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A lattice Boltzmann model for solute transport in open channel flow

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A B S T R A C T

A lattice Boltzmann model of advection–dispersion problems in one-dimensional (1D) open channel flows is developed for simulation of solute transport and pollutant concentration. The hydrodynamics are calculated based on a previous lattice Boltzmann approach to solving the 1D Saint–Venant equations (LABSVE). The advection–dispersion model is coupled with the LABSVE using the lattice Boltzmann method. Our research recovers the advection–dispersion equations through the Chapman-Enskog expansion of the lattice Boltzmann equation. The model differs from the existing schemes in two points: (1) the lattice Boltzmann numerical method is adopted to solve the advection–dispersion problem by mesoscopic particle distribution; (2) and the model describes the relation between discharge, cross section area and solute concentration, which increases the applicability of the water quality model in practical engineering. The model is verified using three benchmark tests: (1) instantaneous solute transport within a short distance; (2) 1D point source pollution with constant velocity; (3) 1D point source pollution in a dam break flow. The model is then applied to a 50-year flood point source pollution accident on the Yongding River, which showed good agreement with a MIKE 11 solution and gauging data.

1. Introduction

A coupled hydrodynamic and solute transport lattice Boltzmann model is investigated for 1D open channel flow. The lattice Boltzmann method (LBM) is a newly developed numerical approach to solve the incompressible Navier–Stokes equations (Chen and Doolen, 1998). It is a entirely explicit, easy to parallelize, and can handle complex fluids and geometries (Shan et al., 2006). It uses a different solver for the nonlinear partial differential equations, compared to traditional Computational Fluid Dynamics (CFD) methods, such as the finite difference method (FDM), finite volume method (FVM) and finite element method (FEM), which discretize the equations in time and space directly (Zhang et al., 2002). For example, Gurarslan et al., 2013 derived a compact finite difference method solution for 1D Advection–Diffusion (AD) equation, which is sixth-order in space and fourth-order in time accuracy. Gurarslan (2014) also compared high-order finite difference method two-dimensional (2D) AD model to a fourth-order Runge–Kutta scheme, and verified its accuracy and efficiency. The LBM simulates the macroscopic dynamics indirectly, by calculating microscopic molecular particle movements, and integrates them to form physical variables (Zhou, 2004). The unique features of the LBM brings significant benefits for calculation and programming, especially for high computational density problems in engineering.

The LBM is used in many fluid dynamics engineering applications, especially in solving the advection–dispersion equation (ADE). Advection–dispersion problems have been an important area of research for many years, due to applications in practical engineering. For example, pollutant transport in open channel flows, heat transfer in multi-phase fluid flows, nutrition transport in organism colonies, and cell movement in blood vessels, etc (Merks et al., 2002). Hughes et al. (1989) presented a finite element formulation for advection-diffusive equations in computational fluid dynamics. Leveque (1996) used a wave-propagation finite volume approach to solve the advection–diffusion equation in second-order accuracy. Meerschaert and Tadjeran (2004) developed an practical numerical finite difference method to approximate the fractional advection–dispersion equations in groundwater, and modeled the passive tracers transport in porous medium properly.

In previous research, most lattice Boltzmann schemes for advection–dispersion problems focused on improving the accuracy

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and stability in 2D fluid flows. O'Brien et al. (2002) compared experimental data to a 2D lattice Boltzmann method for advection–diffusion model in porous media flow. Ginzburg (2006) proposed a lattice Boltzmann scheme to advection and anisotropic dispersion equations (AADE) to solve Richard's equation in saturated flow. Zhou (2009) studied the LBM for the ADE in 1D area based on solve the 2D shallow water equations. Li and Huang (2008) coupled a hydrodynamic model with advection and anisotropic dispersion using the LBM in shallow water flows. Servan-Camas and Tsai (2009) analyzed the stability constraints for the LBM for the ADE, and illustrated that the negativity equilibrium distribution function values do not necessarily lead to instabilities. Peng et al. (2011) investigated a 2D LBM solute transport model in shallow water, showing that the multiple-relaxation-time (MRT) terms have better stability than the Bhatnagar-Gross-Krook (BGK) terms. Hammou et al. (2011) focused on the analysis the relation between kinetic parameters and stability of two-relaxation-times (TRT) lattice Boltzmann scheme. Ginzburg (2013) presented several anisotropic collisions for a lattice Boltzmann model dealing with the ADE, and introduced many different anisotropic schemes to remove numerical diffusion. Patel et al. (2014) reported a discontinuous Galerkin lattice Boltzmann scheme to solve heat transfer advection–dispersion problems. Ginzburg and Roux (2015) analyzed the truncation effect of TRT-LBM scheme on advection–diffusion equations, and further compared the accuracy and stability of different boundary schemes with variable Peclet number (Pe). Most recently, Markl and Korner, 2015 derived a Neumann boundary condition for no-flux free surface, which expanded the study area of the LBM for the ADE problems.

