

DISPERSION OF CARBON NANOTUBES IN RESIN SYSTEMS USING CHAOTIC MIXING

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ABSTRACT: Carbon nanotubes reinforced polymer nanocomposites have been the subject of much investigation in recent literature. Uniform distribution and dispersion of carbon nanotubes in polymer matrices is critical for realizing the full potential of composites incorporating the nanotubes; however, dispersion of carbon nanotubes remains a challenging problem. This paper explores the use of chaotic fluid mixing phenomenon for dispersing carbon nanotubes in resin systems. Chaotic advection exponentially stretches and folds fluid in situ and the trajectories of the periodic points in the flow form a braid that leads to topological chaos. It is expected that topological chaos could significantly enhance the chaotic mixing of carbon nanotubes. Computational simulations are used to analyze dispersion effectiveness and the flow features as a function of the dispersion process parameters.

KEYWORDS: carbon nanotubes, nanocomposites, dispersion, chaotic mixing, polymer matrix composites

INTRODUCTION

Carbon nanotubes have novel properties that make them potentially useful as reinforcements in many applications of composite materials. They exhibit extraordinary strength and unique electrical properties, and are efficient thermal conductors. Measurements show single-wall nanotubes room-temperature thermal conductivity is about nine times higher than copper, which is well-known for its good thermal conductivity [1]. Electrical conductivity can increase with improved nano fiber dispersion with appropriate surface treatment on carbon nanotubes. It is possible to produce a resin system with carbon nanotube dispersion that has high thermal conductivity. Nanofibers can be uniformly dispersed into polymers to produce significant changes to the physical properties of the host matrix. Surface treatment of the nanotubes could be used to improve interfacial bonding and increase tensile strength, therefore, it is possible to achieving true super-strong materials based on carbon nanotubes [2].

Uniform dispersion of nanoparticles in the resin is necessary to realize the full potential of the nanoscale reinforcements. Currently, mechanical methods such as ultrasonic dispersion or chemical methods such as functionalization of the carbon nanotubes are used to promote dispersion. In this paper, a new method using the fluid flow phenomenon of chaotic mixing is explored to disperse the nanoparticles in a thermosetting resin system. The phenomenon

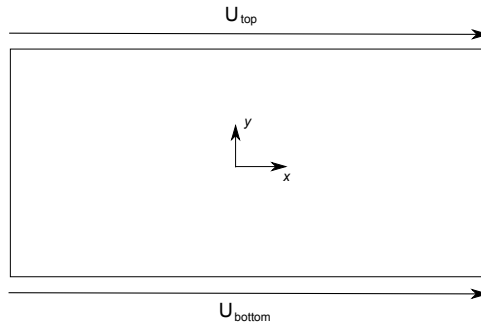


Figure 1: Schematic of lid-driven cavity flow

that passive particles advected by a periodic velocity field exhibit chaotic trajectories is often known as *chaotic advection* [3, 4]. It usually stretches and folds of material interfaces, increases the fluid-fluid interfacial area across which diffusion occurs and meanwhile decreases the diffusion distance, therefore, typically leads to significantly more rapid mixing in laminar flows. Chaotic mixing is thus expected as an efficient technique to produce resin systems with uniform carbon nanotube dispersion. Chaotic advection can occur in a large range of laminar flows, from creeping flow to potential flow, from Newtonian flow to non-Newtonian flow, and in a number of different flow systems, including unsteady two-dimensional flow and both steady and time-periodic three-dimensional flow.

Preliminary experimental studies on chaotic mixing for nanofiber dispersion has been reported in refs. [5, 6]. The present goal is to conduct a computational study of particle dispersion in a chaotic flow with the aim of identifying conditions that lead to better dispersion.

CHAOTIC MIXING MODEL

The two-dimensional lid-driven cavity system has been widely used to generate chaotic motions in a viscous fluid. Flow inside the cavity is driven by time-dependent uniform tangential motion along the entire length of each boundary, as shown in Fig. 1. By applying certain boundary motions on the top and bottom walls, topological chaos can be generated in an incompressible lid-driven cavity flow with fixed side walls in the Stokes flow regime, so as to achieve efficient mixing in the flow. However, suitable boundary conditions need to be determined for the occurrence of topological chaos [7].

