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## Accepted Manuscript

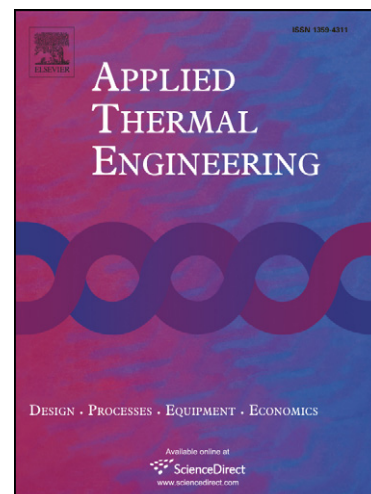
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# Discrete modeling of granular flow with thermal transfer: application to the discharge of silos

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## Résumé

Heat transfer in particulate beds has an important impact for many industrial processes as well as for the storage of particulate material. This study is aimed at modeling the granular flow and heat transfer between particles during the discharge of a silo. A numerical model based on the detection of contacts and the evolution of heat transfers in particle flow has been developed by using Discrete Element Method (DEM). Through this study, we model the heat flows generated by friction and its transfer by conductance. Influence of the friction coefficient and discharging velocity on the granular flow and heat transfer has been investigated through some numerical examples. This modeling enables to understand better the phenomena at the contact point between particles as well as the heat transfer for a great number of particles in motion from their intrinsic mechanical properties and contact conductance.

*Key words:* heat transfer, contact, friction, silo, DEM, particulate beds

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## 1 Introduction

The published literature analysis has shown the importance of heat in granular media for industrial processes in applications as diversified as powder metallurgy, chemical reactors [1], food technology [2], thermal insulation [3]

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or even simply storing particles in a silo after drying [4]. But few studies are interested in the understanding of thermal transfer during sliding contacts. However these complex phenomena with multi-physical characteristics are an essential element in the understanding of the discharging silo process. One of the difficulty is to be able to predict the forces of friction and the temperatures in the friction zone from the intrinsic properties of grains in contact.

From a thermal energy point of view, the sliding contact is the source of a heat generation, whose distribution between the different bodies is difficult to estimate [5]. Besides, the determination of the contact area, which plays an important role in the value of the transferred heat flow is also difficult to estimate. It depends on various parameters like porosity, particles state, the distribution of contact forces, the nature of each phase and the structure of media. Mechanical engineers are at the origin of the greatest number of works. Slavin *et al.* [6], Bahrami *et al.* [7] and Filali [8] have developed models to estimate the effective thermal conductivity of a particles packing, from the intrinsic properties of solids and fluids materials. These models enable to determine the apparent thermal conductivity evolution of a granular media depending on the mechanical forces applied to the particle bed. Vargas *et al.* [9] has studied more particularly the influence of contact pressure on the apparent conductivity of the bed with a small, but finite area of contact. All these models are considering the state surface of the spheres but only the heat transfers by contact are studied. Laguerre *et al.* [10] have presented a heat transfer model which took into account radiation phenomena in a packing so as to simulate the cooling of a fruit pile in a cold chamber. In all the above mentioned works, it is assumed that the study is realized in a static bed.

The first part of this work consists in using the Discrete Element Method (DEM) for the contact detection, the determination of contact forces and the kinematic parameters. A computational software MULTICOR, that can treat an important number of particles ( $10^6$  particles in 2D plane), has been developed to solve the mechanical equations. In a second time, the energy dissipation generating by friction and its transfer by contact have been studied and implemented in MULTICOR software. In the last part, through some experimental data and simulations, we underscore the phenomena of thermal and mechanical interaction during the discharge of the silo. We have investigated the influence of friction coefficient in the case of forced flow of granular media. Some phenomenon such as vault effect arising during the discharge of silo are observed and their influence on the heat dissipation into the granular media has been studied throughout numerical simulations.

## 2 Mechanical resolution by DEM

The conventional DEM allows to model really deformable particles as well as complex shapes (from the ellipsoid to the polygon). Here, we have studied the simple case of non-deformable and non-penetrable particles in 2D plane with the computational programme MULTICOR, developed by Fortin *et al* [11]. The coordinates and the rotations of Euler are the configuration parameters  $q$ . The gyroscopic and centrifugal terms are equal to zero in 2D. The matrix of generalized mass  $\underline{M}$  of the system doesn't depend on  $q$  that is diagonal block. The mechanical equation can be written in the following form (Eq. 1):

$$\underline{M}\ddot{q} = F_{ext}(q, \dot{q}, t) + R^\alpha \quad (1)$$

where  $F_{ext}$  represents the known external forces and  $R^\alpha$  the unknown interior forces related to contact reactions with  $\alpha$  the number of contacts for the considered particle.