Our study couples the 1D hydrodynamics model with AD model based on solving the Saint–Venant equations (SVE) and the advection–dispersion equations, which could improve the practicality of using LBM for dealing with flux and wetted boundaries when simulating solute transport in open channel flow. It also introduces a more efficient method to deal with 1D ADE problems for engineering applications, e.g. dam break flow, which is a typical hydrodynamic problem in engineering, can cause significant loss of human life (Zhou, 2004). And it is much faster than 2D models in computation.

Section 2 introduces the lattice Boltzmann equations and the ADE, using the Chapman-Enskog expansion. Section 3 simulates three benchmarks to validate the method. Section 4 presents an application to a pollution accident, demonstrating the utility of the formulation.

2. Lattice Boltzmann method

2.1. Lattice Boltzmann Equation

The lattice Boltzmann method was derived first by McNamara and Zanetti (1988) from a lattice-gas-automata (LGA) model, and further developed using the Bhatnagar-Gross-Krook (BGK) collision operator (Bhatnagar et al., 1954), which is also called the single-relaxation-time (SRT). The SRT collision operator is simpler and more efficient compared to two relaxation times (TRT) and multiple relaxation times (MRT) collision operators (Peng et al., 2016). The LBM considers particle movement as two separate steps, streaming and collision. In streaming, particles move forwards or backwards to neighboring lattices according to velocity vectors in a D1Q3 scheme (Zhou et al., 2004) (Fig. 1). The streaming is governed by

$$f_\alpha(x + e_\alpha \Delta t, t + \Delta t) = \bar{f}_\alpha(x, t) + \frac{1}{2}\Delta t e_\alpha F(x, t), \tag{1}$$

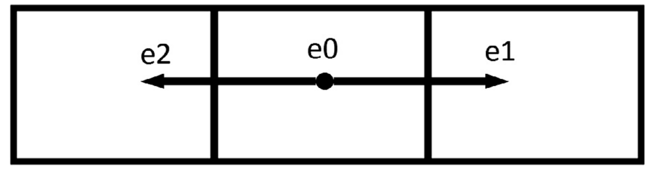

Fig. 1. D1Q3 Lattice Scheme.

where f_α is the particle distribution function and $\bar{f}_\alpha$ is the initial f_α before the streaming step. e_α is a particle velocity vector defined by

$$e_\alpha = \begin{cases} 0, & \alpha = 0 \\ e, & \alpha = 1 \\ -e; & \alpha = 2 \end{cases} \tag{2}$$

where $e = \Delta x/\Delta t$. Δx is the lattice size and Δt is the time step, and $F(x, t)$ is the external force term.

In the collision step, particles collide with each other and reach equilibrium according to a scattering rule within each lattice, which is defined by

$$\bar{f}_\alpha(x, t) = f_\alpha(x, t) + \Omega_\alpha[f(x, t)], \tag{3}$$

where Ω_α is the collision operator, which controls the collision speed of f_α. It can be linearized to the BGK collision operator (Bhatnagar et al., 1954)

$$\Omega_\alpha(f) = -\frac{1}{\tau}(f_\alpha - f_\alpha^{eq}), \tag{4}$$

where τ is the single relaxation time coefficient and f_α^{eq} is the local equilibrium distribution function. Combining the two steps together gives the lattice Boltzmann equation (LBE)

$$f_\alpha(x + e_\alpha \Delta t, t + \Delta t) - f_\alpha(x, t) = -\frac{1}{\tau}(f_\alpha - f_\alpha^{eq}) + \frac{1}{2}\Delta t e_\alpha F(x, t). \tag{5}$$

The derivation of f_α^{eq} is listed in Appendix A, which is similar to the conduction of shallow water LBM model by Zhou (2004). The solution of f_α^{eq} is

$$f_\alpha^{eq} = \begin{cases} \frac{1}{2}\lambda cA + \frac{e_\alpha Qc}{2e^2}, & \alpha = 1, 2 \\ (1 - \lambda)cA, & \alpha = 3. \end{cases} \tag{6}$$

where λ is

$$\lambda = \frac{K_d}{\Delta t\left(\tau - \frac{1}{2}\right)e^2}. \tag{7}$$

2.2. Advection–dispersion equations

The solute transport and pollutant concentration variation in an open channel flow can be described by ADE. Advection describes the pollutant or solute particles moved from one place to another due to the local velocity of the water. In dispersion, solute molecules move from high concentration regions to lower concentration according to a dispersion coefficient K_d, proportional to the negative of the concentration gradient according to Fick's law (Garcia-Navarro et al., 2000). These phenomena can be described by the advection–dispersion equation. As the wetted area-averaged concentration is to be considered, a simple form of the 1D advection–dispersion model is (Holly, 1975)

$$\frac{\partial(cA)}{\partial t} + \frac{\partial(Qc)}{\partial x} = \frac{\partial}{\partial x}\left[K_d \frac{\partial(cA)}{\partial x}\right]. \tag{8}$$

The recovery of advection–dispersion equation is a well-known process and listed in Appendix B, which verified the accuracy of the conduction. Hence, the concentration is expressed as