In this study, the flow is investigated in the two-dimensional rectangular domain shown in Fig. 1, with the dimensions of $2 \text{ cm} \times 1 \text{ cm}$. The tangential motion of the top and bottom boundaries is very slow such that the Reynolds number is about 10. A carbon nanotube bundle with 1000 carbon nanotubes is placed in the fluid, initially with an equilibrium distance between two neighboring carbon nanotubes of about 2.93 \AA . For this study, there are no interactions between particles and the particles are treated to move individually. Particles are small enough not to agitate the flow, but large enough not to exhibit Brownian motion, moving only with the surrounding flow itself. The effects of the particles on the fluid rheology are neglected in this initial study, as also the effects of all body forces. Under these assumptions, the governing equations for conservation of mass and momentum are:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

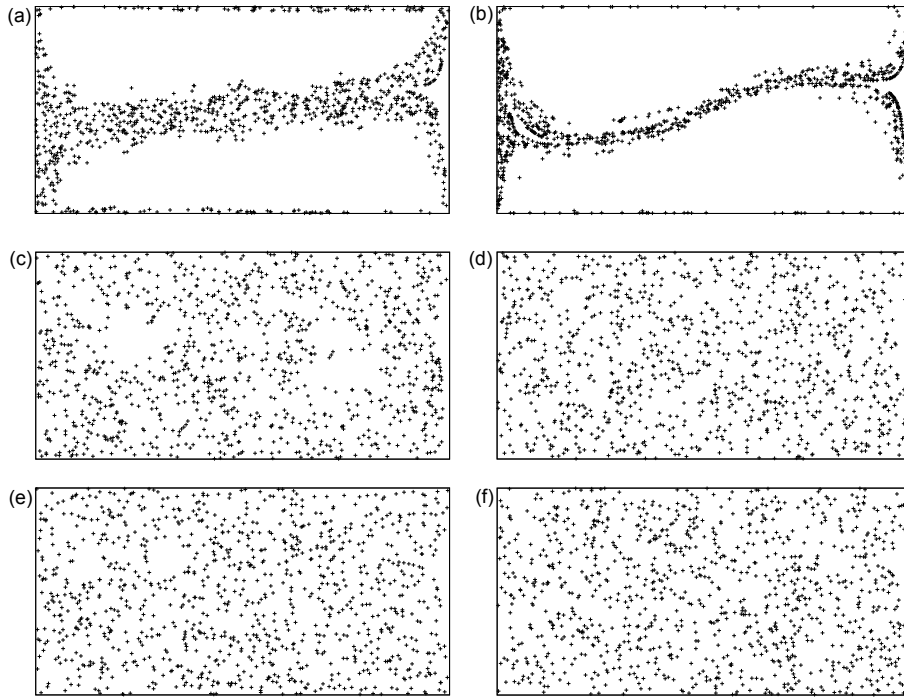


Figure 2: Carbon nanotube dispersion for $(\tau, T) =$ (a) (20, 1600 s); (b) (30, 3000 s); (c) (42, 3360 s), (d) (50, 3000 s), (e) (60, 3600 s) and (f) (80, 4800 s).

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} \quad (2)$$

where ρ is the density, \mathbf{u} is the velocity vector, p is the pressure and μ is the viscosity.

Periodic boundary conditions are applied to generate chaotic mixing,

$$\begin{aligned} U_{top}(x) &= 3 \text{ mm/s}; U_{bottom}(x) = 1 \text{ mm/s}, 2n\tau \leq t < (2n+1)\tau \\ U_{top}(x) &= 1 \text{ mm/s}; U_{bottom}(x) = 3 \text{ mm/s}, (2n+1)\tau \leq t < (2n+2)\tau \end{aligned} \quad (3)$$

where, τ is the time interval and n is any non-negative integer. The side walls are assumed to be fixed with no-slip boundary conditions. The flow field $\mathbf{u}(\mathbf{x}, t)$ is numerically solved for using the commercial computational fluid dynamics package FLUENT, and the particle trajectories are obtained through a numerical solution of the particle dynamics equation using a fourth/fifth order adaptive Runge-Kutta method:

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t) \quad (4)$$

The solution is based on a one-way coupling between the macroscopic fluid flow equations (Eqs. (1) and (2)) and the dynamics equation above, with a quasi-steady-state assumption on the flow field during each time cycle.

RESULTS AND DISCUSSION

Considering the initial location of the carbon nanotube bundle to be at the center of the domain, the effects of the mixing period τ on the dispersion is shown in Fig. 2. For mixing periods of 20 s and 30 s (Figs. 2(a) and (b)), two large islands are seen in the flow which

