform for modeling materials and structures, consisting of several main modules. This software includes the Digimat FE module, which uses the numerical homogenization method. In order to carry out an advanced micromechanical analysis, the geometric data of the fiber were defined in the software (Table 2). Based on the introduced data, six micromechanical analyses were performed for six different types of fiber geometry: ellipsoid, cylinder, sphero-cylinder, curved cylinder, beam and curved beam. For all the types of fiber shape, the same RVE (representative volume element) dimensions were defined. The representative volume element was digitized with the same number of Voxel finite elements (FE) (Table 2) for each of the six analyses. The presented issue belongs to difficult non-linear problems. This work adopted the strategy of minimizing the size of the RVE due to the limited calculation possibilities of the PC. The task was to put as many fibers in the RVE as possible, while maintaining their actual size. The numerical homogenization method was applied due to the possibility of analyzing various fiber geometries.

TABLE 2. **Input data for micromechanical analysis using Digimat FE**

TABELA 2. **Dane wejściowe do analizy mikromechanicznej wykonanej za pomocą programu Digimat FE**

Fiber diameter	0.01 mm
Fiber length	0.1 mm
Fiber length to diameter ratio (l/d)	10
Fiber volume content	0.106445
RVE dimensions	0.2x0.1x0.1 mm
Number of Voxel FE in RVE	250 000
Orientation tensor values: a[1,1] a[2,2] a[3,3]	 0.73 0.18 0.09

RESULTS AND DISCUSSION

One of the computational problems was proper distribution of the fibers in the RVE for the defined volume content of 0.106445 (approx. 10 vol.% WF). Fiber location calculations were performed for each geometry type. Very high compatibility was obtained between the preset volume content and the calculated volume content for the adopted fiber shapes. As we can see (Fig. 6), there are slight differences in the volume content obtained for different types of geometry. The biggest difference in the obtained volume content was the RVE whose fibers were characterized by sphero-cylinder geometry. The calculated value of 0.11 volume content deviates by 3.34% to the entered value, which indicates the very high accuracy of the software, even for the smallest compatibility for the selected shape of fiber (sphero-cylinder).

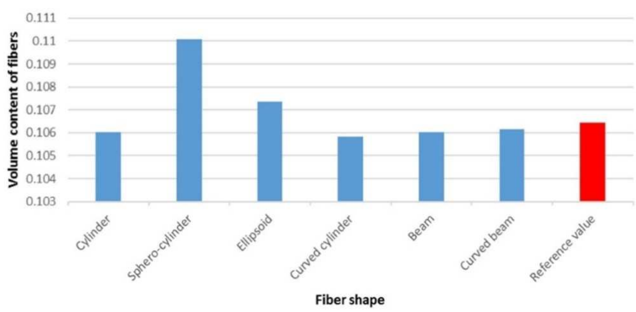


Fig. 6. Calculated volume content of fibers in analyzed RVE (for reference fiber content of 0.106445 set as input value)

Rys. 6. Obliczona zawartość objętościowa włókien w reprezentatywnym elemencie objętościowym (REO) dla referencyjnej zawartości włókna 0,106445, która została ustawiona jako wartość wejściowa

It is also worth analyzing the actual number of packed fibers in the RVE for the given volume share (Fig. 7). By analyzing the results, it can be seen that for the curved beam, beam, curved cylinder and cylinder geometries, 27 fibers in the RVE were recorded. In turn, the largest number of fibers in the RVE with ellipsoid geometry was 41.

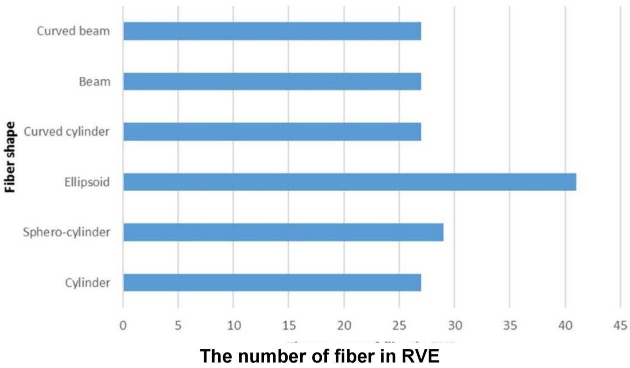


Fig. 7. Generated number of fibers in RVE as consequence of prescribed fiber content i.e. 0.106445, at same fiber length and diameter

Rys. 7. Ilość włókien wygenerowana w REO dla przypisanej zawartości włókien, tj. 0,106445, przy tej samej długości i średnicy włókna

One of the most important parameters determining the micromechanical properties of composite materials is the fiber orientation. The value of the 1-, 2- and 3-order orientation tensor values was added to the Digimat software using the injection molding simulation results. By generating the RVE, the fiber placement algorithm also had to orient the fibers accordingly, trying to ensure that the resulting fiber orientation was consistent with the input values. The highest correlation was found in the orientation tensor value for the curved cylinder geometry (Table 3).

