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NUMERICAL INVESTIGATION OF SCALING EFFECTS ON GRANULAR MATERIAL DYNAMICS

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Abstract.

We investigate by direct simulation the problem of scaling for a rectangular tank partly filled with granular material. The work is a step in a longer - term effort aimed to developing a mathematical model addressing coupled motions of ships in waves, having loose tanks wherein cargos in bulky form are transported. The developed discrete - particle fluid model is based on the "soft sphere" Molecular Dynamics method with nonlinear frictional forces. Material particles are considered at this stage as spherical (3mm) and dry. They can be translated or rotated in any direction. Simulation results for geometrically similar containers of three different sizes are presented, assuming horizontal harmonic vibration of the container. In another type of test is investigated the avalanching phenomenon of the free surface during slow tilting, in containers of different size. Preliminary conclusions are drawn about the influence of scaling on these motions.

1 INTRODUCTION

Materials in granular form (powders, sands, grains, metal ore etc.) are basically conglomerations of discrete and solid macroscopic particles (Brown & Richards 1970). Their behaviour is of great interest, since they can present the physical properties of two or more states of matter. Coulomb, Faraday, Reynolds, Brigadier Bagnold and other eminent scientists have set the foundations of this field. When a collection of grains form a pile in a container, it can be compared to a solid (static state). If the container is sufficiently tilted, the granular material starts to flow, resembling a liquid (dynamic state). Between these two states a granular assembly may experience a quasi - static state. For example, when the container is vibrated at a relatively high frequency, the grains rearrange themselves in the packing (decrease of volume). On the other hand, if the container is very strongly vibrated, the grains display free motion and the granular assembly behaves like a dissipative gas (Lumay et al, 2012). Subsequently, their handling often needs special attention.

Further to its scientific interest, granular matter's behaviour is of great practical significance. Statistics suggest that, 40% of the capacity of many industrial plants is wasted because of problems related to materials' transport (Ennis et al., 1994). Moreover, In the field of maritime transportation it is well known that, loose bulky material inside ship holds can become perilous (Spandonidis & Spyrou 2012). Cargo shift represents a major threat for ship safety and probably the most common cause of capsize of large ships. It is notable that more than 800 seamen lost their lives in the last two decades on bulk carrier vessels (INTERCARGO 2012). International regulations have been developed and they are regularly updated, aiming to control the method of transport of these materials and to specify testing techniques suitable for verifying that a certain cargo can be safely transported (IMO 2012). At the same time, computational methods have progressed and they can be potentially very useful for better understanding the behaviour of these materials and for creating more effective testing procedures.

In the current paper we present a computational method and some preliminary results on the problem of model scaling, that is faced in practice when one employs an apparatus of a certain small size for testing a granular cargo's suitability for transport. The dynamic behaviour of particles inside three geometrically similar rectangular containers is simulated. The containers are subjected to: a) horizontal vibration and b) tilting with a relatively slow angular velocity.

2 SIMULATION APPROACH

The calculation scheme is based on the method of Poeschel & Schwager (2005). Concerning the interaction force model, several options are available (Schafer et al 1996, Zhou et al 2001). Normally to the line of contact during collisions we have considered nonlinear elastic and frictional forces; while transversely we have assumed acting a purely frictional force (Figure 1). Granules were considered as smooth dry spherical particles with fixed diameters (3 mm) that can be translated or rotated on a vertical plane.

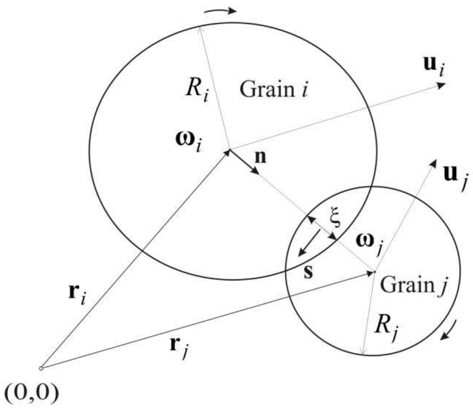

Figure 1 Grains penetration.

