Direct Numerical Simulation of Carbon Nanofibre Composites Under Shear Flow

João M. Maia, Mikio Yamanoi
I3N-Institute for Nanostructures, Nanomodeling and Nanofabrication
Department of Polymer Engineering, University of Minho
4800-058 Guimarães, Portugal
jmaia@dep.uminho.pt ; yamanoi@dep.uminho.pt

The mechanical and transport properties of carbon nanofibres, CNF, in combination with their low production costs make them a promising material for use in polymer composites. However, the level of these properties is largely dependent on the fibres' dispersion state and aspect ratio, which, in turn, depend on the processing history of the composites. Due to strong Van der Waals interactions, CNFs tend to agglomerate, reducing their effectiveness in polymer composites. Applied shear during processing can break up the agglomerates and disperse the CNFs, but excessive shear can lead to fibre breakage, which negatively affects final properties. It is therefore crucial to 'tailor' the level of shear to obtain good dispersion, without fibre length reduction.

The current work studies the effect of simple shear flows (dominant in typical polymer processes) on the dispersion state of CNF composites and consists in a direct simulation method based on the Particle Simulation Method developed by Yamamoto et al. to analyze fiber dispersed systems. In the present work fibers are modelled as a series of connected spheres, with stretching force, torsion and bending torques being considered. Also studied is the effect of van der Waals interactions on the state of aggregation of the nanofibres. In addition our code allows the simulation of the effects of both near-field and far-field hydrodynamic interactions with relatively short computational times.

The method is a very powerful one, currently allowing the semi-quantitative prediction of the dynamics of the fibre suspensions as well as the correct prediction of the kinematics, including some previously unexplained orientation effects observed experimentally.