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MODELING AND SIMULATION OF THE GRANULAR FLOW INSIDE THE PRESSURE VESSEL OF A SHOT PEENING MACHINE

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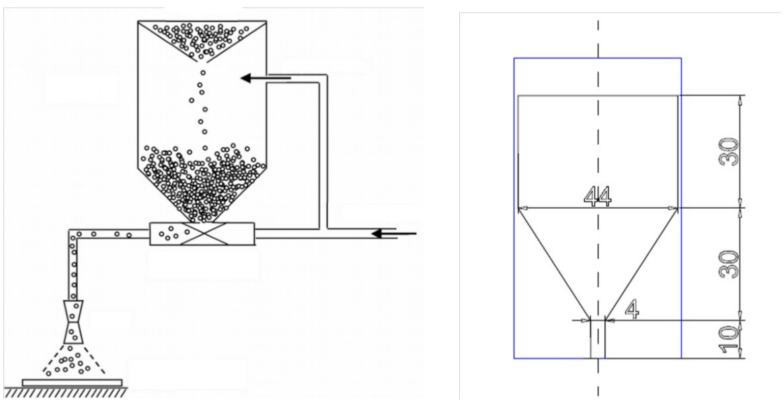
Abstract. *This article use the molecular dynamical approach to simulate the granular flow occurring inside the pressure chamber of a shot peening machine. The model was implemented with the aid of LAMMPS, a molecular dynamics simulation software. The microcanonical ensemble was used, with contact forces estimated by the theory of Hertz. The results were confronted with the flow predicted by Beverloo correlation, over a range of exit diameters. The molecular dynamics model proved to be very accurate, even without experimental data concerning the friction factor.*

Keywords: *granular flow, molecular dynamics, microcanonical ensemble, shot peening, LAMMPS.*

1. INTRODUCTION

Peen forming is a cold working process in which small metallic spheres are propelled by a line of compressed air towards the surface of the part to be shaped. The impacts of the shot against the surface give rise to a thin layer of residual stresses equivalent to a bending moment that keeps the part permanently deformed (Fathallah et al. 1996). Peen forming is widely used by the aeronautics industry, especially in the manufacture of wing skin panels integrated with stringers (Yamada et al. 2002).

In a pneumatic shot peening equipment, schematically illustrated in Fig. 1a, the particles accumulated within the pressure vessel, after passing through a dosing valve, flow along a pipeline towards a venturi nozzle, from where they are expelled as a jet impinging on the part. After the impact, the spheres are collected, submitted to a separation process to eliminate the fragments and returned to the pressure vessel. Figure 1b shows the dimensions, in centimeters, of the pressure vessel analyzed.



(a) (b)

Figure 1. (a). Pneumatic shot peening equipment. (b). Dimensions of the pressure vessel, in centimeters.

Along the process, very distinct granular flow regimes can be observed. Inside the pressure vessel a dense, quasistatic flow is observed. In this region, the main dissipation mechanism is friction, as the particles tend to maintain in contact with each other. In the pipeline, the velocity is much higher, as well as the average distance between particles. The main dissipation mechanism is impact, due to collisions being quite frequent between the particles and the wall, and between the particles themselves. Down-stream the venturi nozzle exit the flow evolves to a solid particulate jet.

This article focus exclusively on the quasi-static granular flow inside the pressure vessel. There are, however, numerous articles in the literature that explore other aspects of the peen forming process (Meguid et al. 1999, Wang et al. 2008, Kato et al. 2014).

2. GRANULAR FLOW MODEL AND SIMULATION

The peculiar physical behavior of granular flows has attracted the attention of researchers for a long time. As described in Sperl (2006), the experiments conducted by Janssen in 1895 in a corn grain storage silo showed that the outlet pressure was much lower than that which would be measured if the granular material had behaved as a liquid. Janssen concluded that this was due to the frictional forces between the corn and the inner wall of the silo. These frictional forces become so great that if the height of the column exceeds a certain threshold value, the pressure on the bottom of the silo remains practically invariant.

