



# Lattice Boltzmann simulation of polymer melt flow with a low Reynolds number



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## ABSTRACT

The lattice Boltzmann method (LBM) has been used in various fluid flow analyses as an alternative to the traditional method of computational fluid dynamics. In the study reported here, the LBM was used to simulate a simple Hele–Shaw melt flow of polymers considering their actual physical properties, whereas the Carreau fluid model was used to evaluate the polymer melt viscosity. Since the Reynolds number of a polymer melt flow is typically quite low due to its high viscosity, which in turn lowers its convergence rate in the LBM, introducing a new density offset method improved that rate. In this paper, cases of simulations with pressure or velocity inlet boundary conditions are discussed in which the density offset method is applied.

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## 1. Introduction

Manufacturing plastic components using thermoplastics often requires considering the melt flow of polymers, upon which processes such as injection mold, extrusion, and blow molding depend to form the desired shapes of components. Among those processes, injection molding requires injecting a polymer melt into a cavity in a close mold and solidifying it by cooling in order to replicate the shape of the cavity. The most important property of the polymer melt flow is its high viscosity, which resulting in a low Reynolds number.

Extensionally analysis and modeling have been done on the injection molding process in the early time [1–5]. Recently, Microinjection molding technology was developed to fabricate micro scale plastic components. It can be designated to the fabrications of components with micro features or components with size in milligrams. Their applications include the products as diffractive optical elements, high density information storage, micro fluidics, micro mechanical parts, etc. In general, plastic components with such small features require a substrate of normal size and are built with different predefined microscale features to perform their functions. The effective simulation of the micro injection molding process has been reported in terms of the polymer melt flow and aspects of temperature analysis [6–8]. In modeling polymer flows, the polymer melt refers to a non-Newtonian fluid, usually assumed to be a generalized Newtonian fluid, defined as an idealized fluid whose shear stress depends only on the shear rate at a given time,

as applied in studies on plastic production processes that consider polymer melt flows.

Given the simplicity of its computations, the lattice Boltzmann method (LBM) has been applied in various fields [9–12], especially in various fluid flow analyses as an alternative to the traditional method of computational fluid dynamics. From a certain perspective, the LBM is a mesoscopic numerical approach situated between nanoscopic (i.e., molecular dynamics) and macroscopic (i.e., computational fluid dynamics) methods of analysis. In recent decades, the LBM has received considerable attention in studies on complex flow phenomena such as phase separation, condensation, multicomponent flow and flows in porous media together with thermal analysis.

In analyzing non-Newtonian flows, the relaxation time in the Bhatnagar–Gross–Krook collision term can be adjusted to suit the viscosity, which depends on the shear rate at each time step [13–17]. As an example, Gabbanelli et al. [18] employed variable relaxation time for the power-law fluid in LBM simulations with truncated upper and lower shear rates. Since the relaxation time in the LBM depends on the fluid viscosity, the low viscosity of power-law fluid in the high shear rate region will result in numerical instability with a relaxation time of approximately 1/2. In response, a lower viscosity limit was applied in their study to ensure stability, and a limit value was used for viscosity near the zero shear rate due to the unrealistically high viscosity proposed by the power-law model. A lattice kinetic scheme, as an extension of the LBM, was used to study non-Newtonian, power-law, and Carreau fluids and was reported to be more stable than the LBM [19]. Briefly, the power-law fluid can be a shear thinning or thick-

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ening fluid, depending on the power-law exponent, whereas Carreau fluid is a shear thinning fluid with upper and lower viscosity limit values as the shear rate tends to infinity or 0. Although the power-law fluid is an idealized model, the Carreau model satisfies the behavior of a real fluid in regions of low and high shear rates. To improve numerical stability, multi-relaxation-time LBM has been introduced to the non-Newtonian fluid flow [9], and studies with the Bingham plastic or pseudo-plastic fluid flows have used the LBM as well [20,21].

Most studies on LBM simulation have focused on modeling different flow behaviors with pseudo-material properties in LBM units. Some simulations have involved water- and air-based materials, but none have performed LBM simulation using the properties of real plastics. In response, to apply the LBM to the simulation of plastic processes such as injection molding, the study reported here involved performing an LBM flow simulation of the polymer melt. The LBM, developed to an alternative approach for solving complex fluid dynamic problems, was deemed suitable for the flow simulation in micro injection molding compared to conventional methods. The direct kinetic formulation can facilitate the implementation of LBM in complex geometry, and in micro-scale simulations, the LBM can capture physical behaviors easily, including heat transfer, surface tension, and air trapping, in the free surface interface of the mold filling flow. Since polymer melt flows require exceptionally low Reynolds numbers given the high viscosity of the melting polymer and since LBM flow simulations of polymer melts pose a similarly low speed of convergence, a density offset method for LBM simulations was proposed to accelerate convergence in the simulations. Two plastics materials—polystyrene (PS) and acrylonitrile butadiene styrene (ABS)—were used in the simulations.

