DIRECT NUMERICAL SIMULATION OF CARBON NANOFIBRE COMPOSITES UNDER SHEAR FLOW

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ABSTRACT

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. [1] 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 [2], collision interactions [3] and fibre orientation [4].

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.

This work focuses on the flocculation structures that form under shear flows for different fiber flexibilities. Thus, Young moduli, *E*, of 6, 60, and 600 G Pa were selected for flexible, semi-flexible, and rigid fibers, respectively. Table 1 shows details of the model nano-fiber composites.

Volume fraction, ϕ	0.01
Radius of fiber, a	25 nm
Aspect ratio	20
Number of fiber	50
Shear rate, $\dot{\gamma}$	10
Viscosity of matrix, η_0	1000 $Pa \cdot s$
Young modulus, E	6, 60, 600GPa

Table 1: Materials parameters used for simulation.

The randomly oriented, perfectly dispersed, no contact between fibers state shown in the figure 3 was used as an initial condition for the simulations. Figure 4 shows the snapshots of fiber structures of (a) *E*=

6 GPa, (b) *E*= 60 GPa, and (c) *E*= 600 GPa under simple shear flows. Figure 4a shows small round flocculation, consisting of a few fibers. There is not only flocculation but also isolated S-shaped fibers that tumble periodically along their axis. Figure 4b shows cylindrical flocculation from many fibers, with the bundles essentially aligned in the vorticity direction. Figure 4c shows flocculation parallel to the flow direction, with percolation conditions occurring. The percolation volume fraction threshold for rigid fibers of aspect ratio 20 is 0.0415 [6]. Although the present simulation is for a volume fraction 0.01, which is less than the threshold, it is conceivable that VDW interactions effectively decrease it, thus allowing percolation to occur. The behaviors shown in Figures 4b and 4c have also been observed experimentally [5].

Figure 5 shows the orientation of fibers under simple shear flows. At strain $\gamma = 0$, the components of orientation a_{xx}, a_{xx}, a_{xx} are 0.33, from which it is obvious that the initial state is an isotropically oriented one. After the application of the flow field, the maximum oriented state is achieved for every case at a strain γ around 20. After that, differences are observed, with both Figure 5a and 5b showing that a_{xx} decreases and a_{yy} and a_{zz} are gradually increasing (at strain 200 a_{yy} and a_{zz} are almost equal).

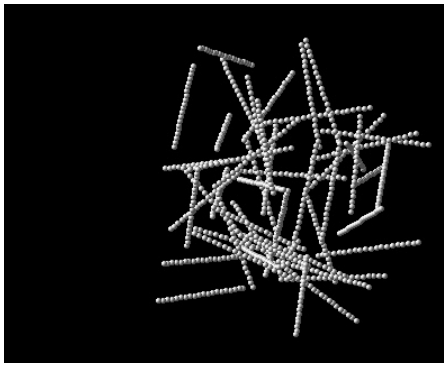
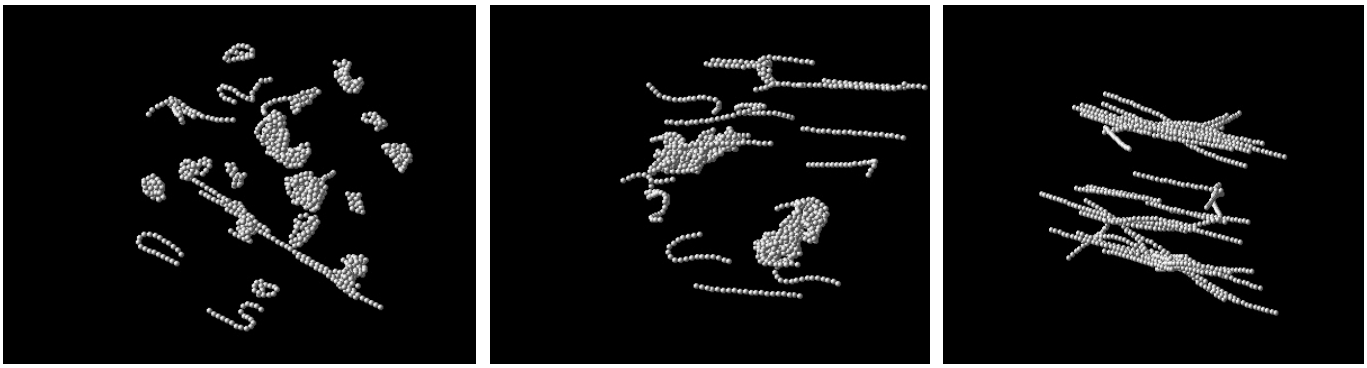


Figure 1: Initial condition



(a) *E*= 6 GPa (b) *E*= 60 GPa (c) *E*= 600 GPa

Figure 2: Aggregated structures of nano-fibers at γ=200 under simple shear flows.

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