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DISCRETE ELEMENT METHOD APPLIED FOR SOYA BEAN FLOW PREDICTION AND ANALYSIS

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Abstract. *Soya bean is a very important product for many countries and there are many equipments to manipulate this product in bulk during the post harvesting process. In this work, the discrete element method (DEM) was applied to predict and analyze the soya bean flow by modeling each seed as a sphere. The values of the material properties necessary for simulation (Poisson coefficient, Young modulus, fraction angle and rolling stiffness) were obtained from the literature. Comparison between the simulation results and the experimental data showed a good agreement. Simulation analysis permitted to identify the non-uniformity of the grain flow that could occur in equipments such as dryers and conveyers that can represent loss in grain quality or security risks for their operation.*

Keywords: *DEM, soya bean, particulate flow, flow analysis)*

1. INTRODUCTION

Soya beans are a very important crop and the world's most important source of oil and vegetable protein. Good soybean post-harvest processes are of vital importance to improve the world food supplies (Mounts *et. al.* 1979). The main post-harvest processes are: threshing, when the beans are separated from the portion of the plant that holds them and is done in the harvesting combine; cleaning, that consists in the elimination of impurities from the grain mass and can be done in more than once through the post-harvest process; drying, when the beans are rapidly dried until they reach the safe storage moisture level; and storage, where the grains are kept in large storage bins, with aeration temperature control systems to maintain its quality (Weber 1995). During this processes, the soya seeds pass trough various devices, including those used for the grain transportation such as elevators and conveyers, which can cause damage that lowers the seed quality and its ability to germinate (Parde et al. 2002). The mathematical modeling of the soya beans flow is an important tool to predict the flow behavior and identify possible problems such as points of high speed impacts that cause damage to the grain or to the equipment, and uneven flow that can reduce the efficiency of the equipments. One method to model and simulate the grain flow is the discrete element method (DEM).

The DEM, introduced by Cundall and Strack (1979) for geotechnical mechanics, has been applied in different fields, such as pneumatic transport (Tsuji *et. al.*, 1992), fluidized beds (Kawaguchi et al, 1998), and has been recently applied for the flow prediction of food grains such as corn, wheat and soya by Vu-Quoc *et. al.* (2000), Iroba *et. al.* (2011), Melmann *et. al.* (2011), Keppler *et. al.* (2012), Gonzáles-Montellano *et. al.* (2001), Boac *et al.* (2012) and

Khatchatourian *et. al.* (2014), where DEM was applied for the problem of grain flow in mixed flow dryers (MFD) and conveyers. In Khatchatourian *et. al.* (2014), DEM was applied, using the software Yade (Kozicki and Donzé 2008), for the prediction of soya bean flow. In Boac *et. al.* (2012), for instance, DEM was applied for the investigation of soya bean flow in a bucket elevator.

In order to apply DEM it is necessary to assign a series of parameters to the material being simulated. Some parameters are physically based properties and can be obtained by running experiments with the actual material, examples are: density, Poisson coefficient, Young modulus and friction angle. Other parameters are related to the numerical method and are not directly related to a single physical phenomenon, but are used to compensate details not predicted in the mathematical model. One example is the numerical damping, used in Woo/Yade to dissipate the kinetic energy of particles (Kozicki and Donzé 2008) and follows the form proposed by Cundall and Strack (1979). Different works have targeted the damping parameter in DEM, trying to build more sophisticated models and investigating its influence in simulation accuracy. In Hu *et. al.* (2011) a general form of damping coefficient is proposed through dimensional analysis, trying to solve unrealistic behaviors in simulations. In Sitharam and Vinod (2010) the influence in the damping ratio of the simulation of various parameters, such as number of cycles and initial confining pressure, is studied. In Khatchatourian *et. al.* (2014) the flow of soya bean in MFD was investigated using Yade, and the numerical damping coefficient for this particular flow was estimated.

The objectives of this work are to:

a) Conduct experiments of soya bean flow under non trivial flow conditions.
b) Carry out numerical simulations of the experimental cases using YADE.
c) Analyze the results considering the simplifications made in the problem modeling.

