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A lattice Boltzmann model for the non-equilibrium flocculation of cohesive sediments in turbulent flow

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ABSTRACT

Microflocs, which are the first-order aggregates of cohesive sediment, are formed during early-stage flocculation through random collisions in turbulent flow. This study proposes a numerical model to describe the non-equilibrium flocculation of cohesive sediments in homogeneous turbulent flows using the lattice Boltzmann method. The validity of the model is verified by analytical results. The influence of suspended sediment concentration and turbulence on the early-stage flocculation phenomena of cohesive sediments at the mesoscale is examined, and it is found that the number of microflocs increases with sediment concentration up to an optimum concentration of 2.0 kg/m^3, after which it decreases with sediment concentration. The mean settling velocities of the suspension sediments in the computational domain first increase with increasing shear rate, then decrease, and the optimum shear rate is approximately 17.6 s^{-1}. Additionally, the turbulence-induced flocculation process can have an influence on the turbulent flow.

1. Introduction

The rate of natural fine sediment aggregation depends on the fluid flow, sediment properties and concentration of the particles in suspension. There are three principle particle collision mechanisms: Brownian motion, turbulent shear and differential settling. Turbulent shears generated on coasts and in estuaries are recognized as having an influence on both the formation of cohesive sediment flocs and aggregate break-up (Winterwerp et al. [1]). McCave [2] finds that turbulence determines the maximum floc size in tidal waters. Tambo and Hozumi [3] show that the aggregate breaks up when the floc diameter is larger than the length-scale of the energy dissipating eddies. Flocculation is a dynamically active process that readily reacts to changes in estuarine turbulence. At low shear rates, the floc size increases with shear rate, whereas the opposite trend is expected at larger shear rates (Dyer et al. [4]; Winterwerp et al. [1]).

In high-energetic conditions at high suspension sediment concentrations, such as those encountered in many estuaries and coastal seas, Dyer [5] suggests that the floc size changes with suspension sediment concentration and turbulent shear. Experimental results and field studies indicate a strong dependence of flocculation on the suspension sediment concentration (Winterwerp [6]). The average floc size and settling velocity increase with increasing sediment concentration up to an optimum concentration, after which they decrease with increasing concentration. This optimum concentration varies between estuaries, ranging from 50 to 20,000 g/m^3 (Dyer et al. [7]; van Leussen [8]; Winterwerp [6]).

Although numerous theoretical analyses, experimental measurements and field observations exist on the turbulent-induced flocculation of cohesive sediments (Li and Logan [9]; Manning and Dyer [10]; Dyer et al. [7]; Dyer et al. [4]; Ha and Maa [11]), there are few numerical simulations due to the inherent complexities in the flocculation processes of cohesive sediments. Usually, numerical modeling of flocculation involves determining the particle collision frequency function and

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estimating the sediment distribution based on the Smoluchowski framework with principal assumptions (Winterwerp [12]; Lee et al. [13]; Maggi et al. [14]). A Lagrangian population balance equation to describe the time evolution of the floc size distribution is proposed to simulate the flocculation processes (Winterwerp [12]). Maggi et al. [14] successfully promote a modified method of changing the capacity dimension of fractal flocs during flocculation within a population balance equation. Other research in the literature investigates floc formation and breakup in simple shear flow by considering the hydrodynamic interactions between flocs and fluid through the discrete element method (Higashitani et al. [15]). However, the ways in which the flocculation is promoted at low shear stresses and the flocs are disrupted at larger shear stresses have not yet been described from a mesoscopic viewpoint. Furthermore, the method in which the suspension concentration affects the floc size and floc settling velocity during turbulence-induced flocculation requires further research.

Cohesive sediments have the potential to flocculate into larger aggregates or flocs. Cohesive material in a river inevitably aggregates into "microflocs", which, upon arrival in the estuary, aggregate into large "macrofloc". The small particle clusters (microflocs) are generally considered to be the building blocks of larger macroflocs (Stone and Krishnappan [16]), which are defined as a stable element and a first-order aggregate of cohesive sediment (Mikeš and Manning [17]). Therefore, the microfloc properties play an important role in the formation of macroflocs and the prediction of cohesive sediment transport. However, the lack of clear understanding of microfloc properties is a key gap in the current knowledge of the flocculation process.

