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A 3D DEM-LBM approach for the assessment of the quick condition for sands

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Abstract

We present a 3D numerical model to assess the quick condition (the onset of the boiling phenomenon) in a saturated polydisperse granular material. We use the Discrete Element Method (DEM) to study the evolution of the vertical intergranular stress in a granular sample subjected to an increasing hydraulic gradient. The hydrodynamic forces on the grains of the sample are computed using the Lattice Boltzmann Method (LBM). The principal assumption used is that grains remain at rest until the boiling onset. We show that the obtained critical hydraulic gradient is close to that defined in classical soil mechanics. ***To cite this article: M. Mansouri et al., C. R. Mecanique 337 (2009).***

Résumé

Approche couplée DEM-LBM 3D de prédiction de la boulance des sables. Cet article présente un modèle numérique 3D pour évaluer le début de boulance dans un milieu granulaire polydisperse saturé. Le modèle est basé sur l'étude de l'évolution de la contrainte intergranulaire verticale à l'intérieur d'un échantillon granulaire soumis à un gradient hydraulique ascendant croissant. Cette contrainte est calculée moyennant la Méthode des Eléments Discrets (DEM). Les forces hydrodynamiques sur les grains sont calculées en utilisant la Méthode Lattice Boltzmann (LBM). L'hypothèse principale utilisée est que les grains restent immobiles tant que l'état de boulance n'est pas atteint. Le gradient hydraulique critique obtenu par le modèle est en bonne concordance avec celui défini en mécanique des sols classique. ***Pour citer cet article : M. Mansouri et al., C. R. Mecanique 337 (2009).***

Keywords: Granular media; Soils; Discrete elements; Lattice Boltzmann; Sand boiling

Mots-clés : Milieux granulaires ; Sols ; Éléments discrets ; Lattice Boltzmann ; Boulance du sable

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1. Introduction

Discrete element modeling of granular materials containing a liquid phase has received a great interest in recent years. In the case of non-saturated materials supplemental forces are added to model the liquid phase effects [1,2]. For saturated materials, the straining leads to fluid flow in the pores spaces, therefore a convenient fluid modeling is required in addition to discrete element modeling of grains. In the last decade, the LBM has emerged as a powerful tool to model fluid flows in complex geometries. This method has been recently coupled with DEM to study saturated granular materials [3,4]. In this work, we propose a simplified coupled DEM-LBM model to analyze the onset of the boiling phenomenon of a granular material. We focus particularly on the assessment of the critical hydraulic gradient that corresponds to the quick condition (the onset of boiling). As a first step, we construct a granular material sample, then we submit it to an upward hydraulic gradient, that is increased step by step until the limit value that triggers the boiling. To quantify this limit, which represents the critical hydraulic gradient, we analyze the evolution of the vertical intergranular stress under the increasing hydraulic gradient. This stress is computed at any time using DEM with including grain weights and hydrodynamic forces on grains computed by the LBM.

2. Sample construction

The Discrete Element Method (DEM) is used to construct a densely-packed sample of polydisperse spherical particles. We use the statistical model proposed by Voivret et al. to obtain a set of particle diameters according to the cumulative beta distribution [5]. This distribution has the advantage to be bounded on both sides and capable of representing double-curved distributions similar to the soil grain-size distributions encountered in practice. We use the reduced diameter $d_r = \frac{d-d_{\min}}{d_{\max}-d_{\min}}$ where $d \in [d_{\min}, d_{\max}]$ and $d_r \in [0, 1]$. The size distribution is given by $\beta(d_r) = \frac{1}{B(a,b)} \int_0^{d_r} t^{a-1}(1-t)^{b-1}\,dt$, where $a > 0$, $b > 0$, Γ is the Gamma function and $B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$.