Attempts to predict the mass flow resulting from a granular flow with bulk density ρ_B, particle diameter *d,* exiting from an orifice with a diameter D, on a flat bottom silo showed that the curve seemed to be of the form presented in Eq. (1).

$$W = C * \rho_B * \sqrt{(g)} (D - kd)^{2.5} \quad (1)$$

showed that *C* falls between the range of 0.55 to 0.65. The *k* factor depends on the geometry of the particles, and for spheres it is known that *k=1.5.* Rose and Tanaka studied the influence of the angle of the walls, in the case of a conical hopper, and showed that in the case of a wall angle α and a repose angle ϕ, the flow can be adjusted with a simple factor, as shown in

The literature reports that experimental results Eq. (2).

$$W = C * \rho_B * \sqrt{(g)} (D - kd)^{2.5} (\tan\alpha \tan\phi)^{-0.35} \quad (2)$$

Jenicke and Johanson (1969) made a series of experiments to investigate the two types of granular flow that can arise in the convergent region of a storage silo: 'funnel flow', when occurs partial stagnation of the granular material close to the walls, and 'mass flow', in case all particles keep moving. The analytical model developed by these authors allows determining the conditions for one of the two types of flow to be established. Furthermore, they arrived at an algebraic equation that calculates the particle velocity field in mass flow regimes.

Although the above referred empirical and analytical models are capable of identifying relevant physical characteristics of quasi-static granular flows, they are not able to provide accurate velocity and pressure fields, since they rely on many simplifying assumptions. For this reason, numerical models based on different approaches have been proposed in an attempt to investigate this class of flows (Patankar and Joseph, 2001; Cleary and Sawley, 2002).

One of the techniques that can be applied to simulate granular flows is the so-called molecular dynamics (MD) (Haile, 1997). In this computer simulation paradigm, a very efficient algorithm (Verlet's algorithm, for instance) is used to simultaneously integrate a large set of second order differential equations representing the dynamical behavior of the system according to Newton's second law. During the simulation, particles are individually followed on a Lagrangian basis, and the system phase point $P(x_1, y_1, z_1, \dot{x}_1, \dot{y}_1, \dot{z}_1, \ldots, x_N, y_N, z_N, \dot{x}_N, \dot{y}_N, \dot{z}_N)$ gradually traverses the 6N-dimensional system phase space. Admitting the validity of the ergodic hypothesis, it is expected that P will eventually assume all possible micro-states of the system. Thus, the statistical mechanical framework (Schwabl and Brewer 2006) can be used to determine the macroscopic properties of the granular flow. MD simulations are performed in the micro-canonical, or NVE ensemble, as suggested by the work of Edwards (1989).

The use of equilibrium ensembles to represent granular systems may not seem fit at first sight. After all, due to their characteristic meta stability, they are intrinsically out of equilibrium. However, the slow flow of particles can be seen as a succession of jammed states. Edwards then proposed that each jammed state is equally probable in the volume ensemble, and thus can be treated by the same method proposed by Gibbs in his statistical mechanical theory.

The crucial step is setting the variables, as those used by Gibbs are not suitable for granular systems, as friction is a dissipative mechanism. On the other hand, the volume is clearly one of the state variables, and is a function of each of the *N* particles positions r_i and orientations $\hat{t}_i$. We can thus define a volume function $W = W(r_i, \hat{t}_i)$ as a replacement for the Hamiltonian in the equilibrium ensembles. The temperature-like parameter is called by Edwards *compactivity,* and is defined as a measured of how much the material can be compressed. Fluffy powders will have a high compactivity, and compact packings will have a low compactivity.

Edwards also defines the jammed meta stable state, expressing it analytically, so a statistical mechanical approach to granular matter can proceed by analogy with equilibrium systems. The jammed state then becomes a constraint satisfaction problem, governed by the non overlaping principle, the force balance, torque balance, Coulomb friction, repulsive forces and Newton's third law (Baule et. al. 2018).

In our model, the forces of contact f_a are that predicted by the Hertz-Mindlin theory (Deresiewicz, 1958). When two nonconforming solids are brought into contact they touch initially at a single point or along a line. Due to elasticity, they deform around their first point of contact so that they touch over a small finite area. In the simplest case, of two identical spheres of radius R compressed statically by a force N directed along the line formed between the centers, the contact area is circular. Deresiewicz (1958) shows that the radius *c* of the contact area is also dependent on the Poisson's ratio *ν* and the Young's modulus of the material *E,* as shown in Eq. (3) and Eq. (4).

$$c=(\vartheta N R)^{\frac{1}{3}} \tag{3}$$

$$\vartheta=\frac{3(1-\nu^2)}{4E} \tag{4}$$

As shown in Zhang and Makse (2005), the normal compressive contact force between two spheres can be given by Eq. (5).