More specifically, for the normal force we adopted the dissipative Hertz - type force for viscoelastic materials proposed by Brilliantov et al (1996):

$$F_n = -k_n \xi^{3/2} - \gamma_n \xi^{1/2} \dot{\xi} \tag{1}$$

where γ_n is a damping constant connected to the radii of the spheres and the coefficients of bulk viscosity. k_n is a non-linear stiffness of a spring whose elongation is ξ (ξ = max (0, $R_i + R_j - |\mathbf{r}_i - \mathbf{r}_j|$)), the deformation of the grain, connected to the elastic properties (Young Modulus, Poisson ratio) and to the radii of the spheres. This model was originally developed for stiff particles as is the case of our investigation.

As for the transverse force, the following model by Haff & Werner (1986) was adopted:

$$F_t = -\min\left(|\gamma_s \cdot u_s|, |\mu \cdot F_n|\right) \cdot sign\ (u_s) \tag{2}$$

γ_s is shear damping constant; u_s is the shear velocity component that for a 2D case is expressed as:

$$u_s = (\mathbf{u}_i - \mathbf{u}_j) \cdot \mathbf{s} + \omega_i R_i + \omega_j R_j \tag{3}$$

μ stands for the dynamic friction coefficient and $\mathbf{s}$ is the unit vector that for spheres is along the perpendicular to the line of contact. Kuwabara & Kono (1987) argued that simulation results based on Equation 2 are in good agreement with experimental results when γ_s receives high values (e.g. 20 Ns/m). Particles' motions are governed by Newton's second law for translational and rotational motions.

Trajectory generation refers to the paths of a large number of particles and it is divided into three major steps: initialization, equilibration and production. Of the large number of available finite - difference schemes, Gear's (1971) predictor - corrector was used which is suitable for MD due to its numerical stability.

Verification of the code was based in conservation principles during both the initial equilibration and the subsequent execution of the code and on systematic error, while its validation involved comparison of characteristic obtained results with experimental data (Spandonidis & Spyrou 2013). The results are processed in order to assess the computed trajectories and we calculated the quantities that are representative of the targeted collective phenomenon (e.g. shift of cargo's centre of mass). For trajectory visualization we have used the open-source multi - platform ParaView 3.12 (Sawley et al, 2007) whose flexible and intuitive front - end graphical user interface (GUI) is amenable to complex and "fine – grained" data manipulation.

3 SIMULATION RESULTS

We consider a mobile, rectangular, smooth and rigid tank, filled partly by dry granular material. The origin of the coordinate system is placed at the left side of tank's bottom (Figure 2). Tank is free to move in any possible direction, depending on the desired excitation. Following Schafer et al (1996) and basically what is a standard practice, our tank walls are built of particles, to model surface roughness. Motion of the walls is prescribed and it can be periodic or random. Cellulose acetate spheres with diameter 3 mm were used. Table 1 summarizes the material properties.

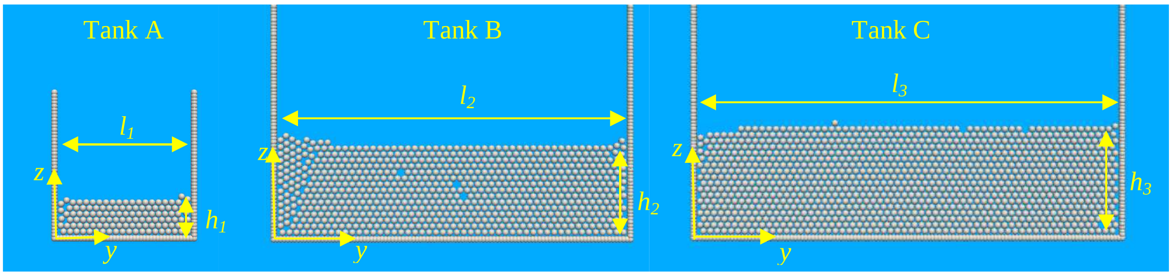

Figure 2. The origin of the coordinate system is placed at the left corner of each tank's bottom. The height-to-width-ratio h_i/l_i, $(1 \le i \le 3)$ is fixed to a constant value.

Three different tank configurations (tank A, B and C in Figure 4)) are used in order to investigate the scaling effects in the dynamic behaviour of the material. Tank widths are: $l_1 = 6\ cm$ for tank A, $l_2 = 15\ cm$ for tank B; and $l_3 = 18\ cm$ for tank C. The height-to-width–ratio was kept fixed ($h/l = 0.256$).