Once the diameters are generated, the particles are placed on a regular grid in a rectangular column as a dilute sample, and deposited under gravity. The following procedure is used: The force $\mathbf{F}$ between two grains has a normal component $\mathbf{N}$ and a tangential component $\mathbf{T}$ due to friction. For the force law between a pair of particles i and j in contact, we use the linear-elastic approximation: $\mathbf{N} = (-k_n\delta + 2\alpha\sqrt{mk_n}\dot{\delta})H(-\delta)\frac{\ell}{\|\ell\|}$, where $\delta = \|\ell\| - \frac{1}{2}(d_i + d_j)$ is the gap or the overlap between the two particles, ℓ is the branch vector, H is the Heaviside function, k_n is the normal stiffness, $m = \frac{m_i m_j}{m_i + m_j}$ is the reduced mass and $\alpha \in [0, 1]$ is a damping parameter which controls energy dissipation due to inelastic collision. Since we are interested in the equilibrium state, the parameter α has a very weak influence on the final results, but high values of α reduce the simulation time. For the friction, we use the simple Coulomb law expressed as a non-linear relation between the friction force $\mathbf{T}$ and the sliding velocity $\dot{\delta}_t$ with a viscous regularization around the zero velocity: $\mathbf{T} = -\min\{\eta\|\dot{\delta}_t\|, \mu_f\|\mathbf{N}\|\}\frac{\dot{\delta}_t}{\|\dot{\delta}_t\|}$, where η is the tangential viscosity and μ_f is the coefficient of friction.

Once the sample deposited, the average stress tensor in a control volume V can be expressed as:

$$\sigma_{rs} = \frac{1}{V}\sum_{c=1}^{n_c} N_r^c l_s^c \tag{1}$$

where $r, s = 1, 2, 3$, c is the contact label, n_c is the total number of contacts in the volume V, N_r^c is the r component of the contact force N^c and l_s^c is the s component of the branch vector ℓ^c.

3. Modeling of the fluid flow and the fluid–grain interaction

3.1. Modeling of the fluid flow

The Lattice Boltzmann Method (LBM) is a powerful tool for the computation of fluid flows. This method was proposed for the first time in the 1980s and is based on general lattice gas modeling techniques. LBM can be described as a time-stepping Eulerian micro-particle based procedure. Hence, the fluid is modeled as particles moving on a fixed regular grid. An interesting point of LBM with respect to the conventional computational fluid dynamics methods lies in its ability to take into account complex fluid domains without extensive computation time. Although the LB scheme used in this work is 3D, it is easy to present an illustrative 2D formulation.

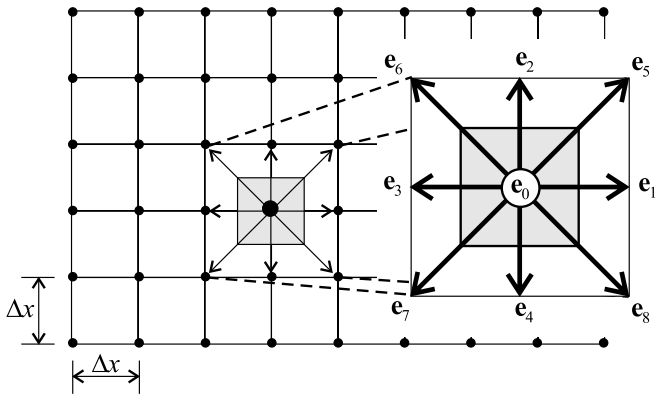

Fig. 1. Discretization of the flow domain according to the D2Q9 scheme.

We consider a 2D fluid flow within a rectangular domain (Fig. 1), with fluid density ρ and kinematic viscosity ν. First, the domain is discretized into a finite number of sites (nodes) that are located on a regular grid (lattice). The fluid particles located at each node can naturally move in all directions, however it is assumed that the number of velocities of motion is finite so that fluid motion is possible only through prescribed paths going from one site to another. Hence the fluid mass density at each node can be understood as a sum of partial densities corresponding to the discrete selected velocities. The time is divided into increments Δt so that at each time step, the particles located at all nodes move to the neighboring nodes along the corresponding directions, therefore we define the lattice speed of the model as $c = \frac{\Delta x}{\Delta t}$.