## 2. Numerical method

### 2.1. Lattice Boltzmann method

Implementing the LBM involved applying the Boltzmann equation on a discrete lattice with a set of velocity distribution functions

$$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i(f(\mathbf{x}, t)) \quad (1)$$

in which  $f_i$  refers to the density distribution functions of a fluid particle along the  $i$ th direction in the discrete lattice,  $\Omega_i$  to the collision operator,  $\mathbf{x}$  to the position vector of the particle,  $\mathbf{e}_i$  to the lattice velocity, and  $\Delta t$  to the time step increment. With the Bhatnagar–Gross–Krook approximation, the lattice Boltzmann model can be expressed as

$$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) - \frac{f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)}{\tau} \quad (2)$$

in which  $\tau$  is the time that the distribution function takes to relax to the local equilibrium distribution function  $f_i^{eq}$ . The value of  $\tau$  relates to the kinematic viscosity of the fluid per the equation  $\nu^* = (\tau - 1/2)/3$ . To maintain numerical stability, the relaxation time is usually 0.5–2 X; for the D2Q9 model, the equilibrium distribution function was

$$f_i^{eq}(\mathbf{x}, t) = \omega_i \rho(\mathbf{x}) \left[ 1 + 3 \frac{\mathbf{e}_i \cdot \mathbf{u}}{c^2} + \frac{9}{2} \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{c^4} - \frac{3}{2} \frac{u^2}{c^2} \right] \quad (3)$$

in which  $\omega_i$  is the weight coefficient with 4/9 for  $i = 0$ , 1/9 for  $i = 1-4$ , and 1/36 for  $i = 5-8$  and  $c$  is the lattice velocity. The macroscopic density and velocity were

$$\rho = \sum_{i=0}^8 f_i \quad (4)$$

$$\mathbf{u} = \frac{1}{\rho} \sum_{i=0}^8 f_i \mathbf{e}_i \quad (5)$$

### 2.2. Non-Newtonian fluid

The plastic materials PS and ABS were used in the LBM simulations. The Carreau fluid model was employed for the polymer melt flow, following several macroscopic flow simulations for injection molding [1,22,23]. Polymer viscosity is a function of shear rate, temperature, and pressure and can be expressed as

$$\eta = \frac{\eta_0}{1 + \left[ \frac{\eta_0 \dot{\gamma}}{\tau^*} \right]^{1-n}} \quad (6)$$

in which  $\eta_0$  denotes the zero shear rate viscosity,  $\dot{\gamma}$  the shear rate,  $n$  the power index, and  $\tau^*$  a material constant. A Williams–Landel–Ferry-type equation was used to represent the zero shear rate viscosity:

$$\eta_0 = D_1 \exp \left[ - \frac{A_1 (T - T^*)}{A_2 + (T - T^*)} \right] \quad (7)$$

in which

$$T^* = D_2 + D_3 P \quad (8)$$

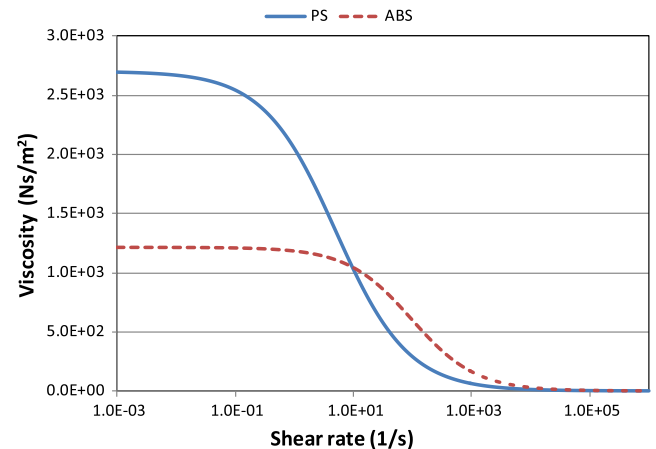
and

$$A_2 = \tilde{A}_2 + D_3 P \quad (9)$$

The corresponding material constants in the viscosity model for PS and ABS appear in Table 1. The densities of PS and ABS were 1040 and 1027.7 kg/m<sup>3</sup>, respectively. The viscosity for PS and ABS appear in Fig. 1, as calculated by Eq. (7) with melt temperatures of 473 and 513 K, respectively. In consideration of the isothermal flow, the polymer’s melting temperature was set. The

**Table 1**  
Constants for viscosity model.

	PS	ABS
N	0.293	0.203
$\tau^*$ (Pa)	13,680	$1.175 \times 10^5$
$D_1$ (Pa s)	$7.44 \times 10^{10}$	$1.669 \times 10^5$
$D_2$ (K)	373	443
$D_3$ (K/Pa)	0	0
$A_1$	25.97	13.15
$A_2$ (K)	51.6	117



**Fig. 1.** Viscosity of Polystyrene (PS) and Acrylonitrile Butadiene Styrene (ABS) based on the Carreau model.

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