Annals of DAAAM for 2010 & Proceedings of the 21st International DAAAM Symposium, Volume 21, No. 1, ISSN 1726-9679
ISBN 978-3-901509-73-5, Editor B. Katalinic, Published by DAAAM International, Vienna, Austria, EU, 2010
Make Harmony Between Technology and Nature, and Your Mind will Fly Free as a Bird
DAAAM Symposium

THE ESTIMATION OF THE YOUNG'S MODULUS OF THE COMPOSITE FOR DIFFERENT TYPES OF MATRIX

MAJER, Z[denek]

Abstract: *The main goal of this paper is the numerical estimation of the tensile properties in the particulate composite. The composite was modelled as a two-phase continuum (finite elements method - ANSYS). The final results are confirmed with experimental data as well as the data for modeling primary matrix was determinate from experiment.*
Key words: *particulate composites, rigid particles, soft polymer matrix, two-phase model, numerical calculations*

1. INTRODUCTION

In this paper particulate composites are studied. The particulate composites, especially with the polypropylene matrix (PP) and rigid particles (mineral fillers, e.g. H_2MgO_2 or $Mg(OH)_2$), are of great practical importance due to the possibility both of modifying many diferent mechanical properties and reducing the price/volume ratio of resulting material (Pukánszky, 2005). The properties of the matrix and rigid particles (size, shape, material properties) can have a significant effect on the global behaviour of the composite. The change of these general material properties of the particulate composites, especially elastic modulus or yield stress, is the usual motivation for investigation particulate filled composites. Generally, the addition of rigid particles to a polymer matrix will have an embrittling effect on the particulate composite.

The model was created with respect a few general terms (Zuiderduin et al., 2003): (i) particles should be of small size (less then 5 μm), (ii) aspect ratio must be close to unity to avoid high stress concentration, (iii) particles must debond prior to the yield strain of the matrix polymer in order to change the stress state of the matrix material and (iv) particles must be dispersed homogeneously in the matrix polymer.

This article is focused on the global particulate composite characteristics response. Numerical calculations on condition the perfect homogeneous distribution of the particles in the matrix are solved (Jančář et al., 2007). At the other side, it is obviously impossible in reality to have a perfect homogeneous distribution. It is possible that particles can create clusters and distribution of the particles can certainly change the global behaviour of a particulate composite (Kiss et al., 2007). It was studied that the random distribution of the particles has no significant effect on the global behaviour (mechanical characteristics) of the composite (Prod'Homme et al., 2008).

2. NUMERICAL MODEL

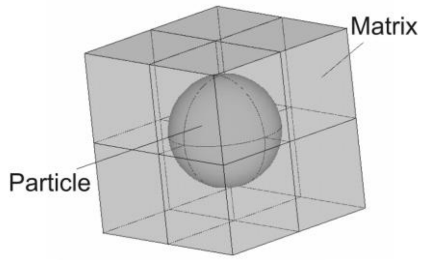


Fig. 1. Used unit cell

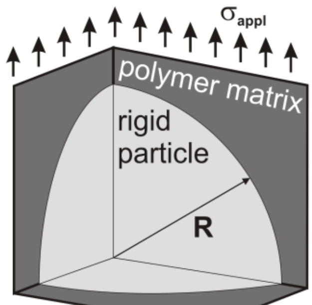


Fig. 2. One eight of the unit cell = FEM model

The deformation behaviour of a two-phase composite with homogeneously distributed coated particles was numerically simulated on a microscopic scale. For the calculation the finite element program ANSYS was used. Full model according the following assumptions was created: the spherical shape of the particles, the regular distribution of the particles and the perfect adhesion between particle and matrix. The finite element model was three dimensional with periodic boundary conditions. From this model the unit cell was segregated, see Fig. 1. For simulations only one to eight model was used (see Fig. 2).

