



Contents lists available at ScienceDirect

Particuology

journal homepage: [www.elsevier.com/locate/partic](http://www.elsevier.com/locate/partic)



## CFD–DEM simulation and experimental investigation of the flow behavior of lunar regolith JSC-1A

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### ARTICLE INFO

#### Article history:

Received 27 January 2017

Received in revised form

10 November 2017

Accepted 8 December 2017

Available online xxx

#### Keywords:

CFD–DEM simulation

Flow behavior

Lunar regolith JSC-1A

Experiment

### ABSTRACT

Rovers on Mars and the Moon analyze the local geology by collecting samples of the upper layer in containers and ovens. After the analysis, the complete discharge of samples from the reservoir must be ensured. Because of the low atmospheric pressure, reduced gravity, and different grain shapes of the bulk material, the discharge process is very different compared to that on Earth. In this study, the behavior of lunar regolith JSC-1A in closed containers during discharge was investigated by analyzing the flow in an hourglass under the Earth's atmosphere. Reproducible fluidization of the top particle layer was observed during the outflow of the upper half of the hourglass. These particles were fluidized by the displacement flow initiated by falling particles in the completely closed container. This complex problem was simulated by coupling computational fluid dynamics (CFD) with the discrete element method (DEM). A CFD–DEM simulation with 1 million particles was performed. Because billions of particles are present in the actual system, the use of a coarse graining approach was required. In addition, high-speed camera measurements were used to determine the velocities of individual particles to validate the simulation. The fluidization effect was successfully simulated using the coupled method.

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### Introduction

In recent decades, the exploration of celestial bodies has rapidly developed. However, missions to the Moon and Mars have proven challenging for engineers and scientists because the material properties are often completely different owing to the different physical environments. Corrias, Licheri, Orrù, and Cao (2012) described the optimization of the in situ self-propagating high-temperature process for fabricating lunar construction materials, and He (2010) characterized lunar regolith simulants. However, further studies pertaining to bulk material characteristics on other celestial bodies are scarce in the scientific literature. Autonomous aerospace rover and robots such as the Mars Science Laboratory (“Curiosity”) are used to explore the atmosphere, radiation, and geology of extraterrestrial celestial bodies. All rovers are equipped with various analytical instruments. Small excavator booms are often used to extract a sample of rocks and regolith, which make up the upper dust layer, for the analysis of geological samples. For some analy-

sis methods, the sample is placed into a container or small oven, where it is heated to investigate the released gases. After the heating process, it is critical to ensure that the contents of the sample container are completely discharged. If material remains in the container, further tests may not be feasible. In the worst case scenario, a complete blockage of the container or device could occur, preventing any further investigation and leading to an interruption of the mission. The discharge of the excavator bucket as well as the filling and discharge of the container are critical steps in ensuring the safe functionality of the rover.

Appropriate container design strongly depends on the bulk material behavior. In this study, a substitute material with the same properties as the regolith on the Moon was employed. Astronauts involved in the Apollo Program collected soil and regolith on the surface of the Moon and brought it back to Earth. This material was characterized by a very rough appearance because the grains were not rounded by erosion as they would be on earth. Only impacts from asteroids, radiation, and temperature formed their shape. Consequently, the material behavior differed from that of sand found on Earth with the same grain size. NASA developed the material “JSC-1A”, which has the same bulk density, friction, grain size distribution, and shape as lunar regolith (McKay, Carter, Boles, Allen, & Allton, 1994) for this reason. This material has been used for

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further investigations. On Earth and several larger celestial bodies, the atmosphere cannot be neglected when studying the dynamic behavior of fine powders and bulk material. Reiss, Hager, Hoehn, Rott, and Walter (2014) investigated the bulk material discharge of lunar regolith in an hourglass during parabolic flights. Fluidization was observed in the top particle layer and occurred under varying atmospheric pressure and gravity. During the fluidization, the air-flow decreased the inner pressure of the bulk material and reduced the density of the particle phase, causing the particles to move away from each other. The inner friction of the bulk material was reduced because of the diluted particle bed, leading to an increased air flow rate. The fluidization was reproducible; however, the point in time at which particles were fluidized varied as a stochastic value in the experiments. At low pressure, the fluidization effect was no longer observed. The experimental tests conducted by Reiss et al. (2014) under varying gravitational conditions were extremely difficult and expensive, and different gravitational effects can be easily considered using simulations. Hence, several research groups, including Kuang, LaMarche, Curtis, and Yu (2013) and Metzger, Smith, and Lane (2011), are working to develop a simulation model of the flow behavior of lunar regolith. The aim of this study was to adapt the previously presented methods and use a coupled simulation to reproduce the observed effects of the bulk material flow in a simulation.