2. MATERIALS AND METHODS

This section describes the materials am methods used in this study. First there is a brief explanation about the DEM, flowed by the software used for the computational simulations. This section also describes the apparatus used for the experimental study and the methodology adopted.

2.1 Discrete Element Method

The discrete element method, introduced by Cundall and Strack, (1979), calculates the interactions between a finite set of particles applying the Newton's second law of motion in successive small time steps. This method assumes that, if a sufficiently small time step is considered, the disturbances can only propagate to the particle immediate neighbors. Each particle, designed as an element, is modeled by a geometric entity (or a set of them), that approximates the particle actual geometry. The geometry entities used are usually simple, such as the sphere for 3D simulations, or circles, for 2D simulations. The method iteratively applies the following steps:

a) For each element, determine which neighboring elements are colliding (interacting) with it, and using a contact model, determine the forces action on the elements.
b) For each element, applying Newton's second law, integrate the forces for the time step.
c) Update the position of all elements.

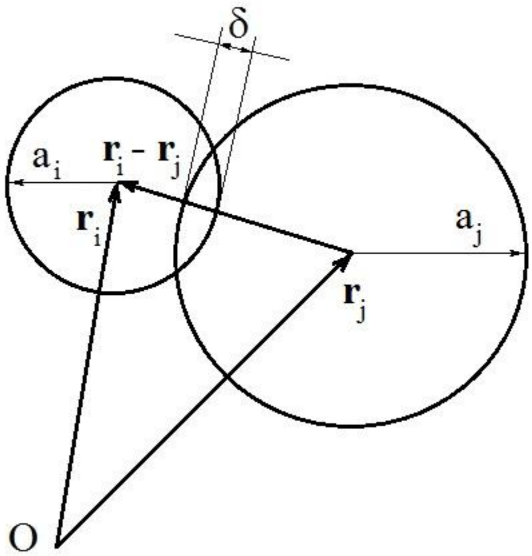

Figure 1. Elements interaction

The forces acting on each particle can result from the contact with other particles, with walls or produced by external forces. Considering the forces f_i acting on the particle *i*, the problem is than reduced to the integration of Newton's equations of motion for the translational and rotational degrees of freedom (Luding, 2008):

$$m_i \frac{(d^2)}{(dt^2)} r_i = f_i + m_i g \tag{1}$$

$$I_i \frac{d}{dt} \omega_i = t_i \tag{2}$$

where m_i is the element *i* mass in *kg*, r_i is the position vector in *m*, f_i is the sum of all forces acting on element *i* in *N*, g is the acceleration of gravity in ms^{-2}, I_i is the moment of inertia in kgm^2, ω_i is the angular velocity in $rads^{-1}$, t_i is the total torque in Nm.

A very important step in DEM implementation is the collision detection, when the system detects which elements are interacting. Two spherical elements with radii a_i and a_j are considered to be interacting if their geometries overlap, according to

$$\sigma = (a_i + a_j) - (r_i - r_j) \cdot n \tag{3}$$

when $\sigma > 0$, where $n = n_{ij} = (r_i - r_j)/|r_i - r_j|$, as illustrated in Fig 1.

2.2 Software tool

Among various tools used for DEM simulations, Woo stands out for being free software under GNU public license (GPL). Woo is derived from other DEM GPL tool, the Yade. The code used by Woo and Yade has been validated by numerous works (Belheine e*t. al.*, 2009), (Bourrier *et. al.*, 2013) and (Harthong et al., 2012). Yade was initially developed by Kozicki and Donzé (2008). Being an open software, the scientific community is able to look at the source codes, validate the implementations and spot possible flaws that can be corrected by the scientific community, not depending on a specific specific software company. Woo, the DEM tool used for the simulations in this work, is than a fork from the Yade project and uses the same core DEM code.

