FORMULATION, PROCESSING AND NUMERICAL MODELLING OF POLYPROPYLENE/CLAY NANOCOMPOSITES

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Introduction

Polypropylene (PP)/clay nanocomposites have quite a high potential to form a group of innovative materials and replace the conventional plastics in many automotive and packaging applications. Notwithstanding the merits of nanocomposites, such as high stiffness, light weight and good heat resistance, the growth of PP/clay nanocomposites faces the problem of hydrophobic polymer's low interaction with the hydrophilic clays. Maleic anhydride grafted PP (MAPP), commonly used as a compatibiliser, has been proven to facilitate a good dispersion of clays in PP matrix through its functionalised groups. However, despite the great attention from the industry and researchers in recent years, commercial PP/clay nanocomposites with reliable properties are still limited in availability. The major problem stems from the complex influence of the material selection and the processing methods.

The present work introduces a comprehensive approach towards determining optimised formulation, materials processing and numerical modelling that is based on the scanning/transmission electron image processing of morphological structures of PP/clay nanocomposites.

Formulation

The initial formulation work focused on the optimisation on property enhancement of PP/clay nanocomposites using Taguchi design of experiments (DoE) [1]. Three grades of PP with various melt flow indices (MFI), denoted as PP-Co M710 (MFI=0.6g/10min), PP-Hom Y130 (MFI=4.0g/10min) and PP-Hom H380F (MFI=25g/10min), were obtained from Clariant New Zealand Ltd. Three organoclays, NANOLIN™ DK1N (d-spacing d_{001}=2.29nm), DK2 (d_{001}=2.25nm) and DK4 (d_{001}=3.56nm), were obtained from Zhejiang Feng Hong Clay Chemicals Co., China. The compatibiliser MAPP Exxelor™ PO1020 (MFI=430g/10min), was supplied by ExxonMobil Chemical (Germany). Table 1 shows the factors and levels in the nine trials of the DoE work.

Table 1. Factors and levels in the DOE work [1]

Factor	Level		
	1	2	3
A: Clay type	DK1N	DK2	DK4
B: Clay content (wt%)	3	5	10
C: MAPP Content (wt%)	5	10	20
D: PP type	PP-Co M710	PP-Hom Y130	PP-Hom H380F

DoE results show some significant effects of PP type and clay content on the property enhancement, particularly with PP-Hom H380F being found to be the best performing grade [1]. Consequently, the optimised formulation is based on using MAPP and PP-Hom H380F, DK4 clay of 3wt%, 5wt%, 8wt% and 10wt% (weight ratio of MAPP:clay, α=2:1).

Processing

PP/clay nanocomposites were prepared by melt compounding PP and MAPP pellets with downstream feeding of clay powder using a co-rotating intermesh twin screw extruder DSE20 (D=20mm, L:D=40, BRABENDER OHG, Germany) at 200 rpm and a temperature profile of 185-210°C. The initial nanocomposite batches were then recompounded at 100rpm in the same conditions to extend the residence time. PP and the prepared nanocomposite pellets were both fed at 3.0 kg/hr and the final dried nanocomposite pellets were further injection moulded to prepare the mechanical test samples using a BOY 50A machine at 190-210°C with die temperature of 25°C and injection pressure of 60-80 bars.

Mechanical Properties

Mechanical testing was carried out at room temperature to determine the tensile, flexural and impact properties of PP/clay nanocomposites according to ASTM D638, D790 and D6110, respectively. Final results are based on the average data of five samples with calculated standard deviations.