The most common 2D LB discretization is the so-called D2Q9 model (2 dimensions, 9 velocities). In this scheme, fluid particles at each site can move to the 8 nearest neighboring nodes with the velocities $\mathbf{e}_i$ $(i = 1, \ldots, 8)$. A site may include particles at rest that are associated to a zero velocity denoted $\mathbf{e}_0$. We note $f_i(\mathbf{x}, t)$ $(i = 0, \ldots, 8)$ the mass density distribution of the particles moving in direction $\mathbf{e}_i$, at time t and position $\mathbf{x}$.

During each time step Δt, the particles located at all nodes move to the neighboring nodes along the corresponding directions, where collisions occur and new particle distributions take place. The change of the density distributions before and after collisions is usually computed through the single relaxation time approximation (BGK kinetic model). In this way, computationally, there are two operations at each time step, namely "streaming and collision". Let $f_i^{\text{in}}(\mathbf{x}, t)$ be the distribution of incoming particles to the site $\mathbf{x}$ at time t^- and $f_i^{\text{out}}(\mathbf{x}, t)$ the distribution of outgoing particles from the site after collision (at time t^+). The algorithm works as follows:

- Collision operation (after BGK model):

$$f_i^{\text{out}}(\mathbf{x}, t) = f_i^{\text{in}}(\mathbf{x}, t) - \frac{1}{\tau}\left(f_i^{\text{in}}(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{u}, \rho)\right)$$

  The parameters τ and f_i^{eq} are defined below.
- Streaming operation:

$$f_i^{\text{in}}(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i^{\text{out}}(\mathbf{x}, t)$$

The parameter τ is the dimensionless relaxation time and the f_i^{eq} $(i = 0, \ldots, 8)$ are the equilibrium distribution functions that depend on the macroscopic variables ρ and velocity $\mathbf{u}$ at position $\mathbf{x}$ and time t.

For the D2Q9 model, the equilibrium functions are:

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

where w_i is a weighting factor given by: $w_0 = 4/9$, $w_i (i = 1, \ldots, 4) = 1/9$ and $w_i (i = 5, \ldots, 8) = 1/36$.

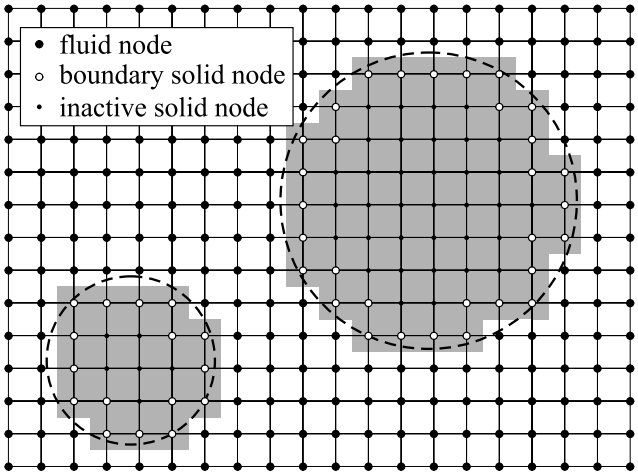

Fig. 2. Discretization of a domain containing the fluid and solid particles.

The macroscopic fluid variables are obtained from the moments of the distribution functions:

$$\rho = \sum_{i=0}^{8} f_i; \qquad \rho \mathbf{u} = \sum_{i=0}^{8} f_i \mathbf{e}_i \tag{2}$$

The fluid pressure field p is related to the fluid density by $p = c_s^2 \rho$, where c_s is the speed of the sound of the model given in terms of the lattice speed c as $c_s = \frac{c}{\sqrt{3}}$. Note that, in the LBM the fluid viscosity is implicitly taken into account through τ. So the kinematic viscosity is expressed as: $\nu = \frac{1}{3} c \Delta x (\tau - \frac{1}{2})$.

