MOLECULAR DYNAMICS SIMULATION METHODOLOGY TO RHEOLOGY POLYMER NANOCOMPOSITE THROUGH A CONTRACTION-EXPANSION GEOMETRY.

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Polymer industry and academic area have put attention in material redesign to obtain new version of old materials with improve properties. In this sense, the nanocomposites have become the best option due its specific and extraordinary properties and because they have a great variety of applications1. The enhanced properties have improved owing to high surface of nanocomposites and the intermolecular-intramolecular interactions. Nevertheless, because of entropic driving force, the nanoparticles come together defined agglomerate structures; this spatial organization of fillers impose negative effect on nanocomposite properties. Many investigations, either experimental or simulation, have focused in impose a good dispersion of nanoparticles in the matrix, being the best options: varying polymer radius of gyration, such that, the radius of nanoparticles must be bigger than the former, chemical modification of nanoparticle surface, through grafted short matrix polymer chain that enable implant further interactions between components of the system, and flow effects which kinetic energy can breaks up agglomerations, and even Flory parameter. For these reasons, we deepened the molecular simulation methodology and carried out an equilibrium and a non-equilibrium molecular dynamics simulation of polymer melt nanocomposite through a 4:1:42,3,4 contraction-expansion geometry, with the aim to observe the response of material of nanoparticles dispersion and rheological properties. Furthermore, we include no homogeneous equilibrium molecular dynamics results as a way to relate surface area and dispersion degree.

Keywords: nanoparticle, molecular dynamics, rheology

References:


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