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Analytical and numerical investigation of the advective and dispersive transport in Herschel–Bulkley fluids by means of a Lattice–Boltzmann Two-Relaxation-Time scheme

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HIGHLIGHTS

- Analytical derivation of the Taylor dispersion coefficient for various rheologies.
- Dispersion coefficients of the Herschel–Bulkley fluids can now be determined.
- Fluid rheology influences displacement distributions and dispersion coefficients.
- Time necessary to reach the Taylor regime does not depend on the fluid rheology.

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ABSTRACT

Dispersion of a passive tracer in a tube has been extensively studied in the case of Newtonian fluids since the pioneer work of Taylor (1953). However, the influence of more complex rheological behavior on the transport has only be scarcely investigated. Non-Newtonian fluids are increasingly used in the industry and transport in this type of fluid merits therefore thorough investigations. An example of industrial application is Enhanced Oil Recovery, that is based on the injection of non-Newtonian fluids as polymers or surfactant solutions in porous media, which are then submitted to dispersion phenomena.

This work deals with transport of a passive tracer in shear thinning fluids with and without yield stress whose constitutive behaviors are representative of a large number of industrial fluids. We focus on transport in capillary tubes, essential for the understanding of dispersion in porous media. Transport is investigated at different time scales by solving the advection–diffusion equation using a Two-Relaxation-Time Lattice–Boltzmann method. We also derived an analytical expression of the Taylor dispersion coefficient for a large range of fluid rheologies. Dispersion coefficients of all fluids described by the Herschel–Bulkley model can now be determined. Analytical and numerical results are compared and very good accordance is obtained.

We discuss the characteristic time scales of the transport before reaching steady state as a function of fluid rheology and Péclet number. We show that the time to reach the dispersive regime is nearly independent of the fluid rheology whereas the effective dispersion coefficient is a function of the rheological parameters.

We also present the displacement distribution of the tracer molecules (propagators) as a function of time and show that they are strongly conditioned by the fluid rheology. Indeed, propagators give valuable information on the temporal evolution of the concentration profile towards the stationary Taylor regime.

1. Introduction

Passive tracer transport in simple geometries has attracted the attention of many researchers since the pioneering work of Taylor (1953). For many applications, it is indeed very useful to have a deep understanding of the interplay between advection and diffusion at different time scales and to take into account transient dynamics of tracer transport. For this purpose, both analytical expressions and numerical simulations have to be used. Surprisingly, for Newtonian fluids and despite a very large number of publications, it is only recently that an exact analytical expression is available for calculating the evolution of the displacement variance in a pipe for vanishing Neumann boundary conditions (Camassa et al., 2010). Here we are interested in non-Newtonian fluids, particularly Herschel–Bulkley fluids, circulating in a pipe under various conditions. Moreover, our

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final objective is to relate analytical and numerical results to quantities that are directly measurable by Nuclear Magnetic Resonance (NMR) velocimetry techniques (Callaghan, 1993). Indeed, using the NMR propagator technique, one can measure the displacement distribution of water molecules in a section of the tube (propagator) and extract for example its variance as a function of time. Particularly, displacement distributions in combination with concentration profiles allow further understanding of the temporal evolution of the tracer transport. For example for a Newtonian fluid, Codd et al. (1999) measured the propagators at different times in a capillary tube near the Taylor regime and could reproduce the observations with simple numerical simulations without any fitting parameter.

The mechanisms at the origin of dispersion have been first described and modeled by Taylor (1953), and later by Aris (1956), both works being now referred to as the Taylor–Aris theory. Essentially, in Poiseuille flow, the effective longitudinal diffusivity, also called effective dispersion, can be much larger than the molecular diffusivity because molecules can move randomly from one streamline to another in the radial direction due to molecular motions. This enhanced diffusivity depends on the Péclet number (defined later) but also on the configuration of the velocity field. In Poiseuille flow, the velocity field is different when considering non-Newtonian fluids, yielding different dispersion coefficients.

Dispersion in non-Newtonian fluid has been studied by only few researchers. Fan and Wang (1965, 1966) were the first to consider non-Newtonian fluids in the framework of Taylor theory. They first considered an Ostwald de Waele fluid (Fan and Wang, 1965) and later a Bingham plastic fluid and an Ellis model fluid (Fan and Wang, 1966). Later on, dispersion coefficients were computed for fluids with distinct rheologies (Goshal et al., 1971; Sha and Cox, 1974). Close to our consideration, Booras and Krantz (1976) and Sharp (1993) developed analytical expressions of the effective dispersion coefficient for shear thinning fluid but without taking into account the yield stress. Sharp (1993) computed then the effective dispersion coefficient for a particular yield stress fluid ($n=1$). More recently, Ramana et al. (2012) derived analytical expressions of the time dependent dispersion for Herschel–Bulkley, power law and Bingham fluids to calculate when a stable dispersion coefficient is reached.