TABLE 3. **Calculated orientation tensor values after transformation from Moldflow to RVE from Digimat**

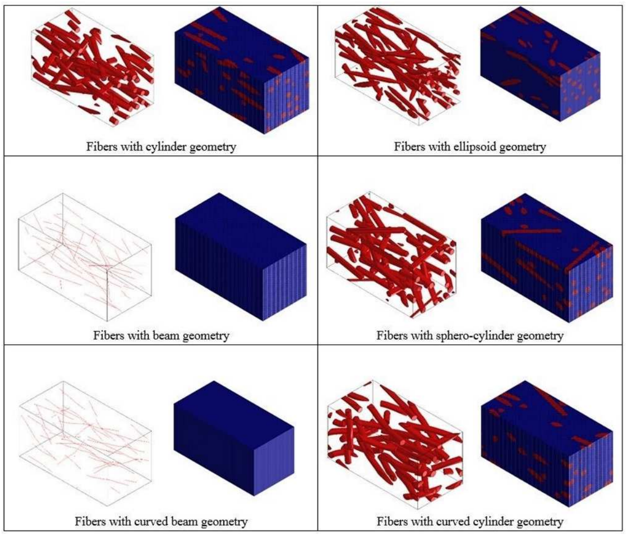
TABELA 3. **Obliczone wartości tensora orientacji po transformacji z Moldflow do REO w Digimat**

Reference value of fiber orientation tensor (introduced from Moldflow analysis): **a[1,1] 0.73 a[1,2] 0 a[1,3] 0; a[2,2] 0.18 a[2,3] 0; a[3,3] 0.09**	
Ellipsoid: a[1,1] 0.86 a[1,2] -0.079 a[1,3] 0.045; a[2,2] 0.084 a[2,3] 0.0026; a[3,3] 0.52	Beam: a[1,1] 0.85 a[1,2] -0.062 a[1,3] -0.039; a[2,2] 0.13 a[2,3] 0.0013; a[3,3] 0.015
Sphero-cylinder: a[1,1] 0.71 a[1,2] -0.028 a[1,3] -0.086; a[2,2] 0.19 a[2,3] 0.026; a[3,3] 0.099	Curved beam: a[1,1] 0.83 a[1,2] 0.056 a[1,3] 0.032; a[2,2] 0.11 a[2,3] 0.015; a[3,3] 0.056
Curved cylinder: a[1,1] 0.74 a[1,2] 0.0006 a[1,3] 0.046; a[2,2] 0.18 a[2,3] 0.001; a[3,3] 0.09	Cylinder: a[1,1] 0.75 a[1,2] -0.055 a[1,3] -0.001; a[2,2] 0.18 a[2,3] -0.012; a[3,3] 0.072

The visualizations of the RVE before and after discretization for the specified six types of fiber geometry are shown in Table 4.

TABLE 4. **Visualization of fiber distribution in RVE for defined orientation tensor value: before (left) and after discretization (right)**

TABELA 4. **Wizualizacja rozkładu włókien w REO dla zdefiniowanej wartości tensora orientacji: przed (po lewej) i po dyskretyzacji (po prawej)**



A comparative analysis of the stress-strain characteristics for the given fiber geometry types was performed (Fig. 8). The greatest compatibility was found for the curved cylinder geometry. The relative error values for the following deformation values were approximately: 12.5% (at strain - 0.01), 6.84% (at strain - 0.03), 6.98% (at strain - 0.05). Satisfactory compliance of the results for this type of geometry may be the result of the most consistent fiber orientation tensor in the RVE relative to the set value. The fact that the selected geometry is characterized by a degree of curvature also further reflects the real problem of a non-standard, individual type of wood fiber geometry. In turn, the smallest compatibility of the characteristics is noticeable for the beam and curved beam geometry types. This may indicate that the software interprets these types of geometry as a fiber with very low body mass.

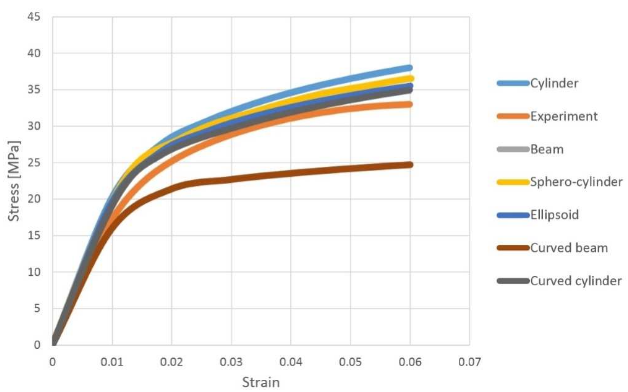


Fig. 8. Calculated stress-strain characteristics of WPC for various shapes of wood fibers compared with experiment result

Rys. 8. Obliczona charakterystyka naprężenie-odkształcenie kompozytu WPC dla przyjętych różnych kształtów włókien drzewnych w porównaniu z wynikiem eksperymentu

CONCLUSIONS

The influence of the fiber geometry selection determines the effective volume content of fibers in the RVE. The highest compatibility was obtained for the cylinder shape (the percent error was about 0.395%). The worst compatibility was obtained for the spherocylinder shape (the percent error was about 3.34%).