In Woo, the dissipation of the particles kinetic energy is done using a numerical damping coefficient. It is a numerical coefficient because it is introduced directly in the numerical method used and is not physically based. It is based in the form proposed by (Cundall and Strack, 1979) and the general principle is to decrease forces which increase the particle velocities and vice versa by the factor $(\Delta F)d$. This damping scheme is non-physical because is done separately by component and is not invariant in respect to coordinate system rotation. The damping scheme follows the form (Hentz 2003):

$$\frac{(\Delta F)_{dw}}{F_w} = -\lambda_d sgn\left(F_w \dot{u}_w^{\theta}\right), \quad w \in \{x, y, z\} \tag{4}$$

where λ_d is the damping coefficient. According to (Hentz 2003), the use of numerical damping has some advantages: a) it acts on forces, not constraining uniform motion; b) it is independent of eigenfrequencies of elements, making the damping uniform, and c) it needs only the dimensionless parameter λ_d . The damping factor is implemented inside the *NewtonIntegrator* software component.

2.3 Experimental apparatus

In order to carry-out experiments for the validation of the soybean flow mathematical modeling, an apparatus was built. This apparatus consists a MDF and acrylic plates arranged according the depiction on Figure 2. The apparatus is fixed at a specific angle to the ground and its fins are also configured at a desired angle, as seen if Figure 3. The angle of the apparatus in relation to the ground can be set to any angle from 0 to 90 degrees. For the fins there are three possible configurations: 90, 30 and 60 degrees. The experiments are carried out by filling the apparatus with soybean seeds and than opening the gate at its base, the discharge flow is recorded by a digital camera for further analysis. For the experiments in this study, the fins were configures at an angle of 90 degrees and the apparatus was fixed at 90 degrees, *i.e.* perpendicular to the ground. The gate opening at the equipment base was of 0.04 m.

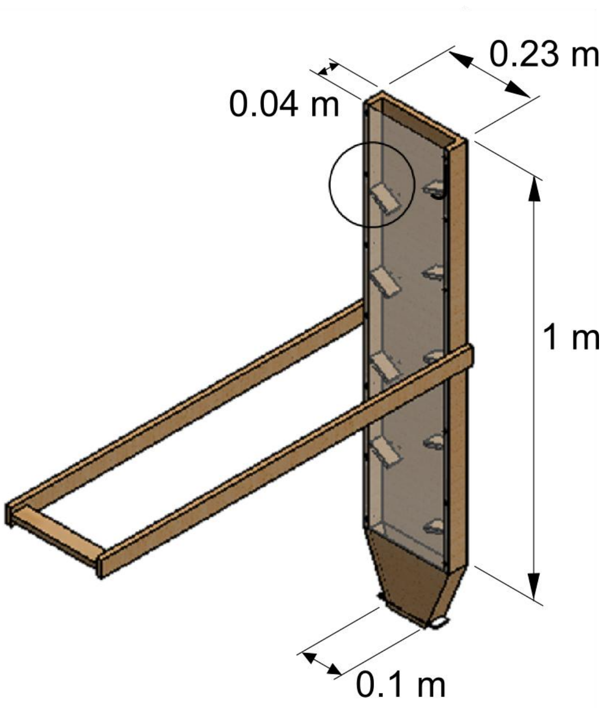

Figure 2. Experimental apparatus

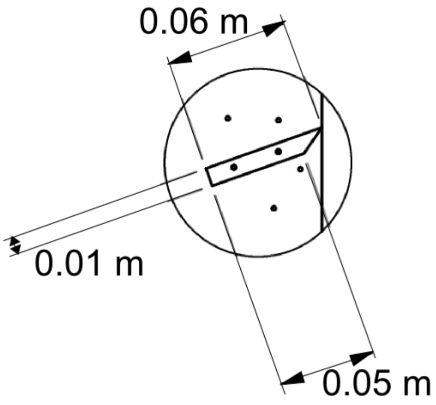

Figure 3. Configurable fins

3. NUMERICAL SIMULATIONS AND RESULTS DISCUSSION

The simulations are defined in Woo using a python script the defines the geometries of the elements involved and the simulations engines used. The geometries for this simulations are of two kinds, the fixed walls defined by a series of triangular elements, and the granular elements, defined by spheres. While the spheres interact with each other and the walls, the walls interact with the spheres but not with each other. Along with the definition of the elements, it is necessary to define their materials. In this work two materials are defined, one for the walls e one for the grains. Even dough the walls are made of two different materials (wood and acrylic plates), their properties are close enough so that the definition of a single material for the walls sufficed. The material properties for the soya beans were the same used by Khatchatourian *et al.* (2014) and are detailed in Tab. 1.