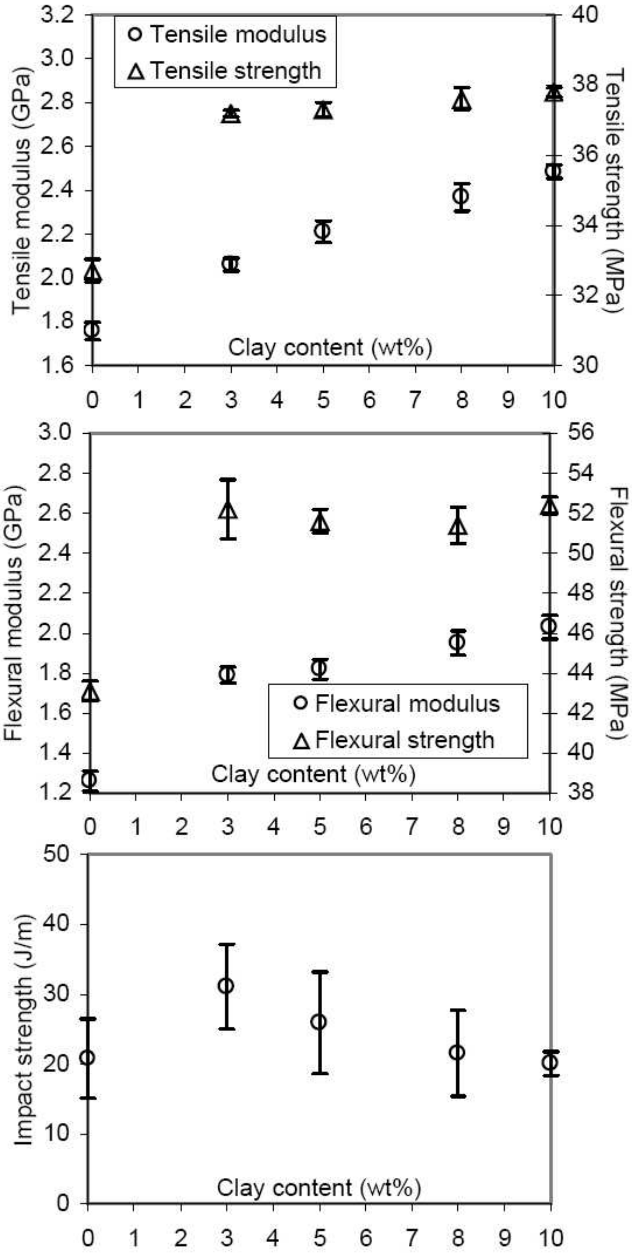

Fig.1 Mechanical properties of PP/clay nanocomposites (weight ratio α=2:1).

Fig.1 depicts the mechanical properties of nanocomposites compared with those of neat PP. It is evident that the inclusion of clays into PP matrix yields overall enhancement of properties in the presence of MAPP. Both tensile and flexural moduli significantly improve with the increase of clay content. With 10wt% clay, the enhancements of tensile and flexural moduli reach 41% and 61%, respectively. The strengths also increase by 16% (tensile) and 22% (flexural), but they more or less stay at similar levels irrespective of the clay content. More remarkably, impact strength achieves a 50% improvement at the clay content of 3wt%. However, for 10wt% filled nancomposites, the impact strength is almost the same as that of neat PP. The enhancement of impact strength might be attributed to the right mix of exfoliation and intercalation that can hinder the crack propagation.

Numerical Modelling

Previous modelling work [2] using an object-oriented finite element (OOF) method has already developed a methodology, based on the morphological image analysis, to predict the tensile moduli of PP-CoM710/DK2 clay nanocomposites. Fig.2 exhibits the finite element mesh of a typical 5wt% filled nanocomposite structure. Further development work for OOF modelling of the optimised nanocomposites (quoted in this paper) is currently under way following the OOF imaging approach.

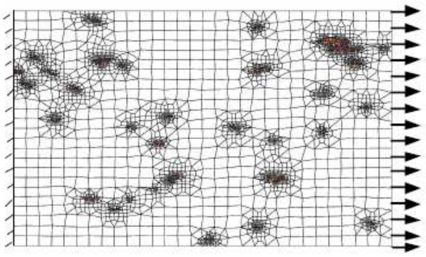

Fig.2 Finite element mesh of 5wt% filled nanocomposites [2].

Conclusion

A comprehensive approach has been successfully developed to achieve significant performance enhancements of PP/clay nanocomposites. The appropriate material selection is achieved through a Taguchi analysis and the property predictions are made by a novel numerical approach based on morphological image analysis.

References

1. Dong, Y., Bhattacharyya, D. and Hunter, P.J. Optimisation of property enhancement of polypropylene/organoclay nanocomposites. 16th International Conference on Composite Materials (ICCM-16), Kyoto, Japan, Jul. 8-13, 2007.
2. Dong, Y., Bhattacharyya, D. and Hunter, P.J. Characterisation and object-oriented finite element modelling of polypropylene/organoclay nanocomposites. *Key Eng. Mater.*, 334-335 (2007) 841-844.