A simulation study of the microstructure evolution of PP-LDHs nanocomposites in melt compounding

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In the context of polymer-based nanocomposites containing layered nanofillers, the achievement of good extents of dispersion and distribution of the dispersed nanoparticles and the obtainment of intercalated and/or exfoliated structures through melt compounding still represents a persistent challenge, especially in the case of anionic layered double hydroxides (LDHs) embedded in non-polar polymeric matrices. Since the microstructure of a nanocomposite strongly depends on the flow field developed during the melt-compounding processing, the selection of the processing parameters during this stage plays a fundamental role in determining the material final morphology. In this work, polypropylene (PP)-based nanocomposites containing 5 wt.% of organo-modified LDHs were formulated through melt compounding using a twin-screw extruder. Different combinations of screw speed (namely, 150 and 300 rpm) and feed rate (namely, 2 and 4 kg/h) were exploited, following the results of the DoE analysis performed through Ludovic® Software. The effects of the different processing conditions on the final morphology of the nanocomposites were assessed through rheological and morphological characterizations, also evaluating the evolution of the material microstructure along the screw.

The rheological results indicated that the introduction of the LDHs, irrespective of the used processing conditions, causes the disappearance of the matrix Newtonian plateau, with a general amplification of the non-Newtonian features and the appearance of a yield stress behavior. This phenomenon can be ascribed to a limited mobility of the polymer macromolecules that, interacting with the embedded nanofillers, are no longer able to fully relax. The yield stress was quantified through the fitting of the experimental data with the modified Carreau model. The highest value of yield stress was obtained for the systems processed with the highest feed rate and highest screw speed; a high extent of LDHs dispersion and distribution is thus expected for the system processed using these conditions. For the nanocomposites obtained using the other exploited combinations of the processing parameters, lower values of yield stress were obtained, suggesting a worst dispersion of the nanofillers. The morphological analyses confirmed what inferred on the basis of the rheological measurements. In fact, the nanocomposite processed at 350 rpm and 4 kg/h showed a quite uniform and homogeneous morphology, indicating that the nanofiller was successfully nanodispersed.

Furthermore, the evolution of the microstructure along the extruder was followed, performing rheological and morphological analyses on samples picked up in two different zones of the screws. A non-monotonic trend of the yield stress as a function of the selected processing parameters was found, indicating the occurrence of concurrent phenomena during the processing (namely, melt intercalation or flocculation and reaggregation) which contribute to determining the final morphology.
Finally, the obtained results were related to the flow parameters derived by the Ludovic® simulations. Some relationships between the processing conditions, the flow parameters and the final morphology of the formulated nanocomposites were disclosed, demonstrating that high shear stresses and low residence times are required to achieve a good extent of LDHs dispersion and distribution and the formation of intercalated/exfoliated hybrids.

Keywords: polypropylene, layered double hydroxides (LDHs), rheology, melt compounding, simulation

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