ORIENTATION PREDICTION OF CARBON NANOTUBES IN DUAL-SCALE POROUS MEDIA DURING RESIN INFUSION

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1 Overview

In this work, we introduce a simple constitutive model for the stress and orientation prediction of the carbon nanotube (CNT) suspensions and apply it to predict the orientation prediction of such a suspension during the resin infusion process (with either RTM or VARTM) through dual-scale porous media.

Recently, Ma et al. [1] reported that a classical kinetic constitutive modeling for Brownian rod-like molecules can be employed to predict the stress and orientation of CNT suspensions formulated with epoxy resin in a simple shear flow. Of course, their CNTs is chemically treated to avoid entanglement and is well defined SWNT of low volume fractions (upto 0.5%wt). In this specific case, they showed that a classical Fokker-Plank (PF) equation

$$\frac{d\psi}{dt}+\frac{\partial}{\partial \mathbf{p}}\cdot\left(\frac{d\mathbf{p}}{dt}\psi\right)=\frac{\partial}{\partial \mathbf{p}}\cdot\left(D_r\frac{d\psi}{dt}\right) \tag{1}$$

can be successfully applied in prediction of the stress (i.e. shear-thinning viscosity) as well as the orientation, if Eq.(1) is correctly solved with equations with the momentum balance and continuity along with the stress contribution of the orientation $\boldsymbol{\tau}^f$ of the form

$$\boldsymbol{\tau}^f = 2\eta N_p \mathbf{a}_4 : \mathbf{D} \tag{2}$$

where $\mathbf{a}_4$ is the fourth-order orientation tensor [2] and N_p is a parameter that depends on the fiber concentrations and aspect ratios. They solved this complicated set of equations with FP equations using PGD (Proper Generalized Deposition) and showed that the rotary diffusivity constant D_r obtained by fitting the experimental data is very close to the classical prediction of Doi and Edward [3] for rod-like molecules.

From their result, one can expect that the tensorial description with the orientation tensor [2] can be an alternative for the FP equation (Eq.1) , which is much easier to solve especially for complex fluid flows in composite manufacturing processes. This is exactly what we have done in this work. We construct the corresponding engineering constitutive model for the evolution of CNT orientation during flow, which is expressed by the orientation tensor. We made comparison for the steady shear viscosity and the orientation in simple shear flow with the prediction in Ma et al. [1]. Then we apply this constitutive model in predicting much complex flow – the flow in dual-scale porous media during resin infusion, considering the application to hybrid composite manufacturing.

2 Results

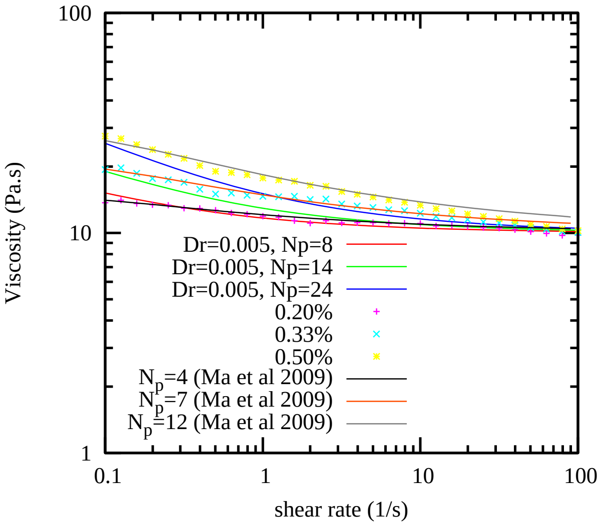

Fig.1. Prediction of the steady shear viscosity and comparison with Ma et al. [1]

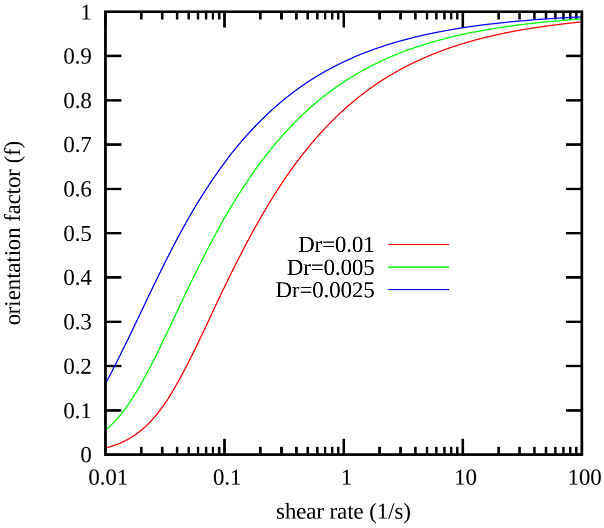

Fig.2. Prediction of the steady state orientation.

Firstly we made comparison for the steady shear viscosity as a function of the shear rate in simple shear flow. As shown in Fig. 1, a single rotary diffusivity coefficient fits fairly well with the experimental results of dilute unentangled SWNT suspension, as was observed in the result of FP solution of Ma et al. There seems to be some discrepancy in the viscosity especially for intermediate shear rate ranges (around 1), which is probably due to our choice of the closure approximation for the fourth order tensor $\mathbf{a}_4$. In the present work, we employed the hybrid closure approximation [2].

Next we observed the steady state orientation distribution. Unlike the short fiber suspensions, we have shear-dependent orientation in steady state and we presented in Fig. 2 the orientation factor *f*:

$$f = 2\mathbf{a}:\mathbf{a} - 1$$

In Fig.2, one can observe that the orientation evolution is faster with lower value of the rotary diffusivity D_r, which is obvious as D_r represents a randomizing force for the orientation.

Finally, we apply the present constitutive model for more complex flow – flows in dual scale porous media that mimics the inter- and intra-tow flows during the resin infusion process. In this work, we use a level-set based numerical scheme to deal with the Stokes-Brinkman coupling for the dual scale porous media flow simulation [4] and, at the moment, it is the decoupled simulation, which means that the stress contribution from CNT orientation does not affect the flow field. In Fig. 3, we present one example: the steady state orientation distribution distribution in a bi-periodic box with two fiber tows in each computation unit.

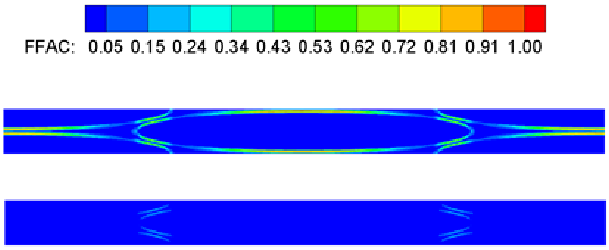

Fig.3. Steady state orientation factor distributions in dual-scale porous media flows in a bi-periodic domain: (up) horizontal flow; (down) vertical flow.

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