Two different simulation results per tank configuration are produced. Firstly, we monitored the movement of the granules' mass centre for various pure sway oscillations when harmonic external excitation is applied. A wide range of excitation frequencies and amplitudes was investigated (0 - 3.7 Hz and 0 - 4 cm, respectively). Based on these simulations, diagrams in comparative form are created for material's dynamical behaviour in the different tanks. Furthermore, in order to determine scaling effect on the *angle of repose*, that is the maximum slope angle of non-cohesive (i.e. free-flowing) granular material, we tested the response of the free surface under a certain rate of tilting, monitoring the initiation of avalanching.

Table 1. Numerical values for particle coefficients.

Parameter	**value**	**Parameter**	**value**
Diameter (*mm*)	3	Young modulus (N/m^2)	3.2×10^9
Density (gr/cm^3)	1.319	Coulomb friction	0.25
Poisson ratio	0.28	Shear damping (*N s/m*)	20

* Cellulose acetate particles

3.1 Horizontal motion under sway excitation

Although less investigated than vertical oscillation, a rich variety of interesting macroscopic phenomena such like convection, segregation and compaction appear when a rectangular tank, filled with granular material is shaken horizontally (Poschel & Rozenkranz 1997). Among all these phenomena what interests us is that of fluidization; that is the transformation of materials behaviour after a critical point of a system's variable (most commonly excitation frequency and amplitude) has been reached, from solid like to fluid - like behaviour. In Figure 3 are presented time instants of material's motion inside tank C (large) for a case where this critical point has been exceeded. In order to investigate differences between the dynamic behaviour of the same material inside different tanks, we performed a great number of simulations for each tank configuration varying the excitation frequency and amplitude. The displacement of material's mass centre both in y and z-axis were captured and graphically presented. In Figure 4 material's mass centre displacement inside tank C, for different excitation frequency and excitation amplitude 4 cm is depicted. There is a critical frequency value close to 1.2 Hz after which the material starts to behave almost like a fluid.

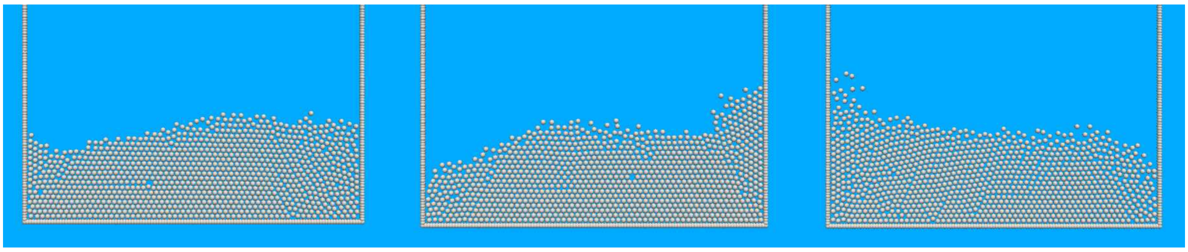

Figure 3. Motion of material inside tank C (excitation frequency 1.5 Hz). Left: time instant little after the beginning of the motion; middle: time instant when the maximum amplitude is reached for the first time; right: time instant after tank crosses the initial point for the first time.