Table 1. Soya beans material properties used in the simulations.

Property	Value
Density (kg m^{-3})	1243
Poisson Coefficient	0.25
Young Modulus (Pa)	2.6×10^6
Friction Angle (rad)	0.45
Rolling Stiffness	0.05
Medium Particle Radius (mm)	3.08
Radius Standard Deviation (mm)	0.305
Damping Factor	0.05

The definition of the geometry was made as close as possible to the actual equipment, except for one important modification, the distance between walls in the actual equipment is 0.05 m, but the distance used in the simulations was 0.01 m. This modification was made in order to reduce the amount of elements in the simulations due to the high computational resources demanded by DEM.

3.1 Simulation Results

As in the experiment, the simulation was carried out with a python script that filled the apparatus geometry with spherical elements generated according to the soya bean radius distribution and material properties defined in Tab 1. After the geometry was filled up to the same level of the experiment, the geometry element correspondent to the 0.04 m gate at the bottom of the simulation body was deleted from simulation geometry list. This step enabled the spherical elements to start flowing trough the opening compelled by the force of gravity.

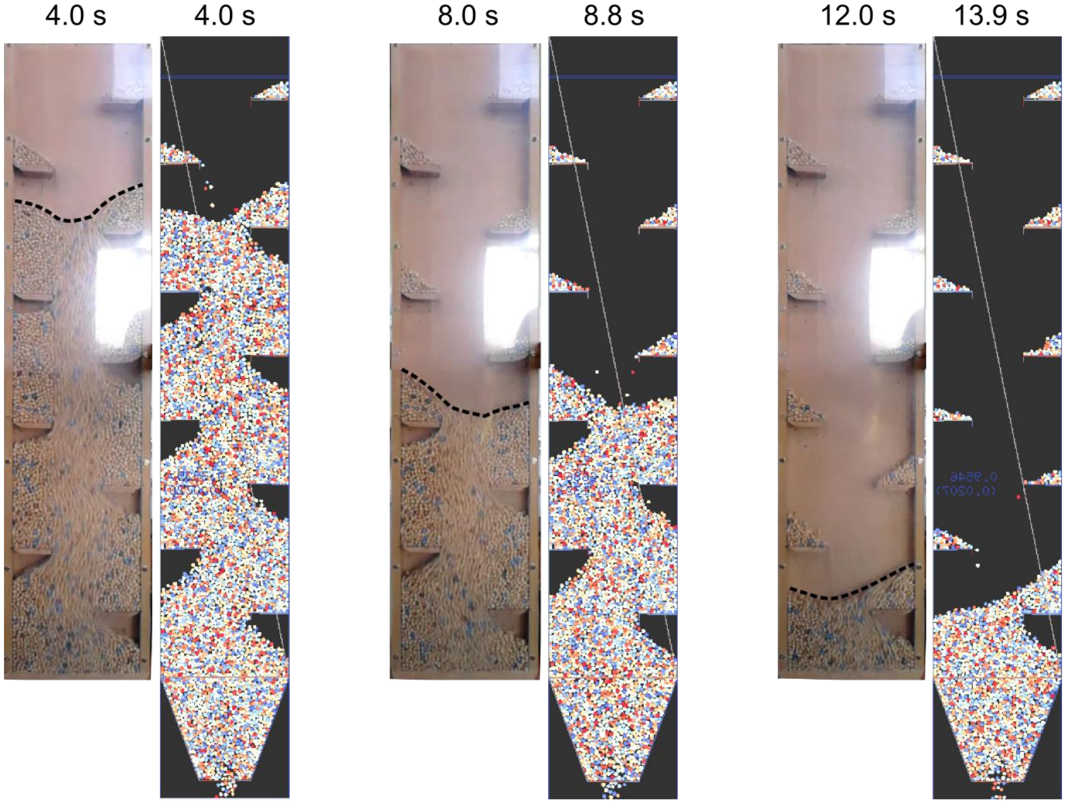

Figure 4. Experimental data

Fig. 4 shows a comparison of the experimental data and the simulation results of the soya bean flow during the discharge process. For each comparison, the image on the left is a frame of the video recorded during the discharge process with a dashed line added for easier identification of the grain level; and the image on the right is a frame of the simulation at the time step corresponding to the experiment according to the grain level. On top of each image is the time counting from the beginning of the discharge process, when the gate at the base of the equipment was opened.

For the first point of comparison, at *4 s* of discharge, there is no discernible difference between the experiment and the simulation. The second point of comparison is when the experimental discharge time is at *8 s*. The corresponding simulation time, *i.e.* the time when the simulation reaches the same grain level, is *8.8 s*, showing a discrepancy of *10%* between the experiment and the simulation. The third comparison is near the end of the discharge, when the experiment discharge time is *12 s*. Here the corresponding simulation time is *13.9 s*, showing an error of *16%*.