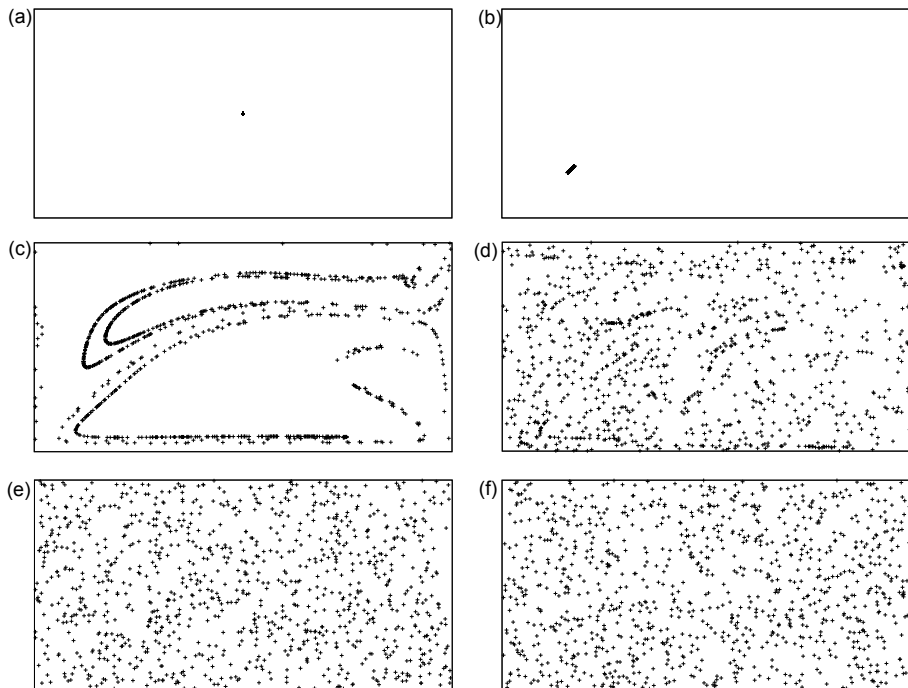


Figure 3: Carbon nanotube dispersion for at different time when $\tau = 50$ s: (a) $T = 0$ s; (b) $T = 500$ s; (c) $T = 1000$ s, (d) $T = 1500$ s, (e) $T = 3000$ s and (f) $T = 5000$ s.

don't have any nanoparticle penetration. As the period is increased to 42 s (Fig. 2(c)), the dispersion is generally good although the remnants of the islands are still evident. With further increase in τ , the dispersion is seen to improve considerably, as shown in Figs. 2(d)–(f), for $\tau = 50, 60$ and 80 s, respectively, where the islands disappear thus promoting dispersion.

The evolution of dispersion of the carbon nanotube bundle with time during the mixing process, for $\tau = 50$ s, is shown in Fig. 3, again with the carbon nanotube bundle initially positioned at the center of the rectangle. During the first 1000 s, the bundle becomes significantly stretched, however, without any significant dispersion, as shown in Figs. 3(a)–(c). After another 500s, the particles are dispersed although still not uniformly, as shown in Fig. 3(d). When $T = 3000$ s, the dispersion seems uniform, as shown in Fig. 3(e). When T further increases, the dispersion cannot be distinguished from the previous case and the state of dispersion is preserved with no re-agglomeration.

The Poincaré section may be used to quantify the dispersion effectiveness in terms of the area of the chaotic sea (the non-island areas). For the case presented in Fig. 3, the time evolution of the area fraction of the chaotic sea is presented in Fig. 4, where the area fraction of chaotic sea increases with increasing τ when $\tau < 50$ s, then decreases slightly after it reaches a maximum suggesting that $\tau = 50$ s is an optimum period for maximizing dispersion effectiveness. For higher values of τ , the dispersion quality is still acceptable; however, it takes longer to reach the steady dispersion state, requiring more power input.

CONCLUSIONS

In this study, chaotic mixing was investigated in a laminar lid-driven cavity flow under a low Reynolds number. Under certain condition, chaotic mixing found to lead to good dispersion.

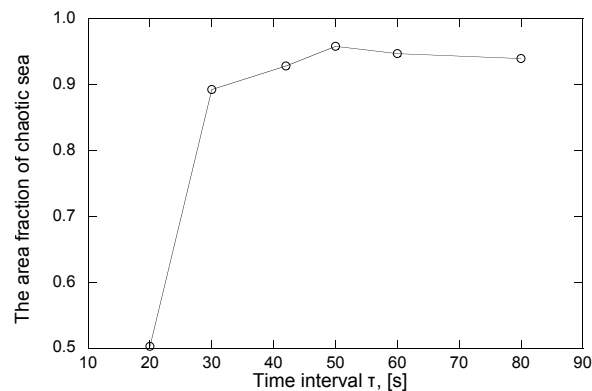


Figure 4: The area fraction of chaotic sea with respect to time interval τ

The study explored the effects of the mixing time period on the dispersion effectiveness, and $\tau = 50\text{s}$ was found to lead to the best dispersion. It is shown that the area fraction of chaotic sea in the Poincaré section can be used as an effective means to quantify the dispersion effectiveness.

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