This research primarily investigates the effects of suspended sediment concentration and turbulence on the non-equilibrium flocculation of cohesive sediments using a three-dimensional lattice Boltzmann (LB) numerical model (Zhang and Zhang [18]) for turbulence-induced flocculation, in which the hydrodynamics, attractive van der Waals forces and electrostatic repulsive force are considered to simulate the formation of microflocs. The LB method is widely used to simulate particle suspensions in fluids (Ladd and Verberg [19]; Cate and Portela [20]; Derksen and Sundaresan [21]), and such a simulation is performed for the collision and aggregation of various size particles and the growth of flocs in isotropic homogeneous turbulent flows. The effects of suspended sediment concentration and turbulence on the flocculation phenomena of cohesive sediments at the mesoscale are also examined.

2. Lattice Boltzmann model

2.1. The lattice Boltzmann method

The basic concept of the LB method is to represent fluid as a particle distribution function located at a lattice node. Fluid particles move to neighboring nodes at discrete time steps, colliding with other fluid particles. In the LB approximation, the fluid is described by a density distribution function $f_i(\mathbf{x}, t)$, which describes the number of particles at a lattice site $\mathbf{x}$, at time t, with the discrete velocity $\mathbf{c}_i$. The Boltzmann equation is used to solve for the collision-induced evolution of the fluid particle velocity distribution function:

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i(\mathbf{x}, t) = \Omega_i(f_i) \tag{1}$$

where $\Omega_i(f_i)$ is the collision operator. The subscript i, represents the directions toward which the particle may move.

The hydrodynamic fields, such as mass density ρ, momentum density $\mathbf{j}$, and momentum flux $\mathbf{\Pi}$, are moments of this velocity distribution:

$$\rho = \sum_i f_i, \qquad \mathbf{j} = \rho \mathrm{u} = \sum_i f_i \mathbf{c}_i, \qquad \mathbf{\Pi} = \sum_i f_i \mathbf{c}_i \mathbf{c}_i \tag{2}$$

where $\Omega_i(f_i)$ is the collision operator, which can be constructed by linearizing about the local equilibrium f_i^{eq}:

$$\Omega_i(f_i) = \Omega_i(f_i^{\mathrm{eq}}) + \sum_j \ell_{ij} f_j^{\mathrm{neq}} \tag{3}$$

in which the non-equilibrium function $f_j^{\mathrm{neq}} = f_j - f_j^{\mathrm{eq}}$ and $\Omega_i(f_i^{\mathrm{eq}}) = 0$.

Here we use the so-called D3Q19 topology, a three-dimensional cubic lattice with 19 velocity vectors. A suitable form for the equilibrium distribution of the 19-velocity model is:

$$f_i^{\mathrm{eq}} = a^{c_i} \left[\rho + \frac{\mathbf{c}_i \cdot j}{c_s^2} + \frac{\rho \mathbf{uu} : (\mathbf{c}_i \mathbf{c}_i - c_s^2 \mathbf{I})}{2c_s^4} \right] \tag{4}$$

where $c_s = \sqrt{c^2/3}$ is the speed of sound and c is the lattice speed, for which $c = \Delta x / \Delta t$ with Δx the lattice spacing, and the coefficients of the three speeds are $a^0 = \frac{1}{3}$, $a^1 = \frac{1}{18}$, $a^{\sqrt{2}} = \frac{1}{36}$.

ℓ_{ij} are the matrix elements of the linearized collision operator, which must satisfy the following eigenvalue equations (Ladd and Verberg [19]):

$$\sum_i \ell_{ij} = 0, \qquad \sum_i \mathbf{c}_i \ell_{ij} = 0, \qquad \sum_i \overline{\mathbf{c}_i \mathbf{c}}_i \ell_{ij} = \lambda \overline{\mathbf{c}_j \mathbf{c}}_j, \qquad \sum_i c_i^2 \ell_{ij} = \lambda_v c_j^2$$