The general solution of the flow problem (pressure and velocity fields) can be obtained from Eqs. (2) after computing the distribution functions f_i at all nodes and at each time step. In the LBM, the boundary conditions cannot be imposed directly since pressure and/or velocity are not explicit variables in the formulation but rather outcomes of the calculation. Hence, equivalent conditions in terms of distribution functions f_i are used. The boundary conditions used in this work are described briefly in the next sections. Details about the boundary conditions topic in the LBM can be found in [6].

3.2. Modeling of the fluid–grain interaction

A domain containing a fluid and solid particles (grains) can also be discretized into nodes located on a regular lattice (Fig. 2). Therfore a solid particle is represented by a set of grouped squares and its boundaries are stairshaped. We call "fluid nodes" the lattice nodes that are occupied by the fluid and "solid nodes" the nodes that are occupied by the grains. The interaction between the fluid and a solid particle is done only through the boundary solid nodes (white nodes in Fig. 2). The internal solid nodes are not taken into account in the computation process and called "inactive nodes".

On grains boundaries the non-slip condition of the fluid should imposed. The simplest way to accomplish this in the LBM is to use the standard bounce-back rule, which means that any incoming fluid particle from a fluid node to a solid boundary node will be reflected back to the node it comes from. Note that this condition implies that the boundary is set halfway along the links between fluid and boundary solid nodes. For moving solid particles the bounce back rule should be modified to take account of the boundary motion.

The hydrodynamic forces acting on grains are computed using the momentum exchange method proposed by Ladd [7]. The fluid particles that are bounced back on grain boundaries transmit forces to the grain proportionally to their momentum change. The implementation of this method is straightforward since particles momenta are known at each time step. The total hydrodynamic forces exerted on a solid particle are obtained by summing up the forces on all boundary nodes of that particle.

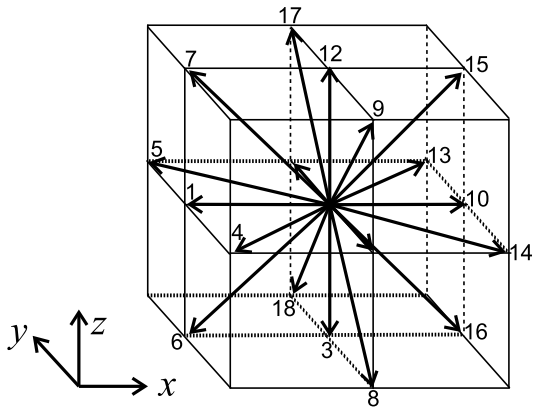

Fig. 3. D3Q19 Lattice Boltzmann model.

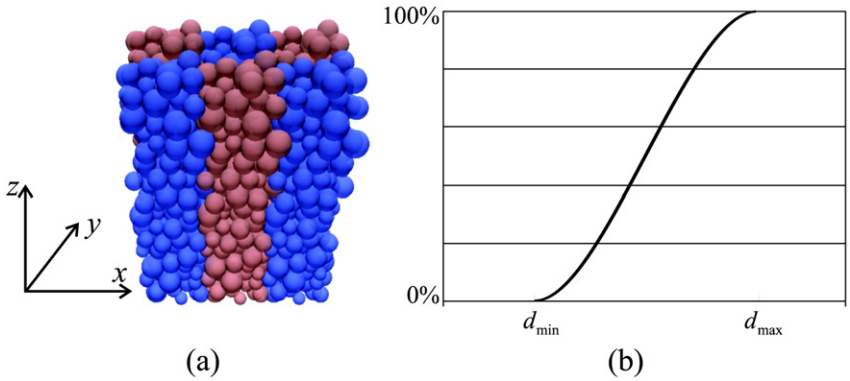

Fig. 4. Polydisperse deposited sample: (a) successive periods with alternating colors in x and y directions, (b) grading curve.

