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Lattice Boltzmann simulation of power-law fluid flow in the mixing section of a single-screw extruder

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ABSTRACT

The single-screw extruder is commonly used in polymer processing where the performance of the mixing section is significant in determining the quality of the final product. It is therefore of great interest to simulate the flow field in a single-screw extruder. In this paper simulations of non-Newtonian fluids in a single-screw extruder are performed using the lattice Boltzmann model.

1. Introduction

A single-screw extruder is commonly used in polymer processing. The mixing performance of the extruder considerably influences the quality and morphology of the final product. For this reason the flow field in the mixing section has been studied by a number of authors to gain a better understanding of the process. Yao et al. (1996, 1997) used the finite difference method (FDM) to determine the flow field in a single-screw extruder geometry. The simulations were shown to be in good agreement with the results of a flow visualisation experiment using high viscosity corn syrup. Horiguchi et al. (2003) used the lattice gas method (LGM) to examine the same problem. The LGM results were found to be in good agreement with visualisation experiments. Horiguchi et al. (2003) also considered a quantitative comparison with theory. This indicated that the LGM produced a more accurate representation of the flow field compared to the FDM; however, there was still a discrepancy between the LGM simulation and the analytic expression. Simulations using the lattice Boltzmann model (LBM) were performed by Buick and Cosgorve (2006). The LBM is a simplified kinetic model (Chen and Doolen, 1998) which has developed from the LGM. The LBM was shown to simulate the flow in the single-screw extruder more accurately and more efficiently than the LGM.

The simulations described above considered the fluid in the single-screw mixer to be a Newtonian fluid. In a Newtonian fluid the viscosity, defined as the ratio of the stress to the velocity gradient of the fluid, is constant. In many practical situations the fluid in a single-screw extruder will exhibit non-Newtonian behaviour. Non-Newtonian fluids have a viscosity which is not constant, it can vary with, for example, shear, temperature or time.

Here we will consider only shear dependent non-Newtonian fluids. A dilatant or shear-thickening fluid has an apparent viscosity which increases with increasing shear, for example corn starch, clay slurries and certain surfactants. A pseudoplastic or shear-thinning fluid has an apparent viscosity which decreases with increasing shear, for example polymer melts such a molten polystyrene, polymer solutions such as polyethylene oxide in water, paint and blood (Quarteroni et al., 2000).

A feature of the LBM is that it is suitable for simulating a non-Newtonian fluid. Gabbanelli et al. (2005) considered a power-law non-Newtonian fluid where the apparent viscosity was calculated as a function of the rate of strain which was found by differentiating the velocity field. The model was found to be first-order accurate for simple flows and was further applied to study flow in a reentrant corner geometry. Kehrwald (2005) considered an LBM for shear-thinning fluids where the rate of strain was determined from known quantities without the need for differentiation. This model was applied to liquid composite moulding. Artoli and Sequeira (2006) also considered a model where the rate of strain was found without differentiating the velocity field. They applied their model to oscillating flows. Non-Newtonian simulations of blood flow using the LBM have also been considered by a number of authors (Ouared and Chopard, 2005; Artoli et al., 2006; Boyd and Buick, 2007; Boyd et al., 2007).

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It has been shown that second-order accuracy can be obtained using the LBM with a non-Newtonian viscosity described by a power-law model (Boyd et al., 2006). Preliminary results have shown qualitative differences between the velocity fields of a shear-thinning fluid and a Newtonian fluid in a single-screw extruder (Buick and Boyd, 2006).

The success of the LBM in simulating flow in a single-screw extruder and in simulating non-Newtonian fluids, coupled with the evidence that there is a significant difference between Newtonian and non-Newtonian flows in a screw-extruder, have motivated the present study. The LBM for a non-Newtonian fluid is described in Section 2. In Section 3 the validity of the model is investigated and simulation results are presented for a range of both shear-thinning and shear-thickening fluids.

2. The lattice Boltzmann model

The LBM (Chen and Doolen, 1998; Succi, 2001; Wolf-Gladrow, 2000) has recently been developed as an alternative technique for simulating fluid flow. Here we describe the Newtonian two-dimensional D2Q9 model and the modifications required to simulate a power-law, non-Newtonian fluid.

2.1. The D2Q9 LBM model

The model evolves according to the kinetic equation

$$f_i(\boldsymbol{x}+\boldsymbol{e}_i, t+1) - f_i(\boldsymbol{x}, t) = \Omega_i \tag{1}$$

for $i = 0, 1, \ldots, 8$, where f_i denotes the distribution function along direction $\boldsymbol{e}_i$ and

$$\boldsymbol{e}_0 = (0,0),$$
$$\boldsymbol{e}_i = \left(\cos\left(\frac{\pi}{2}(i-1)\right), \sin\left(\frac{\pi}{2}(i-1)\right)\right)$$

for $i = 1, 2, 3, 4$ and

$$\boldsymbol{e}_i = \sqrt{2}\left(\cos\left(\frac{\pi}{2}(i-1)+\frac{\pi}{4}\right), \sin\left(\frac{\pi}{2}(i-1)+\frac{\pi}{4}\right)\right)$$

for $i = 5, 6, 7, 8$. The left-hand side of Eq. (1) represents streaming of the distribution functions at unit speed from one site $\boldsymbol{x}$ to a neighbouring site on a regular underlying grid defined by the link vectors $\boldsymbol{e}_i$. The right-hand side of Eq. (1) is the collision function which determines the manner in which the distribution functions interact at each site. The form of Eq. (1) makes the LBM discrete in both space and time.

