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A three-species model for wormlike micellar fluids

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ABSTRACT

We present a new population dynamics-based three-species model for modeling wormlike micellar fluids which incorporates the gelation species. Starting at a homogeneous three-species model (Nestor, 2005), we show that the model is globally stable and approaches to the steady state. We then extend the model to the partial differential equation to incorporate the spatial dependence of the species. Their inhomogeneous effect for the flow behavior is modeled as well, by including populations as a polymeric viscosity in the fluid. Using the newly proposed inhomogeneous three-species model, we tackle the challenge to obtain the shear-thickening transition observed in experiments (Liu and Pine, 1996). Guided by Lerouge and Berret (2010), we design parameters in the model and numerically show that they lead to obtain an appropriate shear-thickening transition. The results are shown to be agreeable qualitatively well with experimental results, thereby confirming the conjecture by Lerouge and Berret (2010) affirmatively.

1. Introduction

A micelle consists of a number of amphiphilic molecules or surfactants and each surfactant consists of hydrophobic carbon tail and hydrophilic head group. A large concentration of amphiphiles in the water, can lead to a spherical and cylindrical micellization (or equivalently "self-organization"). Such self-organization or the micellization occurs due to the nature of hydrophobicity of the carbon tail and hydrophilicity of the head group of the surfactants. Therefore, wormlike micelles are self-assemblies of amphiphilic surfactant molecules in an aqueous solvent [1,2]. Due to the nature of the self-organization, there can be much variations in size in the formation of micelles, thereby making the modeling of wormlike micellar fluids challenging.

Another important aspect in wormlike micellar fluids is the shear-thickening transition. Such transition has been noted to occur above at a critical shear rate and known to be one of the most puzzling phenomena (see [1] and references cited therein). The shear-thickening effect is known to be first observed by Rehage and Hoffmann [3] in 1981. It is only very recent to realize that such a transition is due to a large structure known as so-called the "gelation" or shear induced structure SIS. The first and direct experimental observation for the gelation is made by Liu and Pine [4] using a novel light scattering microscopy technique. In experiments performed by Liu and Pine [4], Taylor–Couette flow is used, in which outer cylinder is rotated with some shear rate, while the inner cylinder is fixed. It is observed that gel bands initially accumulate at the inner boundary after shearing for a few minutes above at a critical shear rate, the gel bands then become unstable, and then finger like gel structures begin to grow from the inner stationary cylinder toward the outer boundary. The emergence of the

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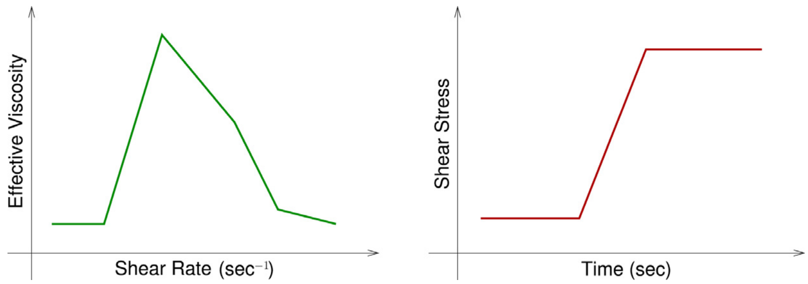

Fig. 1.1. Schematics of effective viscosity as a function of shear rate for CTAB/NaSal in water (Left) and the evolution of the shear stress at an applied shear rate exceeding a critical shear rate (Right) in [4].

shear-induced gel phase is observed to dramatically raise the stress in the solution and gives rise to shear-thickening transition [5]. Typical effects of the shear-thickening transition observed in the dilute wormlike micellar solutions are illustrated in Fig. 1.1. Note that the evolution of the effective viscosity is similar to that of the shear stress.

There has been a lot of attempt to understand the mechanism of shear-thickening transitions in a shear flow for the last three decades. However, none of them are not fully successful [1]. In particular, earlier models have predicted too large shear rates above which the shear thickening occurs, in comparison with experimentally predicted critical shear rates [6,1]. Our aim in this paper is, therefore to mathematically model the generation and the break of the gelation that can reproduce the following physical phenomenon in a shear flow:

1: Shear banding and the generation of gelation are correlated.
2: Shear thickening is predicted above at a critical shear rate, Γ_c as seen in Fig. 1.1 (Left).
3: Evolution of effective viscosity as well as the stress agrees qualitatively well with the experiments as seen in Fig. 1.1 (Right).

The critical shear rate, Γ_c will be built into our modeling, which is shown to achieve the shear-thickening transition exactly at the physically observed critical shear rate. In addition, to the best of authors' knowledge, our work is the first attempt to model the gelation inhomogeneously observed in the wormlike micellar fluids, in the mathematical model. There are in fact two-species model in literatures (see [7] and references cited therein). However, none have taken into account the gelation species in the modelings. We remark that a number of interesting new physical experiments such as the oscillatory falling sphere [8] and jumping bubbles [9] in wormlike micellar fluids have been reported to be conjectured to be correlated with the generation and break of such gelation, SIS. Therefore, our initial attempt to incorporate the gelation due to the shearing in the mathematical model can be an important step toward the modeling of such nontrivial experiments.

The rest of this paper is organized as follows. In Section 2, we investigate and generalize the homogeneous three-species model introduced in the work by Handzy [2] and provide stability analysis for the model. In Section 3, an inhomogeneous version of the three-species model is provided. In Section 4, we present the shear-thickening transition obtained by the proposed three-species model. We conclude our paper with several remarks and future directions in Section 5.

2. Homogeneous three-species model

In this section, we review and generalize the homogeneous three-species model introduced by Handzy [2] for modeling wormlike micellar fluids.

There is a large spectrum of micelle lengths in wormlike micellar fluids. Therefore, it is out of reach to take into account all the variations. In [2], a simple model has been proposed to take into account two sizes of micelles, described as short and long, together with a third species representing *shear induced structure* (SIS) or the "gelation". We denote the short micelles in concentration by $\mathsf{S}(t)$, long micelles in concentration by $\mathsf{L}(t)$, and "gelation" in concentration by $\mathsf{G}(t)$, respectively. There are two main assumptions in the homogeneous three-species model proposed by Handzy [2]. (1) It is based on mass (or concentrations) exchange property of aforementioned species. Specifically, in the modeling, the long micelles are assumed to be p times as long as short micelles. Namely, p short micelles can join into one long micelle or one long micelle can break into p short micelles. On the other hand, it is assumed that q long micelles can be combined into a gelation, or $p \times q$ micelles can be combined to form a gelation. Reversely, the gelation can be broken into a combination of short and long micelles. Note that p and q can be any real numbers that are larger than one. In the treatment of the microscopic dynamics of wormlike micelles by chemical reaction kinetics, an important early study was made by [10]. (2) A scission and reforming of gelation and micelles are crucially dependent on the shear rate and therefore, when considering the three species as chemical reactants, reaction rates are given solely as a function of shear rate. Table in Fig. 2.1 describes the reaction and reaction rates between three species.

Remark 2.1. Physically, one can view the small micelle as a spherical micelle and the long micelle as the cylindrical micelle [2,1,7]. In experiments, it is observed that the shear-thickening transition occurs only for surfactants that self-assemble