The mesh of finite elements was created using 20-node elements; this corresponds to the SOLID95 ANSYS element. These elements are more accurate for structural calculation than basic elements with 8 nodes. It is necessary to have a sufficiently precise mesh to control the number of elements. In fact, the critical locations are situated at the boundary between the particles and the matrix. The mesh was created to be more accurate in these zones and more dispersed in the matrix. Finally, the number of elements depends on the volume filler fraction (from pure matrix up to volume filler fraction 40%); it was included between 100 000 and 300 000 elements. It was checked that further refinement of the finite element mesh has no influence on the results obtained.

3. EXPERIMENT

In the measured particulate composite as the matrix copolymer PP SHAC KMT 6100 was used (produce by Shell International Chemical Co. Ltd.). The density was 0.903 $g.cm^{-3}$ (ISO 1133; 2.16 kg /230°C). This material is using for injection of assorted products (i. e. tools, cars components, equipment of household) (Molliková, 2003).

As rigid filler was used magnesium hydroxide in two commercial available versions (see Tab. 1); company named KISUMA 5AU and MAGNIFIN H 10. In addition MAGNIFIN H 10 was modified by 2,5% stearic acid named ASTRA (Molliková, 2003).

Material	S	F2	F4	F6	S2	S4	S6	N2	N4	N6
Filler	---	KISUMA 5AU company modified			MAGNIFIN H 10 modified			MAGNIFIN H 10 unmodified		
[%] VFF	0	20	40	60	20	40	60	20	40	60

Tab. 1. Different types of materials identification

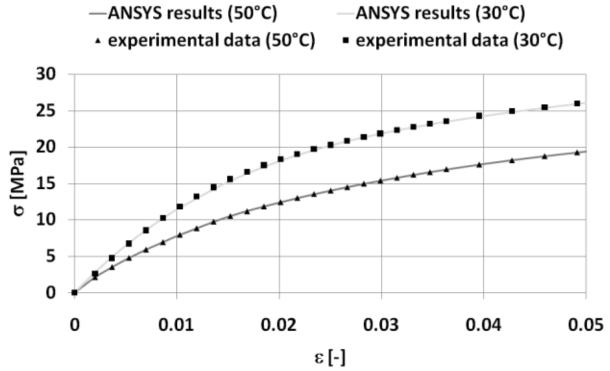


Fig. 3.The comparison of data from experiment and from ANSYS for temperature 30°C and 50°C

The Young´s modulus of the particle is E = 72 GPa, and the value of Poisson´s ratio is ν = 0.29. The material properties characterizing the composite correspond to rigid particle (H_2MgO_2 or $Mg(OH)_2$) filled polypropylene at room temperature was used - elasto-plastic model (i.e. experimental data, temperature 30°C and 50°C, see Fig. 3).

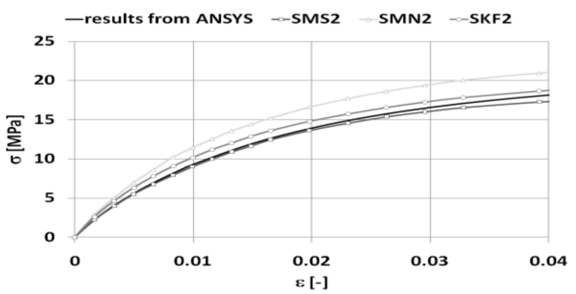
From experiment was determined size of particles too (1 μm).

4. RESULTS AND DISCUSSION

The particulate polymeric composite formed by polypropylene matrix (PP) and mineral fillers (rigid particles) was studied. Generally, the addition of rigid particles to the polymer matrix will have two main efects. The particulate polymeric composite will have significantly greater Young's modulus than self matrix. But at the other side, the rigid particles have sizable an embrittling effect on the composite.