In a system composed of  $p$  heterogeneous particles, the critical parameter for the modelling time is the maximum number of interactions between particles. The more the interaction range is important the more we have to test the possible interactions between particles. MULTICOR uses the partitioning method coupled to a connectivity table [12]. This technique allows to reduce considerably the computational time. In that case, the computational time no longer increases like  $O(p^2)$  but only like  $O(p)$ , which is almost optimal. For each couple of particles  $\Omega_i$  and  $\Omega_j$  which may enter in contact, is associated with a local reference whose axes are oriented according to the two unit vectors  $n$  and  $t$ , respectively normal and tangential vectors in the contact plan (Fig. 1). The normal  $n$  is directed from  $\Omega_j$  to  $\Omega_i$ . The variables put in duality are  $\dot{u}^{ij}$ , the relative local velocity of  $\Omega_i$  compared to  $\Omega_j$ , and the contact reaction  $r^{ij}$  of  $\Omega_j$  on  $\Omega_i$ . In the local base, they are written by:

$$\dot{u}^{ij} = \dot{u}_t^{ij}t + \dot{u}_n^{ij}n, \quad r^{ij} = r_t^{ij}t + r_n^{ij}n, \quad (2)$$

where  $\dot{u}_n^{ij}$  is the normal separation velocity,  $\dot{u}_t^{ij}$  the sliding velocity,  $r_n^{ij}$  the contact pressure and  $r_t^{ij}$  the adherence force.

The introduction of Coulomb's friction  $\mu$  leads to a non linear problem which can't be solved by a linear programming method. Unlike the usual approach, the bipotential method leads to a single variational principle and an inequality [11]. By using Usawa's algorithm, we obtain a resolution algorithm of the constitutive law based on the predictive-corrective scheme expressed by Eq.

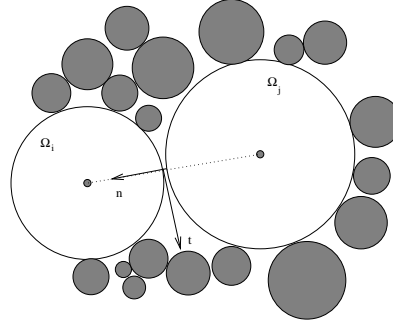


FIG. 1 –. A local referential.

80 3:

$$\begin{aligned}
 &\text{predictor: } \tau^{ij} = r^{ij} - \gamma[\dot{u}_t^{ij} + (\dot{u}_n^{ij} + \mu|| - \dot{u}_t^{ij}||).n], \\
 &\text{corrector: } r^{ij} = \text{proj}(\tau^{ij}, K_\mu)
 \end{aligned} \tag{3}$$

82 where  $\gamma$  is a numerical parameter and  $\text{proj}(\tau^{ij}, K_\mu)$  the projection of Cou-  
 83 lomb's cone which leads, according to the value of  $\tau^{ij}$ , to one of these states:  
 84 non contact, contact with adherence or sliding contact. Conventionally, at each  
 85 time step, the contact forces in the system are determined repeatedly by the  
 86 method of successive balances based on a Gauss-Seidel algorithm for the 2D  
 87 version. Each contact force is calculated by adopting temporary values over  
 88 the other contacts. The convergence is obtained when the force confirms the  
 89 unilateral contact law with dry friction.

90

91 The calculation cycle is a time-stepped algorithm which requires the repetition  
92 of the following resolution scheme (Fig 2).

93

[	$t = t + \Delta t$ Evaluation of the particle positions $q$ Detection of the contact number $\alpha$ in the system Evaluation of the particle velocity (without contact) [ $i = i + 1$ (iteration of solver bipotential) [ $\alpha = \alpha + 1$ (contact loop) Evaluation of the contact reactions $r^{ij}$ Indicator of error ] Evaluation of the velocity
---	--

FIG. 2 –. Algorithm for mechanical resolution.