4. The 3D modeling and boiling state assessment

4.1. The 3D LBM model used

The sample is discretized into a three-dimensional array of identical small cubes whose centers are the lattice nodes, hence a solid particle is represented by grouped cubes (Fig. 3). Three types of boundary conditions are considered: periodic, non-slip and pressure condition. In both horizontal directions, periodic conditions are imposed so that nodes of opposite boundaries are treated as neighboring. Therefore, the outgoing distributions f_i at each boundary are reinjected at the opposite side in the streaming operation. On the sphere-fluid boundary nodes, the non-slip condition is imposed. To drive an upward flow in the sample the horizontal lower and upper boundaries are subjected to a pressure difference. To this end the Zou & He pressure boundary condition [8] is used in both boundaries. This consists in imposing a change of density and computing the distribution functions that satisfy similar equations to Eqs. (2) corresponding to the 3D model.

4.2. Boiling state assessment

We generate polydisperse random close-packed samples by the DEM with periodic boundaries in both horizontal directions (Fig. 4a). The sample is composed of spherical particles with diameters that follow the cumulative beta distribution (with $d_{max} = 2d_{min}$, and $a = b = 2$). The grading curve is shown in Fig. 4b.

After deposition, the sample is subjected to an upward gradually increasing hydraulic gradient while considering that grains are at fixed positions. The hydrodynamic forces acting on the grains are computed for each hydraulic gradient. To assess the boiling state under the upward flow, we study the evolution of the vertical intergranular stress

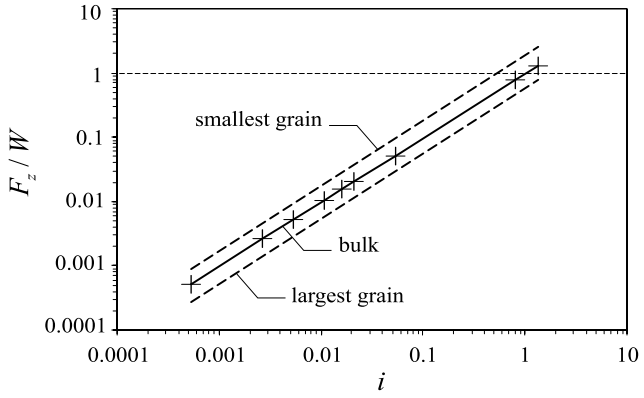

Fig. 5. Hydrodynamic forces vs. hydraulic gradient.

σ_{zz} in the sample with the increasing hydraulic gradient. The vertical intergranular stress σ_{zz} is computed using DEM (Eq. (1)), for each applied hydraulic gradient by taking into account the corresponding hydrodynamic forces and grain weights.

Note that the assumption of fixed-position grains used in computing hydrodynamic forces can be accepted as long as the boiling state is not reached.

In the following, we use a sand sample of 200 spherical grains with grain diameters in the range 0.4–0.8 mm. The grains are represented with sufficient resolution; grain diameters are represented at least by 16 nodes (Lattice Boltzmann nodes). The density of grains ρ_s is set to 2600 kg/m^3 and the fluid properties (water) are set to 1000 kg/m^3 for density (ρ_w) and to 10^{-6} m^2/s for kinematic viscosity. The acceleration of gravity is $g = 9.81$ m/s^2 (opposite to the z positive direction).

The fluid pressure differences Δp applied between inlet and outlet of the sample are varied from 0.333×10^{-1} to 0.833×10^2 N/m^2. Note that this last value causes a total vertical hydrodynamic force (sum for all grains) that can exceed the total weight of the sample. For this reason, we did not consider higher values (see Fig. 5).

The average hydraulic gradient can be defined from the applied pressure as: $i = \frac{1}{\gamma_w}\frac{\Delta p}{\Delta L}$, where ΔL is the sample length (measured in the direction of flow), $\gamma_w = g \times \rho_w$ is the water unit weight.