This study focuses on the described fluidization behavior that occurs owing to particles falling in a closed container and thus displacing the particles in the upper layer. The bulk material and air flow were simulated by coupling the discrete element method (DEM) and computational fluid dynamics (CFD). This problem has a high numerical complexity because a dynamic flow boundary condition (e.g., the inlet–outlet condition) is not defined from outside the system; the flow velocity is directed against the particle flow, and also driven by the displacement of the particle volume. The particle and air flows are strongly coupled; therefore, the solver must adapt to a very stiff system. The flow rates that occur are only dependent on the movement of the falling particles. These constraints exceed the limits of most other conventional multiphase simulation methods, e.g., the discrete particle method (DPM). CFD–DEM simulation is a promising method to simulate both the interaction between particles and their bidirectional effect on the fluid phase. Recently, CFD–DEM simulations have been increasingly applied to engineering problems thanks to an increase in computational power (Brosh, Kalman, Levy, Peyron, & Ricard, 2014; Chen et al., 2015; Salikov et al., 2015). DEM is a meshless method in which the particles are considered free rigid bodies. Contact between the particles is considered by force vectors acting on the center of mass. CFD considers the fluid as a continuous phase by meshing the computational domain. The discretized fluid dynamic conservation equations are computed for each grid cell.

In the present work, a CFD–DEM simulation with one million particles was performed. In the real system, billions of particles are present; thus, coarse graining needed to be applied. In addition, high-speed camera measurements were used to determine the velocities of individual particles to validate the simulation method.

### Model, calibration, and computational details

Coupled CFD–DEM simulations constitute relatively new methods for the simulation of multiphase flow (Harris et al., 1996). Instead of pure DEM simulations (Müller & Tomas, 2014), the effect of the fluid phase is considered (Liu, Wen, Liu, Liu, & Shao, 2015). CFD–DEM computations are so-called four-way coupling methods (Crowe, 2005), meaning that

1. the fluid (continuous phase) affects the particles,
2. the particles affect the fluid flow,
3. the particle disturbance in the fluid locally affects the motion of other particles (an effect known as particle swarm), and
4. the particles can collide with each other and the walls.

The advantages of CFD–DEM simulations over other multiphase models, e.g., DPM simulations, are the direct consideration of particle–particle interactions and the flow modifications due to the swarm effect. In this section, the computational details of the CFD–DEM simulation are briefly described. Further details can be found in, Chen, Zhong, Zhou, Jin, and Sun (2012), Zhu, Zhou, Yang, and Yu (2007), and Saidi, Tabrizi, Grace, and Lim (2015).

### CFD–DEM

The continuity equation and the Navier–Stokes equations (momentum conservation) in modified form are the basis for calculating the flow of an isothermal incompressible fluid with particles:

$$\frac{\partial(\rho_f \varepsilon_f)}{\partial t} + \nabla \cdot (\rho_f \varepsilon_f u_f) = 0, \quad (1)$$

$$\frac{\partial(\rho_f \varepsilon_f u_f)}{\partial t} + \nabla \cdot (\rho_f \varepsilon_f u_f u_f) = -\varepsilon_f \nabla p + R_{f,p} + \nabla \cdot (\varepsilon_f \tau_f) + f, \quad (2)$$

where the index *f* denotes the fluid,  $\varepsilon_f$  represents the volume fraction occupied by the fluid,  $\rho_f$  represents the density of the fluid,  $u_f$  represents the velocity of the fluid, and  $\tau_f$  represents the stress tensor of the fluid.  $R_{f,p}$  represents the semi-implicit momentum exchange between the fluid and particulate phase, which is calculated for each cell and assembled from the particle-based drag forces. Finally, *f* denotes the explicit momentum exchange term.

In practice, if a large number of particles is simulated (as in the present case), a so-called non-resolved explicit approach is used (Di Felice, 1994). In this case, the particles are smaller than the computational grid used for the finite-volume method. Consequently, the particles are not resolved in the CFD simulation. The computation only considers their interaction with the fluid phase (e.g., momentum exchange and the resulting porosity) (Goniva, Kloss, Deen, Kuipers, & Pirkers, 2012).

The drag force in the examined multi-particle-fluid interaction system is considered using the drag model presented by Di Felice (1994). The force balance for a single particle in a fluid environment is

$$F_d - V \frac{dp}{dz} = V \rho_p g - F_c, \quad (3)$$

where *V*,  $\rho_p$ , *g*,  $F_d$ , and  $F_c$  are the volume of the particle, density of the particle, gravity, drag force, and contact forces, respectively. The term  $-\frac{dp}{dz}$  is the pressure gradient force, where *p* represents the fluid pressure.

In the absence of other particles, the drag force  $F_{d0}$  on a single particle is

$$F_{d0} = C_{d0} \frac{\rho_f u_{rel}^2}{2} \frac{\pi d^2}{4}, \quad (4)$$

where  $C_{d0}$ ,  $\rho_f$ ,  $u_{rel}$ , and *d* are the drag coefficient, fluid density, relative velocity, and particle diameter, respectively. For spherical particles, established correlations for the drag coefficient are available such as that proposed by Dallavalle (1948):

$$C_{d0} = \left( 0.63 + \frac{4.8}{Re^{0.5}} \right)^2, \quad (5)$$

which is an empirical function dependent upon the Reynolds number, *Re*.

According to Di Felice (1994), the effect of neighboring particles on the drag force experienced by a single particle may be considered

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