The fluid density, ρ, and velocity, $\boldsymbol{u}$, are determined locally at each site and each time-step as follows:

$$\rho(\boldsymbol{x}, t) = \sum_{i=0}^{i=8} f_i(\boldsymbol{x}, t) \quad \text{and} \quad \rho(\boldsymbol{x}, t)\boldsymbol{u}(\boldsymbol{x}, t) = \sum_{i=0}^{i=8} f_i(\boldsymbol{x}, t)\boldsymbol{e}_i. \tag{2}$$

Conservation of mass and momentum requires that the collision term, Ω_i in Eq. (1) satisfies

$$\sum_{i=0}^{i=8} \Omega_i = 0 \quad \text{and} \quad \sum_{i=0}^{i=8} \Omega_i \boldsymbol{e}_i = 0. \tag{3}$$

This is achieved in the LBM (Qian et al., 1992) using the Bhatnagar et al. (1954) equation

$$\Omega_i = \frac{-1}{\tau}(f_i - \bar{f}_i), \tag{4}$$

which mimics the collisions by a relaxation towards an equilibrium distribution function $\bar{f}_i$ given by

$$\bar{f}_i(\boldsymbol{r}, t) = \rho(1 + 3\boldsymbol{e}_i \cdot \boldsymbol{u} + \tfrac{9}{2}(\boldsymbol{e}_i \cdot \boldsymbol{u})^2 - \tfrac{3}{2}u^2), \tag{5}$$

where $w_0 = \frac{4}{9}$, $w_1 = w_2 = w_3 = w_4 = \frac{1}{9}$ and $w_5 = w_6 = w_7 = w_8 = \frac{1}{36}$. The rate of relaxation is determined by the relaxation time τ. Combining Eqs. (1) and (4) and performing a Taylor series expansion up to second order gives

$$(\partial_t + \boldsymbol{e}_i \cdot \nabla) f_i + \frac{1}{2}(\partial_t + \boldsymbol{e}_i \cdot \nabla)^2 f_i = \frac{-1}{\tau}(f_i - \bar{f}_i). \tag{6}$$

Introducing ε, the Knudsen number (Wolfram, 1986), which is the ratio of the mean free path to the characteristic length of the system; applying a Chapman–Enskog expansion (Frisch et al., 1987):

$$f_i = \bar{f}_i + \varepsilon(f_i^{(1)} + \varepsilon f_i^{(2)}),$$
$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_1} + \varepsilon\frac{\partial}{\partial t_2},$$
$$\frac{\partial}{\partial \boldsymbol{x}} = \frac{\partial}{\partial \boldsymbol{x}_1} \tag{7}$$

and collecting terms up to second order in ε, leads to the mass and momentum equations (Chen and Doolen, 1998)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho\boldsymbol{u} = 0 \tag{8}$$

and

$$\frac{\partial \rho u_\alpha}{\partial t} + \nabla_\beta \Pi_{\alpha\beta} = 0, \tag{9}$$

where the momentum flux tensor is given by

$$\Pi_{\alpha\beta} = \sum_i (\boldsymbol{e}_i)_\alpha (\boldsymbol{e}_i)_\beta \left[\bar{f}_i + \left(1 - \frac{1}{2\tau}\right) f_i^{(1)}\right]. \tag{10}$$

Greek subscripts are used to represent vector components while Roman subscripts label the distribution functions, f_i and $\bar{f}_i$, and link vectors, $\boldsymbol{e}_i$. Using the expression for the equilibrium distribution function, Eq. (5), gives

$$\sum_i (\boldsymbol{e}_i)_\alpha (\boldsymbol{e}_i)_\beta \bar{f}_i = \rho u_\alpha u_\beta + \frac{1}{3}\rho\delta_{\alpha\beta}. \tag{11}$$

In a fluid with pressure p and kinematic viscosity ν the momentum flux tensor takes the form

$$\Pi_{\alpha\beta} = \rho u_\alpha u_\beta + p\delta_{\alpha\beta} - 2\rho\nu S_{\alpha\beta}, \tag{12}$$

where $S_{\alpha\beta}$ is the strain tensor. Thus, expressing the pressure as $p = c_s^2\rho$ we see that the speed of sound is $c_s = 1/\sqrt{3}$ and, following Artoli (2003),

$$S_{\alpha\beta} = -\left(1 - \frac{1}{\tau}\right)\frac{1}{2\rho\nu}\sum_i (\boldsymbol{e}_i)_\alpha (\boldsymbol{e}_i)_\beta f_i^{(1)}. \tag{13}$$

Evaluating Eq. (13) using the first-order Chapman–Enskog expansion of Eq. (6) gives (Chen and Doolen, 1998)

$$\Pi_{\alpha\beta} = \rho u_\alpha u_\beta + p\delta_{\alpha\beta} - \nu\left(\frac{\partial \rho u_\beta}{\partial_\alpha} + \frac{\partial \rho u_\alpha}{\partial_\beta}\right), \tag{14}$$

where

$$\nu = (2\tau - 1)/6. \tag{15}$$

In the incompressible limit, $\partial_\alpha \rho = 0$, the fluid density can be removed from the derivatives in Eqs. (8) and (14). Thus the LBM scheme satisfies the continuity and Navier–Stokes equations for a Newtonian fluid with kinematic viscosity ν. The value of the kinematic viscosity is determined by the free parameter τ (Eq. (15)) which is introduced in the collision function, Eq. (4).