$$F_n=\frac{2}{3}k_n R^{1/2}\gamma^{3/2} \tag{5}$$

where γ is the overlap between the spheres, and the effective stiffness k_n is defined in terms of the shear modulus *G* and Poisson's ratio *ν* of the granular material, according to Eq. (6).

$$k_n=\frac{4G}{1-\nu} \tag{6}$$

The tangential forces are given by Eq.(7).

$$\Delta F_t=k_t(R\delta)^1/2\Delta s \tag{7}$$

The normal forces are completely determined by the geometrical configuration of the packing. In this model, the tangential elastic constant is given by Eq. (8).

$$k_t=\frac{8G}{2-\nu} \tag{8}$$

Given the forces acting on each particle – gravity and contact forces – a Verlet algorithm (Haile, 1997) then use the information from current and previous time steps to evolve the system in time.

The software tool adopted to implement the model and perform the simulations was LAMMPS, a open source code developed by Sandia National Laboratories (https://www.sandia.gov/), initially for MD, and later extended to include the granular models.

Before starting simulation it is necessary to define the system initial kinematic state, i.e., the position and velocity of every particle, as well as the flow boundary conditions. Since the system is considered ergodic, any initial kinematic conditions will lead to the same final statistics. Nonetheless, it is common practice to use the vertices of an infinite grid, called 'simulation box', as the loci of the initial particles positions and to attribute null initial velocities for everyone. It is important to stress that periodic boundary conditions are set up for all the simulation box *x, y, z* axes and that the initial positions of the particles are randomly selected by choosing vertices of the box located in a certain 'insertion region' defined *a priori*. To complete this pre-simulation phase, the limiting surfaces of the flow are defined from the geometry of the storage chamber and suitable mechanical properties are assigned to its walls.

Under the effect of gravity, the initial kinematic state previously described does not correspond to an equilibrium condition. However, once the run starts, equilibrium will eventually be reached after a finite time interval. Ercolessi (1997) stresses that one should always wait for the system to reach statistical equilibrium under clean constant energy conditions before collecting data. During the simulation of the flow focused in this article, the total energy of the system was stabilized after the execution of about 75000 integration cycles (Fig.2).

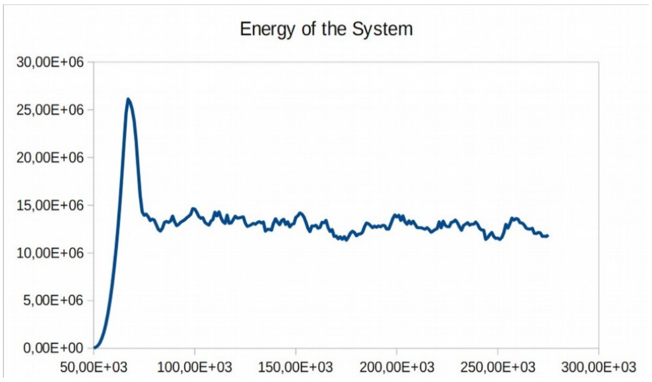
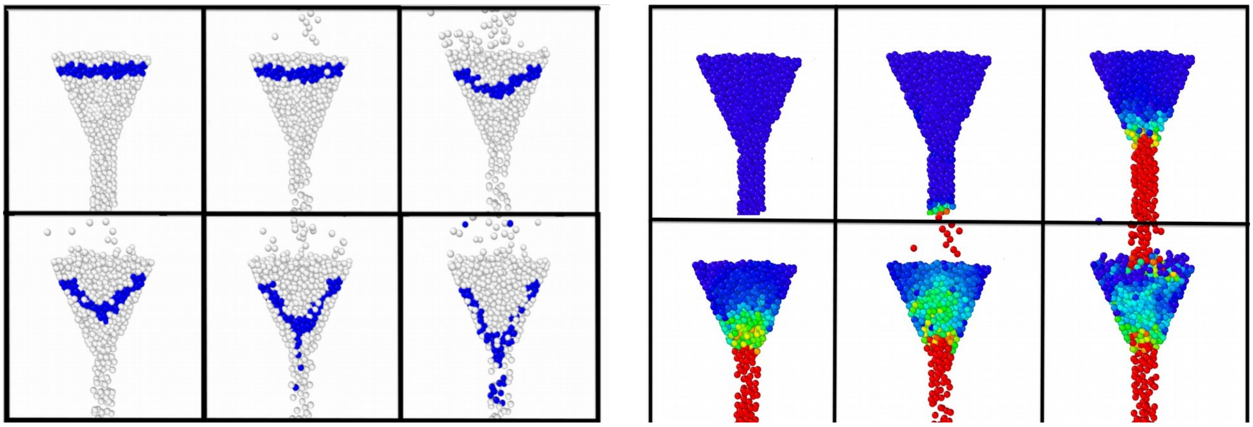