The choice of fiber geometry affects the number of fibers in the RVE ranging from 27 (for cylinder, curved cylinder, beam, curved beam type of geometry) to 41 (for the ellipsoid type of geometry). This significant difference in quantity is due to the fact that the fiber location algorithm in the RVE seeks to achieve the most consistent volume content of fibers in the RVE with the reference value (0.106445).

The resulting orientation tensor values received after transformation from Moldflow to the RVE model in Digimat indicate that the most effective degree of adaptation of the introduced orientation tensor occurs in the case of curved cylinder geometry.

The most consistent result for numerical homogenization (Digimat FE) is associated with the choice of a curved cylinder shape of fiber. This may be due to the greatest convergence of the orientation tensor value received from the numerical simulation of the injection molding process during its transformations to the RVE model. In addition, this result may be due to the fact that the curved cylinder type of geometry is characterized by the most variable shape due to the degree of curvature. This reflects the real, non-standard problems to determine the shape of the wood fiber in the polymer matrix.

The method of numerical homogenization allows good compatibility to be obtained between the results of the experimental research and the numerical analyses. Proper selection of the fiber geometry has a significant impact on the consistency of the obtained results. This is due to the fact that the examined area is analyzed on the micromechanical level, very sensitive to small changes in the input parameters and calculating conditions.

REFERENCES

[1] Niska K.O., Sain M., Wood-Polymer Composites, Woodhead Publishing, Cambridge 2008.

[2] Bledzki A.K., Sperber V.E., Faruk O., Natural and wood fibre reinforcements in polymers, Rapra Review Reports 2002, 13, 8, 1-144.

[3] Bledzki A.K., Letman M., Viksne A., Rence L., A comparison of compounding processes and wood type for wood fibre-PP composites, Composites Part A: Applied Science and Manufacturing 2005, 36, 6, 789-797.

[4] Klyosov A.A., Wood-Plastic Composites, John Wiley & Sons, New Jersey 2007.

[5] Migneault S., Koubaa A., Erchiqui F., Chaala A., Englund K., Wolcott M.P., Effects of processing method and fiber size on the structure and properties of wood-plastic composites, Composites Part A: Applied Science and Manufacturing 2009, 40, 1, 80-85.

[6] Persson K., Micromechanical modelling of wood and fibre properties, Doctoral Thesis, Lund Institute of Technology, Lund 2000.

[7] Bednarz A., Frącz W., Janowski G., The use of image analysis in evaluation of the fibers orientation in wood-polymer composites (WPC), Open Engineering 2016, 6, 1, 737-741.

[8] Bendsøe M.P., Kikuchi N., Generating optimal topologies in structural design using a homogenization method, Computer Methods in Applied Mechanics and Engineering 1988, 71, 2, 197-224.

[9] Abdulle A., Numerical homogenization methods, 2013, 1-18 (No. EPFL-ARTICLE-184958).

[10] Bouchart V., Brieu M., Kondo D., Abdelaziz M.N., Macroscopic behavior of a reinforced elastomer: micromechanical modelling and validation, Mechanics & Industry 2007, 8, 3, 199-205.

[11] Doghri I., Tinel L., Micromechanics of inelastic composites with misaligned inclusions: numerical treatment of orientation, Computer Methods in Applied Mechanics and Engineering 2006, 195, 13, 1387-1406.

[12] Tucker III C.L., Liang E., Stiffness prediction for unidirectional short-fiber composites: Review and evaluation, Composites Science and Technology 1999, 59, 5, 655-671.

[13] Halpin J.C., Kardos J.L., The Halpin-Tsai Equations: A review, Polymer Engineering & Science 1976, 16, 5, 345-352.

[14] Rosen B.W., Hashin Z., Effective thermal expansion coefficients and specific heats of composite materials, International Journal of Engineering Science 1970, 8, 2, 157-161.

[15] Advani S.G., Tucker III C.L., The use of tensors to describe and predict fiber orientation in short fiber composites, Journal of Rheology 1987, 31, 8, 751-784.

[16] Trzepieciński T., Ryzińska G., Biglar M., Gromada M., Modelling of multilayer actuator layers by homogenisation technique using Digimat software, Ceramics International 2017, 43, 3, 3259-3266.

[17] Frącz W., Janowski G., Strength analysis of molded pieces produced from wood-polymer composites (WPC) including their complex structures, Composites Theory and Practice 2016, 16, 4, 260-265.