Fig. 5 shows the evolution of the hydrodynamic forces acting on the grains with increasing hydraulic gradient. The forces are normalized with the weights of the corresponding grains. The middle line represents the total vertical force normalized by the sample weight. This figure shows that the forces are proportional to the applied hydraulic gradient. Although not all grain forces are shown, this was confirmed for all grains. This result is expected since the sample pores and fluid velocities are small, therefore the flow is laminar and the fluid incompressibility assumption used in the LBM formulation is valid for all applied pressures.

This result is important from a numerical viewpoint for computing the intergranular stress with the DEM, since it shows that we can increase hydrodynamic forces proportionally to the applied pressure, without recalculating them at each step.

In the following, the sample is divided vertically into five control slices, in which average vertical intergranular stress are computed for each increment of the hydraulic gradient. Fig. 6 shows the evolution of the normalized vertical stress in the centers of the five slices with increasing hydraulic gradient. These stresses are obtained by dividing average vertical stresses computed from Eq. (1) by the vertical stress at the bottom of the sample. On this plot we can see that the average vertical intergranular stress in all slices decreases linearly with increasing hydraulic gradient until a limiting value, beyond which the intergranular stress becomes fluctuating around an approximately constant low value that is independent of the depth in the sample. This limiting value of the hydraulic gradient corresponds to the beginning of the motion of grains which can be undestood as the boiling onset, therefore this defines the *critical hydraulic gradient* (i_c).

As mentioned above, the plot shows that after the boiling onset the intergranular vertical stress becomes very low and approximately uniform in all the volume of the sample. This final stress cannot be zero because the hydrodynamic forces distribution in the sample creates convergent motions between some grains which leads to continuous collisions during boiling.

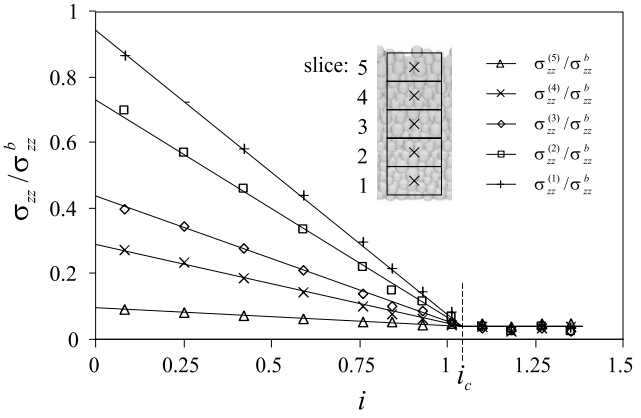

Fig. 6. Intergranular vertical stress vs. hydraulic gradient.

From the plot, the critical value of the hydraulic gradient can be estimated as the point of intersection of the lines corresponding to the fives slices. In the present case, it is about $i_c = 1.040$.

In classical soil mechanics, the critical hydraulic gradient is defined on the basis of the effective stress concept [9]. It corresponds the state where the effective stress vanishes under an upward hydraulic gradient, which leads to the expression $i_c = \frac{(\rho_s - \rho_w)(1-n)}{\rho_w}$ where n is the porosity of the sample. Using this expression for $n = 0.349$ that corresponds to the sample average porosity, leads to the critical hydraulic gradient value $i_c = 1.042$. Note that the sample average porosity is obtained in our case numerically as the ratio of the fluid LB nodes to the total number of LB nodes in the model.

It is clear that the obtained values of the critical hydraulic gradient with the numerical model and the classical formula are very close (1.040 and 1.042).

5. Conclusions

A simplified coupled 3D DEM-LBM model was introduced in view of studying the boiling onset of sand sample composed of polydisperse spherical grains. The model is capable to give the stress distribution in the bulk of a granular material subjected to a fluid flow for low hydraulic gradients up to the beginning of instabilities like boiling for example. Therfore it is capable to define the critical state of the beginning of instability. A comparison on the critical hydraulic gradient was made with a classical formula. It showed that the computed value is very close to the classical one. This result provides a sound basis for further applications of the coupled 3D DEM-LBM method to study the dynamic behavior of saturated sands.

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