144o Microstructure of Multiphase Fluids in Homogeneous Shear Flows

YoChan Kim, Charles A. Petty, and Andre Benard

The prediction of the microstructure of complex fluids, such as liquid crystalline polymers or concentrated rigid rod suspensions, is often based on a moment equation for the orientation dyad, $\langle \underline{p}\,\underline{p} \rangle$. Here the unit vector $\underline{p}$ represents the alignment of a constituent component of the dispersed phase. For homogeneous shear, the velocity gradient is $\nabla \underline{v} = \dot{\gamma}\,\underline{e}_2\underline{e}_1$ with $\dot{\gamma}$ = constant. In a frame of reference relative to the local velocity, the orientation dyad is governed by the following ordinary differential equation (Doi and Edwards, 1986; Bird *et al.*, 1987; Larson, 1999):

$$\frac{d\langle \underline{p}\underline{p} \rangle}{dt} = Pe\left[\underline{e}_1\underline{e}_2 \cdot \langle \underline{p}\underline{p} \rangle + \langle \underline{p}\underline{p} \rangle \cdot \underline{e}_2\underline{e}_1 - 2\underline{e}_1\underline{e}_2 : \langle \underline{p}\underline{p}\underline{p}\underline{p} \rangle\right] + \left[\frac{1}{3}\underline{I} - \langle \underline{p}\underline{p} \rangle + U\left(\langle \underline{p}\underline{p} \rangle \cdot \langle \underline{p}\underline{p} \rangle - \langle \underline{p}\underline{p} \rangle : \langle \underline{p}\underline{p}\underline{p}\underline{p} \rangle\right)\right].$$

The above second order moment equation assumes that the aspect ratio of the dispersed phase is large compared with unity and that the rotary diffusion coefficient does not depend on the microstructure. The Péclet number $Pe = \dot{\gamma}/(6D_r)$ compares the relative importance of a characteristic time scale associated with an external flow field and a characteristic time scale associated with microhydrodynamic fluctuations. The dimensionless group U compares the relative importance of the excluded volume potential and the potential for rotary diffusion. The dimensionless time t° $6D_Rt$, where D_R represents a constant rotary diffusion coefficient in orientation space.

Prediction of the low order statistical properties of the microstructure based on the foregoing moment equation requires knowledge of the local flow field and a closure model for the orientation tetrad, $\langle \underline{p}\underline{p}\underline{p}\underline{p} \rangle$. Unfortunately, the widespread use of moment equations to describe the microstructure has been limited by the absence of a practical and accurate closure model for the orientation tetrad.

A new closure approach for the orientation tetrad that explicitly retains the six-fold symmetry and six-fold contraction properties of the exact fourth order moment has been developed by researchers at Michigan State University (see Petty *et al.*, 1999; Nguyen *et al.,* 2001; Kini *et al.*, 2003; Mandal *et al.*, 2004). At high concentrations (i.e., large U) and in the absence of an external field (i.e., Pe =0), the new theory predicts that all realizable microstructures relax to multiple equilibrium realizable prolate states. Furthermore, in the presence of homogeneous shear flows and for large values of U, the orientation director may show realizable periodic behavior relative to the flow direction.

This presentation will summarize recent results obtained by applying the new microstructure theory to a class of complex fluids subjected to homogeneous shear. The theory is used to predict the allowable microstructures and the concomitant rheological properties of the suspension induced by a simple shear flow. The proposed tetrad closure unifies previous theories of fiber suspensions and theories of complex fluids, such as liquid crystalline polymers.

KEYWORDS:

closure approximation; fiber suspensions; flow induced alignment; liquid crystalline polymers; microstructure; orientation statistics; self-alignment; simple shear; suspensions

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