### 94 3 Heat transfer in granular media and thermal formulation

95 In general, heat transfer in granular media with a stagnant interstitial fluid is  
96 assumed to occur because of the following physical phenomena:

- 97 – Thermal conduction through the particles and thermal conduction through  
98 the fluid between the neighboring particles. Furthermore, in a multi-contact  
99 system considered in this work, we must consider thermal conduction through  
100 the contact area between two particles  $\Omega_i$  and  $\Omega_j$ . Contact conductance re-  
101 fers to the ability of transmitting heat across their mutual interface.
- 102 – Radiant heat transfer between the fluid within neighboring voids and radiant  
103 heat transfer between the surfaces of neighboring particles. For heat transfer  
104 by radiation, contact between surfaces is not required. Radiation is linked  
105 to the production of electromagnetic waves by a heat surface.
- 106 – For flowing fluid, heat transfer by interparticle convection can be considered  
107 if there is a difference of temperature between the particles and the fluid.

108 In frictional granular flow regimes, heat transfer occurs from the phenomenon  
109 presented above. In addition, it is necessary to consider the heat generated  
110 by friction between two particles  $\Omega_i$  and  $\Omega_j$ . Indeed, the sliding contact is an

important source of heat generation for dynamic granular problems considered in this work (Fig. 3a).

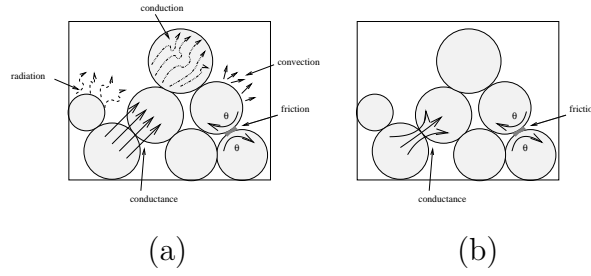


FIG. 3 –. (a) Heat transfer mechanisms in granular media (b) Heat transfer in MULTICOR software.

In this paper, we assume that conduction through the solid phase dominates the thermal conduction. This assumption is verified when:

$$\frac{\lambda_s s}{\lambda_f a} \gg 1 \quad (4)$$

where  $\lambda_s$  and  $\lambda_f$  are respectively the conductivities of the particles and the fluid,  $a$  and  $s$  are respectively the radius of the particle and the contact area.

This expression is checked for high thermal conductivity of solid materials or for solid particles in a vacuum ( $\lambda_f \rightarrow 0$ ) [13]. Under these conditions, the heat transfer between two adjacent particles  $\Omega_i$  and  $\Omega_j$  is only controlled by the contact conductance. In this work, radiant and convective heat transfers are neglected. Therefore, we only consider heat transfer in granular flow by contact conductance and friction effect (Fig. 3b).

### 3.1 Heat transfer by conductance

Contact conductance is directly linked to the constriction of the heat flow lines in the contact point [2]. The thermal contact conductance is defined by the ratio of the heat flow across a contact interface and the magnitude of the discontinuity temperature at the interface (Eq. 5):

$$\varphi_{ij} = H_c^{ij}(T_j - T_i) \quad (5)$$

where  $\varphi_{ij}$  is the heat flow transferred between the particles  $\Omega_i$  and  $\Omega_j$ ,  $T_j - T_i$  the temperature difference between the mid-planes of the spheres and  $H_c^{ij}$  the contact conductance between the particles  $\Omega_i$  and  $\Omega_j$  with  $j$  varies from 1 to



the contact number  $\alpha$ .

The coefficient  $H_c^{ij}$  which is a function of the compression force, refers to the ability for two materials in contact to transfer heat through their mutual interface (Fig. 4). In our work, contact conductance between particles  $\Omega_i$  and  $\Omega_j$  is modeled using Hertz's theory (Eq. 6):

$$H_c^{ij} = 2\lambda_s a_H = 2\lambda_s \left( \frac{3r_n^{ij} a^*}{4E^*} \right)^{1/3} \quad (6)$$

where  $r_n^{ij}$  is the normal force,  $\lambda_s$  the thermal conductivity of the particle,  $a_H$  hertzian contact radius and  $a^*$  is the equivalent radius expressed by  $\frac{1}{a^*} = \frac{1}{a_i} + \frac{1}{a_j}$ ,  $\frac{1}{E^*} = \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j}$  the effective Young's modulus ( $E^*$  expresses an equivalent Young's modulus between the particles in contact) and  $\nu$  Poisson's ratio.