Figure 2. Energy fluctuations

Once this equilibrium condition has been reached, important characteristics of the flow, like the velocity field and the pressure distribution, are statistically estimated and can be periodically dumped in a specified text file while the program is running. These physical properties are periodically stored in a specified text file while the program is running. This file is then post-processed with OVITO software (Stukowski, 2010) and images and videos are created. A Matlab script was also constructed to analyze the number of particles leaving the silo per second, and this results are plotted along with those predicted by the Beverloo correlation.

3. RESULTS AND DISCUSSION

A flow of 6000 spherical particles, with 5 mm radius, was simulated in LAMMPS, using the aforementioned NVE ensemble, with periodical boundary conditions. The dynamic model was constructed using Hertzian contact forces, and integrated with a Verlet algorithm to predict its time evolution. The data generated was then analyzed with OVITO, and the results are presented in Fig.3.



(a) (b)

Figure 3. Simulation results produced with Ovitto (a) Lagrangian evolution of a layer of selected particles; (b) Lagrangian evolution of the velocity of the particles.

The exit diameter varied between 30mm to 43,5mm, in 10 consecutive runs, and the resulting files were processed with Matlab, where a script evaluates the number of particles exiting the silo. These results were then compared with those predicted by the Beverloo correlation, as shown in figure.

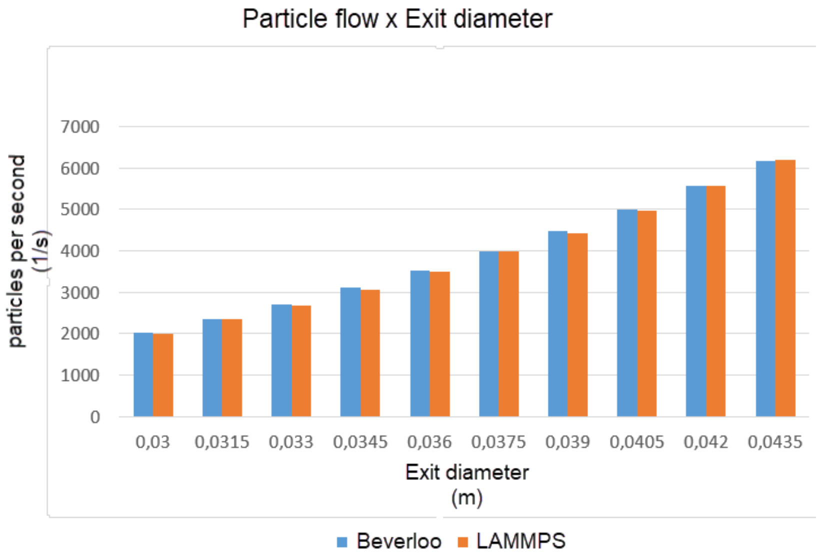


Figura 4. Flow predictions by Beverloo and by the simulation with LAMMPS over a range of exit diameters.

The friction factor used in this simulation is 0.40, and the *C* coefficient of the Beverloo equation was fixed as 0.595. Both values are within the limits encountered throughout the literature (Seireg, 1998;), and the results obtained show an error no greater than 2.5% in all diameters range analyzed. Even when applying a super evaluated friction factor of 0.7, the errors are still bellow 8%, without adjusting the *C* coefficient (*C*=0.595). When adjusting it to its lowest value (*C*=0.55) suggested by Mankoc et al (2007), the errors again fall bellow 2.5%.