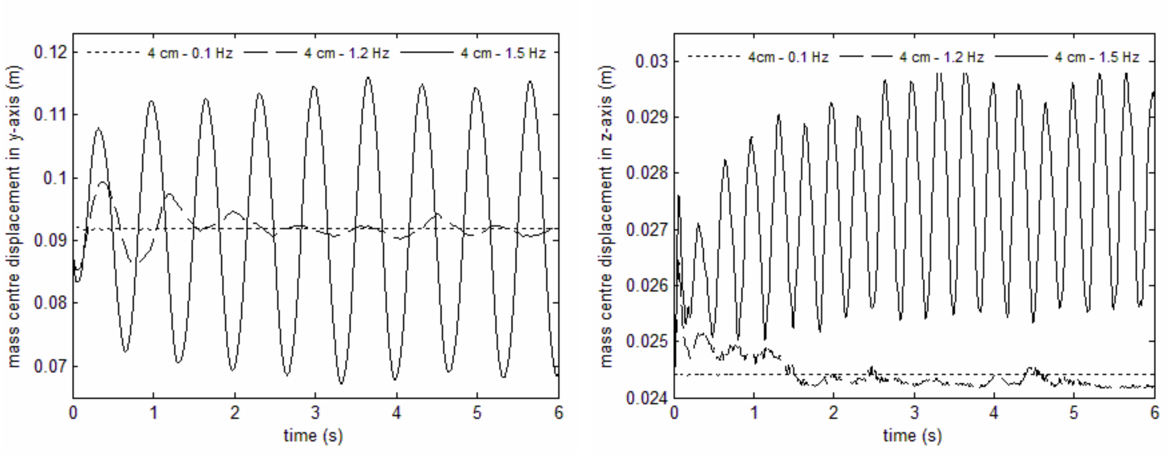

Figure 4. Horizontal (left) and vertical (right) movement of material's centre of mass inside tank C (18 cm width) under sway oscillation for three different excitation frequenc (excitation amplitude is 4 cm).

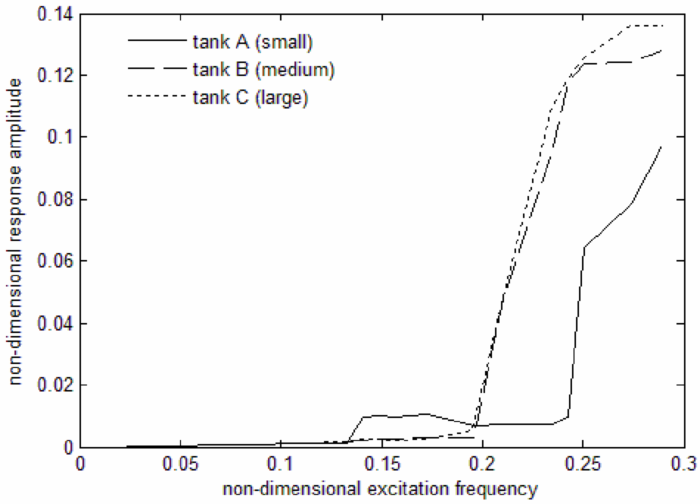

Figure 5. Mass centre response amplitude for various frequency and amplitude excitation values.

By working in a similar manner for more than 300 simulations (for the three tank configurations) we are able to demonstrate the dynamic behaviour of the material inside the tank in the frequency region near to the critical (bifurcating) point. In Figure 5 is shown the mass centre response amplitude y'_{0i} for various frequencies ω'_i. The prime indicates a non - dimensionalised quantity. The excitation amplitude n'_i had a fixed value for all cases. The scaling laws were as follows: $y'_{0i} = y_{0i}/l_i$, $\omega'_i = \omega_i\sqrt{l_i/g}$ and $n'_i = n_i/l_i$, $1 \le i \le 3$ (Lloyd 1989). For small values of excitation frequency the material moves with the tank, but for higher values it starts to flow. What is interesting is that tank's A bifurcating point is at a different place, in comparison to the other two tanks, inside which the material demonstrated almost identical behaviour. Another interesting observation is that, in the tank A there is a second critical point where some limited avalanching is realized, located at lower frequency. Mass centre's shift between these two critical points is relatively small. These observations lead to the suggestion that there must be a critical width, after which the material behaves in an almost identical manner; but before this width (smaller values) the material shows almost no difference in its behaviour. This difference is believed to be due to the fact that friction plays a more crucial role when the dimensions are small, but its role is not so important when the physical dimensions of the problem are large enough.

3.2 Slow tilting of the tank - angle of repose identification

Granular matter is often imagined in the form of a sandpile. Indeed the formation of sandpiles is not only an everyday experience but an event relevant to many practical applications also. Angle of repose is simply the maximum slope angle of non - cohesive (i.e. free - flowing) granular material and one of the most important macroscopic parameters, characterizing material's behaviour. An interesting challenge is to understand the dependence of avalanching when the critical angle has been reached; upon physical parameters of the system (e.g. moisture content, particle diameter, wall - particle friction etc) either by experimental (Dorbolo 2005) or by numerical (Maleki et al 2007) methods. It has been found that this angle strongly depends on material's properties such as particle density and size (Zhou et al, 2001) and also tank's depth (Zhou & Zhang 2009).