The contact between two adjacent particles is assumed to be smooth and sliding. The contact conductance is calculated dynamically at each time step and for all contacts of a particle  $\Omega_i$ .

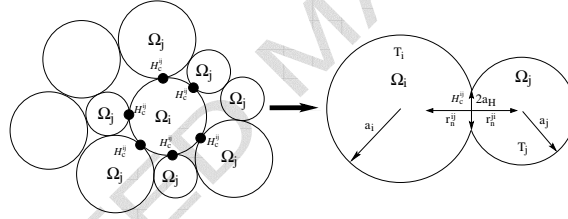


FIG. 4 –. Schematic representation of heat transfer by conductance.

We remind that the considered particles are non-deformable and non-penetrable. The using of Hertz's theory only enables us to compute the contact conductance coefficient  $H_c^{ij}$ . We assume that the particles remain rigid all the time.

### 3.2 Heat generated by friction

In this case, heat flow is generated by dissipation of energy during friction between particles. This assumption of mechanical energy dissipation is well known in thermomechanical field like braking [14] or high speed machining [15]. The deformation is neglected because the particles are assumed rigid. Friction is

understood as continuous mechanical solicitations between two bodies. The heat energy generated by friction  $E_{\mu_{ij}}$  at the frictional interface is:

$$E_{\mu_{ij}} = \mu \dot{u}_t^{ij} r_n^{ij} \quad (7)$$

The modeling of the energy generated by friction requires to share the heat between particles in sliding contact. Therefore, we define the partition coefficient of generated heat flow  $\beta_{ij}$ . This coefficient depends on different microscopic parameters like the thermal properties, the sliding velocity, heat generation parameters and the surface roughness if the contact is not perfect [16]. Research in this area has shown different equations to estimate this coefficient [17] [18]. In our study, this coefficient is obtained from the analytical solution of Varadi *et al.* [19] defined as the ratio of the conductivities:

$$\beta_{ij} = \frac{\lambda_s^i}{\lambda_s^i + \lambda_s^j} \quad (8)$$

We assume that the packed bed is made of only one material. The partition coefficient of generated heat flow  $\beta_{ij}$  is then equal to  $\frac{1}{2}$ .

### 3.3 Thermomechanical resolution

Taking into account the various phenomena of heat generation mentioned above, the energy balance and the variation of temperature for a particle during a low time step  $\Delta t$  can be written as follows (Eq. 9):

$$m_i C_{Pi} \frac{\Delta T_i}{\Delta t} = \sum_{j=1}^{\alpha} \left( H_c^{ij} (T_j - T_i) + \beta_{ij} E_{\mu_{ij}} \right) \quad (9)$$

where  $m_i$  and  $C_{Pi}$  are the mass and the heat capacity for  $\Omega_i$  respectively,  $\alpha$  the contact number.

The temperature evolution between two bodies in contact is governed by the equation (9), representing the balance of the heat energy. This equation is solved with a low time step ( $\Delta t = 10^{-3}s$ ) to assume that the temperature of each particle changes slowly that thermal perturbations do not propagate further than its immediate neighbors during one time step. The second requirement is that the heat transfer resistance through a particle  $\Omega_i$  (conduction) is significantly lower than the contact resistance between two particles  $\Omega_i$  et

188  $\Omega_j$ , proved if:

$$189 \quad Bi = \frac{H_c^{ij}}{\lambda_s a} \ll 1 \quad (10)$$

190 where  $Bi$  is equivalent to the Biot number. The equation used in order to  
191 compute the temperature  $T_i$  at the time  $(t + \Delta t)$  is given as follows:

$$192 \quad T_i^{t+\Delta t} = T_i^t + \frac{\Delta t}{m_i C_{Pi}} \sum_{j=1}^{\alpha} \left( H_c^{ij} (T_j^t - T_i^t) + \beta_{ij} E_{\mu_{ij}} \right) \quad (11)$$