As we can see, the error increases as the simulation time increases. This can happen due to a multitude of reasons. The first reason could the cumulative errors of the numerical integration process. The Woo/Yade DEM core has been well validate for various scientific works, as cited in the introductory section of this work, so numerical integration problems are not likely to be the reason. The second reason could be the material properties and simulation parameters no correctly fine tuned. We have to take care with this approach, since adjusting properties and parameters case by case without a very well grounded reason is not a good practice because it reduces the ability of the mathematical model to predict cases different from those used for the parameters definition. In this case, we prefer to maintain the parameters used by Katchatourian *et. al.* (2014). The third reason is the simplifications in the simulated model, including the fact treat we considered the soya beans as being spherical when in fact they are not; and also the fact the we used a distance between walls five times smaller than the actual experiment, due to computational resources constraints. This third reason is more likely to be the most important factor, in particular the reduced wall distance, since it is the main difference between this work and Katchatourian *et. al.* (2014). Further investigation with the aid of more computational resources is still necessary.

4. CONCLUSIONS

This work presented an experimental study and mathematical modeling of soya bean flow. The software tool Woo was used in order to apply the DEM for the particulate flow modeling. The analysis of the simulation results showed a reasonably good agreement with an error of 16% at the end of the simulation. The errors, when considering the wok of Katachourian *et. al.* (2014), where likely caused by the simplifications in the modeling process, specially the reduced distance between walls. The technique of reducing one of the dimensions, sometimes called quasi-3D simulation, is often used due to computation resources restrictions, and was identified by the authors as the likely reason for this difference.

Even though the simulations presented some discrepancy in relation to the experimental data, the DEM method still proved to be a very useful tool to be applied for soya bean flow prediction. Its application can bring various benefits for the design and operation of post harvesting equipments, such as elevators, conveyers and dryers.

5. REFERENCES

Belheine, N., Plassiard, J. P., Donze, F.-V., Darve, F., and Seridi, A., 2009. "Numerical simulation of drained triaxial test using 3D discrete element modeling". *Computers and Geotechnics*, Vol. 36, pp. 320-331.

Boac, J. M., Casada, M. E., Maghirang, R. G., and Harner, J. P., 2012. "3-D and quasi-2-D discrete element modeling of grain commingling in a bucket elevator boot system". *American Society of Agricultural and Biological Engineers*, Vol. 55, pp. 659-672.

Bourrier, F., Kneib, F., Chareyre, B., and Fourcaud, T., 2013. "Discrete modeling of granular soils reinforcement by plant roots". *Ecological Engineering*, Vol. 61, pp. 646-657

Cundall, P. A. and Strack, O. D. L., 1979. "Discrete numerical model for granular assemblies". *Geotechnique*, Vol. 29, pp. 47-65.