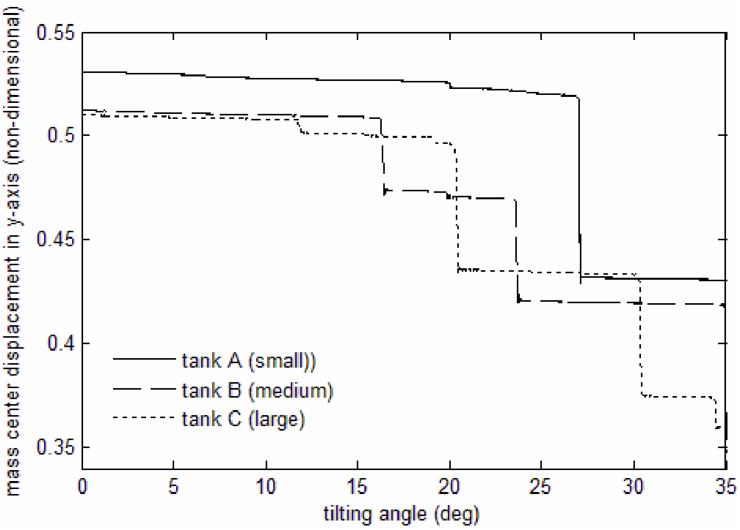

Figure 6 Displacement of material's centre of mass for a tilting rate 0.3°/s. Comparative study for three tank configurations. Sufficiently high tank walls are assumed.

The recommended from IMO test method for determining the angle of repose is the so called "tilting box method" which is suitable for non-cohesive granular materials with a grain size not greater than 10 mm. A standardized box (600mm long, 400mm wide and 200mm high) is filled with the material to be tested and the tilting mechanism is then activated, with rate of tilting approximately 0.3°/s. It is stopped as soon as the material begins to slide. Other common methods include measuring the angle of repose of a pile formed on a fixed bed or inside a revolving cylinder (Train 1958). Even though these methods are adequate for static angle of repose identification, they are largely empirical and many times predict contradictory results due to different angles measured (Liu et al 1991). Furthermore they cannot handle situations where the dynamic motion of the cargo is dominant.

Following the most common definition of angle of repose in the maritime field (IMO 2012) and considering that the critical angle has been reached only when the free surface starts to continually flow (thus excluding initial reordering of the free surface) we tilted the three different tanks with tilting 0.3°/s. In previous work (Spandonidis & Spyrou 2013) we have observed that the value of the angle of repose depends on side wall height and tilting rate. However this dependence is eliminated for slow tilting. Although not the customary practice, predictions seem to be more reliable when the test is performed for high enough side walls (also, this is a more realistic scenario). Figure 6 presents the displacement of the centre of mass along the y-axis, in accordance to the tilting angle, for the three tank configurations. As observed in Fig. 6, there is a slight initial centre of mass offset for all three tanks, owed to different free surface alignment which is a natural occurrence and thus no effort was made to remove it. As the tilting begins, and up to about an angle of 15^0, the particles on the surface show a tendency to be realigned. Also, a small hip is formed near to the wall that is furthest from the rotation axis (Spandonidis & Spyrou 2012). Then the material behaves like a solid, till a critical angle is reached. Suddenly the material behaves almost like a fluid but it soon returns again to a solid - like behaviour (stick slip behaviour); till the next critical angle is reached. In the two smaller tanks the material exhibits a stepped transition. We identified the first critical angle as the angle of repose although this is a matter to be further considered.

Following Lee & Hermann (1993) we repeated each numerical experiment 12 times, with slightly different initial free surface configuration (which also has been found to be crucial in angle of repose prediction) and then we calculated the predicted angle of repose for every tank. Each angle presented in Figure 7 is calculated mean angle over the 12 experiments and the error is the mean square sample-to-sample fluctuation. As noticed, there is a slight dependence of angle of repose on tank's width in the sense that the smaller the tank the larger the predicted value. In order to obtain safer results for this dependency more experiments (not only numerical but physical as well) have to be performed with larger tanks. In this way one could establish a critical width value beyond which every predicted angle is practically the same.