4. CONCLUSIONS

In this paper, we focused in the modeling and simulation of granular flow inside the storage chamber of a pneumatic peen forming equipment. The problem was approached using molecular dynamics, in an NVE ensemble with periodic boundaries. The contact forces were modeled according to the theory of Hertz. The model showed an excellent agreement with the mass flow predicted by Beverloo's correlation. When the friction factor is taken to be 0.40, and we compare this with the Beverloo model with a correlation factor *C*=0.595, the deviation was found to be inferior to 2.5%. With a friction factor as high as 0.70, the molecular dynamical model still keeps its error bellow 7.5%, even when confronted with a Beverloo model in which the C factor remains unchanged (*C*=0.595). When adjusting *C* to its lowest value suggested in the literature (*C*=0.55), the errors again fall bellow 2.5%. The model was verified, and seems to be well adjusted. For an even better accuracy, the friction factor should be experimentally determined for each material.

LAMMPS is not a user friendly tool, as the launching of the program must be made via command prompt, and it does not have a graphic user interface. All interaction with the software must be made through a text file, containing the script directions for the simulation, defining all models and parameters applied. Nevertheless, it can be an important tool in the project and control of shot peening machines, as well as in other fields of granular flows.

5. REFERENCES

Baule, A. et al., 2018. Edwards statistical mechanics for jammed granular matter. *Reviews of Modern Physics*, v. 90.

Blumenfeld, R.; Edwards, S. F., 2014. "Granular statistical mechanics – a personal perspective". *European Physical Journal: Special Topics,* v. 223, n. 11, p. 2189–2204.

Cleary, P. W., Sawley, M. L., 2002. "DEM modeling of industrial granular flows: 3D case studies and the effect of particle shape on hopper discharge". *Applied Mathematical Modeling*, 26, p.89-111.

Deresiewicz, H., 1958. "Mechanics of Granular Matter". *Advances in Applied Mechanics,* 5, C, p. 233-306.

Ercolessi, F., 1997. "A molecular dynamics primer". *Spring college in computational physics*, ICTP, Trieste.

Fathallah, R., Inglebert, G., Castex, L., 1996. "Modeling of shot peening residual stresses and plastic deformation induced in metallic parts". In *Proceedings of the International Symposium on Dynamic Problems of Mechanics*

DINAME2013. Buzios, Brazil.
Haile, J.M., 1997. *Molecular dynamics simulation: elementary methods*. Wiley Interscience, 1st edition
Jenicke, A.W., Johanson, J.R., 1969. “On the theory of bin loads”. Journal of Engineering for Industry, v.91, no.2, p.339-344.
Kato, Y., Omiya, M., Hoshino, H., 2014. “Modelling of particle behaviour in shot peening process”. Journal of Mechanical Enginering and Automation, v.4, no.3, p.83-91.
Meguid, S. A., Shagal, G., Stranart, J. C., Daly, J., 1999. “Three-dimensional dynamic finite element analysis of shot peening induced residual stresses”. Finite Element in Analysis and Design, 31, p.179-191.
Sandia National Laboratories, 2018. “LAMMPS Molecular Dynamics Simulation”. *In*: https://lammps.sandia.gov/. Accessed in 2018, 12.
Schwabl, F., Brewer, W.D., 2006. *Statistical Mechanics*. Springer Berlin Heidelberg.
Seireg, A., !998. “Friction and lubrication in mechanical design,” p. 548.
Sperl, M. 2006. “Experiments on corn pressure silo cells – translation and comment on Janssen’s paper from 1895”. Granular Materials, v.8, no.2, p.59-65.
Stukowski, A., 2010. Visualization and analysis of atomistic simulation data with OVITO – the open visualization tool. Modeling and Simulation in Materials Science and Engineering, 18, 0-15012.
Tang, Y., Zhang, L., Guo, Q., 2015. “A review on numerical models for granular flow inside hoppers and its applications in PBR”. *Journal of Nuclear Science and Technology,* 52, 6, p. 759–768.
Wang, T., Platts, M.J., Wu, J., 2008. “The optimisation of shot peen forming processes”. J*ournal of materials processing technology,* 206 , 1–3, p. 78-82.
Yamada, T., Takahashi, T., Ikeda, M., Sugimoto, S., Ohta, T., 2002. "Development of shot peening for wing integral skin for continental business jets". Mitsubishi Heavy Industries Technical Review, v.39, n.2, 2002, p.57-61.
Zhang, H.P., Makse, H.A., 2005. “Jamming transition in emulsions and granular materials”. *Physical Review E Statistical, Nonlinear, and Soft Matter Physics*. 72, p.1–12.

6. RESPONSIBILITY NOTICE

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