Gonzalez-Montellano, C., Ramírez, A., Gallego, E., and Ayuga, F., 2011. "Validation and experimental calibration of 3D discrete element models for the simulation of the discharge flow in silos." *Chemical Engineering Science*, Vol. 66, pp. 5116-5126.

Harthong, B., Jerier, J.-F., Richefeu, V., Chareyre, B., Doremus, P., and Imbault, D., 2012. "Contact impingement in packings of elastic-plastic spheres, application to powder compaction". *International Journal of Mechanical Sciences*, Vol. 61, pp. 32-43

Hentz, S., Daudeville, L., and Donze, F., 2003. “Modeling of reinforced concrete structures subjected to impacts by the discrete element method.” *Proc., 16th Engineering Mechanics Conf.*, ASCE, Reston, Va.

Hu, G., Hu, Z., Jian, B., Liu, L. and Wan, H., 2011."On the Determination of the Damping Coefficient of Non-linear Spring-dashpot System to Model Hertz Contact for Simulation by Discrete Element Method". *Journal of Computers*, Vol. 6, No. 5, pp. 984-989

Iroba, K. L., Weigler, F., Mellmann, J., Metzger, T., and Tsotsas, E., 2011. "Residence time distribution in mixed-flow grain dryers". *Drying Technology*, Vol. 29, pp. 1252-1266.

Kawaguchi T., Tanaka T., and Tsuji Y., 1998. "Numerical simulation of two-dimensional fluidized beds using the discrete element method (comparison between the two and three-dimensional models)". *Powder Technology*, Vol. 96, pp. 129-138.

Keppler, I., Kocsis, L., Oldal, I., Farkas, I., and Csatar, A., 2012. "Grain velocity distribution in a mixed flow dryer". *Advanced Powder Technology*, Vol. 23, pp. 824-832.

Khatchatourian O. A., Binelo, M. O., de Lima, F. F., 2014. "Simulation of soya bean flow in mixed-flow dryers using DEM". *Biosystems Engineering*, Vol. 123, pp. 68-76.

Kozicki, J., and Donzé, F., 2008. "A new open-source software developed for numerical simulations using discrete modeling methods." *Computer Methods in Applied Mechanics and Engineering*, Vol. 197, pp. 4429-4443

Luding, S., 2008. "Introduction to discrete element methods". *European Journal of Environmental and Civil Engineering*, Vol. 12, pp. 785-826.

Mellmann, J., Iroba, K., Metzger, T., Tsotsas, E., Mszros, C., and Farkas, I., 2011. "Moisture content and residence time distributions in mixed-flow grain dryers." *Biosystems Engineering*, Vol. 109, pp. 297-307.

Mounts, T. L., List, G. R. and Heakin, A. J., 1979. “Postharvest handling of soybeans: Effects on oil quality”. *Journal of the American Oil Chemists’ Society*, Vol. 56, No. 10, pp. 883-885

Pardea, S. R., Kausalb, R. T., Jayasa, D. S., Whitec, N. D. G., 2002. "Mechanical damage to soybean seed during processing". *Journal of Stored Products Research*, Vol. 38, No. 4, 2002, pp. 385–394

Sitharam, T. G. and Vinod, J. S., 2010. "Evaluation of Shear Modulus and Damping Ratio of Granular Materials Using Discrete Element Approach". *Geotechnical and Geological Engineering*, Vol. 28, No. 5, pp. 591-601

Tsuji Y., Tanaka T., and Ishida T., 1992. "Lagrangian numerical simulation of plug flow of cohesionless particles in a horizontal pipe". *Powder Technology*, Vol. 71, pp. 239-250.

Vu-Quoc, L., Zhang, X., and Walton, O., 2000. "A 3D discrete-element method for dry granular flows of ellipsoidal particles". *Computer Methods in Applied Mechanics and Engineering*, Vol. 187, pp. 483-528.

Weber E, 1995. *Armazenagem Agrícola*. Kepler Weber Industrial, Porto Alegre.

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