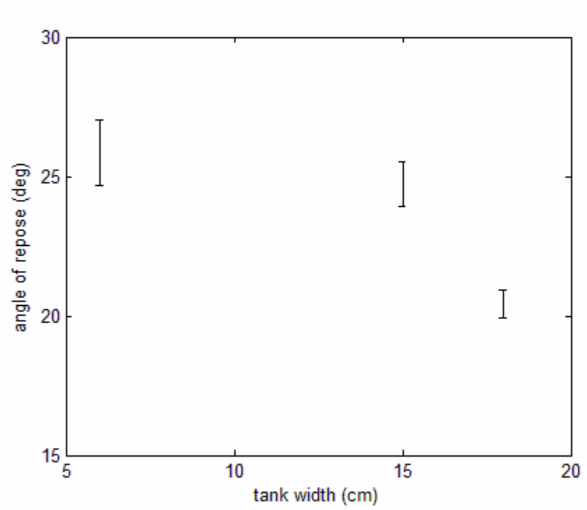

Figure 7 The angle of repose against the width of the tank when the height-to-width ratio is constant.

4 NEXT STEPS

Figure 8 Vibration test system installed at school of naval architecture and marine engineering, National Technical University of Athens.

Experimental reproduction of the performed numerical tests will be attempted in the next stage. A dedicated facility for investigating granular material and fluid dynamics in vibrated containers has been recently installed in our School, consisting of a shaking table that can be driven in six degrees of freedom (6-DOF). It is suitable for producing low frequency excitations like those produced on ship cargos under the effect of waves. Six input time histories are used to describe the desired motions of Roll, Pitch, Yaw, Surge, Sway, and Heave. The table's motions cannot exceed ±40 Degrees and ±0.5 Meters. A supplied Labview interface program reads or generates these time histories and computes the corresponding actuator motions to translate the table platform. Calibration/measurement of table's real motion is done by real time PID loops that control the six actuators and by the use of a table-mounted Miniature Attitude Heading Reference System (AHRS) with GPS (Microstrain 3DM-GX3-35) that reports to the main PC the exact position of the table at any time. A number of square base and cylindrical vessels with various dimensions is getting used. The vessels are made from Perspex of 5 mm thickness to permit direct observation.

Flow visualization is possible by the use of a high speed video system. This system consists of two high speed video cameras (Trouble-Shooter HR - color) with a resolution of 1280 x 1024 pixels and a maximum speed of 16,000 images per second that cooperate in a master/slave mode. A specialized software programme (MIDAS 4.0) is used for event-capture camera control, synchronization with data sources, and automated monitoring.

The use of two PCD-300B sensor interfaces working in a master/slave mode enables the main PC to perform up to 16 different stress and force, pressure, acceleration and displacement measurements through the use of strain gages and transducers, respectively. DCS 100A dynamic data acquisition software enables easy, interactive setting of measuring conditions and sensor information as well as monitoring of measuring data on numeric and various graph windows.

5 CONCLUSIONS

Scaling effects influencing the behaviour (from semi-static to dynamic) of granular matter, placed inside three geometrically similar small size containers were investigated at preliminary level. The investigation was based on simulations relying on the so called “molecular dynamics” method. Cellulose acetate spheres with diameter 3 mm were considering. The tanks were successively i) vibrated in sway assuming prescribed harmonic external excitation and ii) tilted with low tilting rates.

As far as horizontal vibration is concerned, the critical point after which the phenomenon of fluidization occurs was targetted. Observations lead to the suggestion that a critical size of container exists after which the material behaves in an almost identical manner irrespectively of container’s size. It is conjectured that friction plays a greater role in the smaller sizes, hence the apparent difference in the dynamic behavior.

Furthermore, tilting of the three tanks with a slow rate (0.3°/sec), in order to identify the critical angle where avalanching of material’s free surface appears, indicated that there is some dependence of this angle on tank’s width. Specifically, it was observed that the smaller tank leads to a larger critical angle. In order to obtain safer results for this dependency more tests should be performed with a much wider tank. In this way one could establish a critical width value beyond which every predicted angle is practically the same.

Of course, experimental reproduction for both the sway and tilting experiments will be required before the suggested dependency is considered as established pattern of the behaviour of the physical system under consideration.

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