In this work, we focus on the temporal evolution of the propagator as well as its variance for Herschel–Bulkley fluids, in order to gain better comprehension of the transport process. We propose useful analytical expressions not readily available in the literature and perform numerical simulations to cover all regimes, the diffusion, advection and finally dispersion dominated regime. In a first part (theoretical considerations), we give analytical expressions for the displacement variance and the dispersion coefficient for shear thinning fluids taking into account the yield stress starting from various existing formulations. In a second part (numerical approach), we use Lattice–Boltzmann simulations to solve the advection–diffusion equation in a large range of Péclet numbers in order to compute not only the concentration profiles and propagators but also the time dependency of the displacement variance.

2. Material and methods

2.1. Theoretical considerations

2.1.1. Newtonian and non-Newtonian flow fields in a cylindrical channel

The Herschel–Bulkley model (Herschel and Bulkley, 1926) is a simple and general model, that gives a good description of the constitutive behavior of a wide range of non-Newtonian fluids (Coussot, 2014). It relates the shear stress τ to the shear rate $\dot{\gamma}$ by

$$\begin{cases} \tau = \tau_0 + k(\dot{\gamma})^n & \text{if } \tau \geq \tau_0 \\ \dot{\gamma} = 0 & \text{else} \end{cases} \quad (1)$$

with $n \in [0;1]$. τ_0 is the yield stress and k is the fluid consistency expressed in units of $\mathrm{Pa\,s^{-n}}$. The model also includes the description of Newtonian fluid when choosing $n=1$, $\tau_0=0$ and k equal to the dynamic viscosity η.

In the present paper we will focus on fluids flowing through a circular channel. With a negative pressure gradient $\mathrm{d}p/\mathrm{d}z$ oriented along the channel axis (z-direction) the cylindrical symmetry of the channel and the momentum balance give

$$\tau(r) = -\frac{r}{2}\frac{\mathrm{d}p}{\mathrm{d}z}. \quad (2)$$

The shear rate in this unidirectional geometry is given by

$$\dot{\gamma} = \frac{\mathrm{d}v(r)}{\mathrm{d}r} \quad (3)$$

where $v(r)$ is the velocity in the z-direction. Combining Eq. (1) with Eqs. (2) and (3) the expression of the velocity profile $v(r)$, after appropriate integrations, is given by the following expression:

$$v(\tilde{r}) = \begin{cases} V_{\max}\left[1-\left(\dfrac{\tilde{r}-\tilde{r}_0}{1-\tilde{r}_0}\right)^{1/n+1}\right] & \text{if } \tilde{r} \geq \tilde{r}_0 \\ V_{\max} = \left(\dfrac{1}{2k}\left|\dfrac{\mathrm{d}p}{\mathrm{d}z}\right|\right)^{1/n}\left(\dfrac{n}{1+n}\right)R^{1/n+1}(1-\tilde{r}_0)^{1/n+1} & \text{else} \end{cases} \quad (4)$$

where R is the pipe diameter and $\tilde{r} = r/R$. $\tilde{r}_0$ is the radius of the plug flow such that $\tau(\tilde{r}_0)=\tau_0$, it is thus defined as $\tilde{r}_0 = r_0/R$ with $r_0 = -2\tau_0\,\mathrm{d}p/\mathrm{d}z$. For $\tilde{r} < \tilde{r}_0$, the shear stress is smaller than the yield stress τ_0, thus there is no deformation of the fluid and the velocity profile is flat. It is also important to note that if $\tilde{r}_0 \to 1$, $v(r) = 0\ \forall r$. Typical velocity profiles are shown in Fig. 1.

2.1.2. Advection–diffusion equation

The coupling between convective and diffusive transport, generally known as dispersion, is analytically described by the Advection–Diffusion Equation (ADE) which is directly resulting from the mass conservation law. For isotropic diffusion in a unidirectional flow (along the z-axis) in a cylindrical channel, the ADE can be written as

$$\frac{\partial C(r,z,t)}{\partial t} + v(r)\frac{\partial C(r,z,t)}{\partial z} = D_m \Delta C(r,z,t), \quad (5)$$

with $C(r,z,t)$ being the tracer concentration at time t, D_m the molecular diffusion coefficient of the tracer and Δ the Laplace operator. The

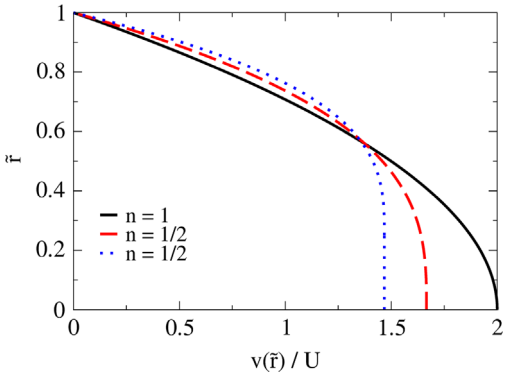

Fig. 1. Velocity profiles used in the simulations. The black continuous line is the Poiseuille curve ($n=1$; $\tilde{r}_0=0$), the red dashed line is the shear thinning profile ($n=0.5$; $\tilde{r}_0=0$) and the blue dotted line corresponds to a shear thinning profile with a yield stress ($n=0.5$; $\tilde{r}_0=0.25$). (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)