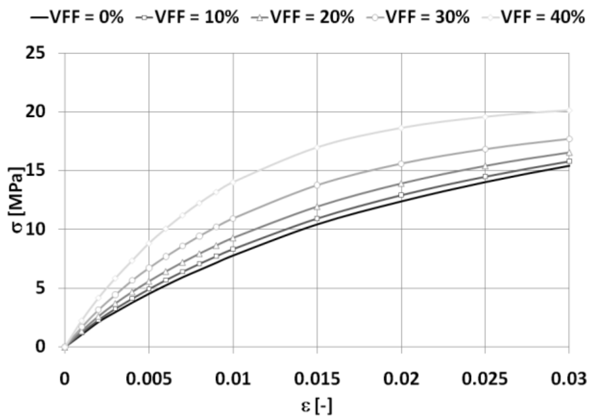
The presented work is mainly focused on the possibility and data reliability of numerical modeling of the particulate polymeric composite. The composite as two-phase continuum with respect regularly distribution of particles in the matrix was modelled. The Young's modulus for different types of composites and several of the volume filler fractions (VFF) was calculated. A special case the configuration corresponding to only matrix (composite without particles) was considered as well.

The comparison between numerical results and experimental data was evaluated (see Fig. 4 for VVF = 20%). Numerical results were confronted by three different types of composites (see Tab. 1). Almost ideal congruity experimental data with numerical results for SMS2 composite is apparent.



	ANSYS	S2	N2	F2
E [MPa]	1231	1225	1550	1450

Fig. 4.Comparison of results from ANSYS with data from experiment (for temperature 50°C and VFF 20%)



VVF	0% (pure matrix)	10%	20%	30%	40%
E [MPa]	987	1078	1231	1484	1942

Fig. 5.Results from ANSYS for different type of composite for temperature 50°C

In the graph (see Fig. 5) set of results from finite element calculations is shown. The smallest Young's modulus is for pure matrix. Whereas the highest value of Young's modulus is for composite with volume filler fraction 40%. With increase of volume filler fraction Young's modulus of composite increase as well.

5. CONLUSIONS

It is shown that mechanical properties of particulate composite using numerical calculations can be use. We are well able to qualitatively predict the Young's modulus of particulate composite for various volume filler fraction.

Significant effect of Young's modulus increasing is above all for volume filler fraction 40%. In this case is Young's modulus of composite more than two times higher than in case of pure matrix (without particles).

6. ACKNOWLEDGEMENTS

This research was supported by grant P107/10/P503 of the Czech Science Foundation.

7. REFERENCES

Pukánszky, B. (2005). Interfaces and interphases in multicomponent materials: past, present, future, *European Polymer Journal*, Vol. 41, pp. 645-662, ISSN: 0014-3057

Zuiderduin, W., C., J.; Westzaan, C.; Huétink, J. & Gaymans, R., J. (2003). Toughening of polypropylene with calcium carbonate particles, *Polymer*, Vol. 44, pp. 261-275, ISSN: 0032-3861

Jančář, J.; Kučera, J. & Veselý, P. (1991). Peculiarities of mechanical response of heavily filled polypropylene composites, *Journal of materials science*, Vol. 26, pp. 4872-4882, ISSN: 0022-2461

Kiss, A.; Fekete, E. & Pukanszky, B. (2007). Aggregation of CaCO3 particles in PP composites, *Composites Science and Technology*, Vol. 67, pp. 1574-1583, ISSN: 0266-3538

Prod'Homme, G.; Majer, Z.; Hutar, P. & Nahlik, L. (2008). The Effect of Particle Distribution in Polypropylene Composites on Mechanical Properties, *Proceedings of 10th International Scientific Conference "APPLIED MECHANICS"*, ISBN 978-83-60102-49-7, Wisla, Poland

Molliková, E. (2003). Vztah mezi technologií výroby, strukturou a mechanickými vlastnostmi polypropylénu plněného hydroxidem hořečnatým, Ph.D. thesis, FSI VUT v Brně, pp. 103 (in czech)