193 The general algorithm implemented in MULTICOR software is represented in  
194 the following scheme (Fig. 5).

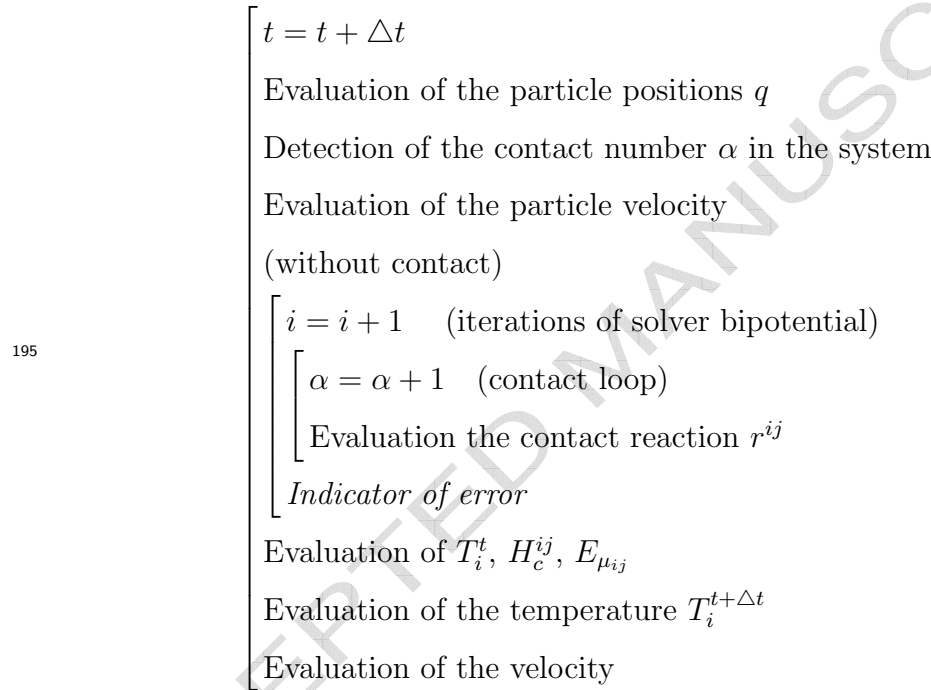


FIG. 5 –. Algorithm for thermal resolution.

196 The resolution of the heat problem requires to compute the contact detection,  
197 the determination of forces and the velocities of particles at each time step.

## 198 4 Numerical simulation

199 MULTICOR software can be used to simulate some industrial processes like  
200 sieving, crushing, filtration, etc. In the next sections, we have focused on the  
201 discharge of a silo both from a mechanical and in a thermal point of view.

#### 202 4.1 Mechanical application

203 In this part, the influence of the initial fill on the discharging process has been  
 204 investigated. Only mechanical equations have been taken into account for the  
 205 granular flow modeling in order to correlate MULTICOR predictions with ex-  
 206 perimental results developed in the works of Ketterhagen [4]. The experiments  
 207 have used bidisperse spheres with a mean diameter of 1.6mm and 0.52mm.  
 208 The dimensions of the silo and the properties of the particles are the same  
 209 than the ones used experimentally by Ketterhagen [4].

210  
 211 The first study is the discharge of the silo with a well-mixed initial charge  
 212 as shown in Fig. 6. The initial charge contains 10% of fine particles. Compu-  
 213 tationally, a well-mixed initial fill is relatively simple to obtain by assigning  
 214 particle positions via a random number generator.

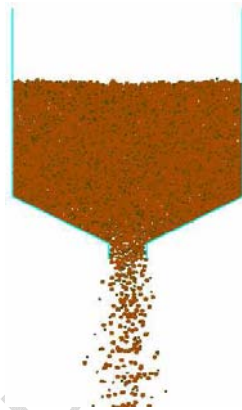


FIG. 6 –. Hopper discharge of a well-mixed initial fill.

215 The comparison of experimental results and computational data of discharged  
 216 fine particles fraction is represented in Fig. 7.  $M$  represents the cumulative  
 217 mass discharge,  $M_{TOT}$  the total mass initially charged in the silo and  $x_i$  the  
 218 fine mass fraction of discharged particles.

219 It should be noted that the discharge of the silo is homogenous but there  
 220 is an over-prediction of the fine particles concentration by MULTICOR for  
 221  $0.4 < M/M_{TOT} < 0.7$ . The main reason may be due to variation in friction  
 222 coefficient, particle shapes or homogeneity of the initial fill [4]. Moreover, the  
 223 simulations have been carried out in two dimensions and do not reproduce  
 224 perfectly the 3D experiments. Despite these differences, analysis of the weight  
 225 fractions of the fine particles shows a quite good adequation between mode-  
 226 ling and experimental data and allows us to provide a realistic prediction of  
 227 granular flow during the discharge of silo.

228

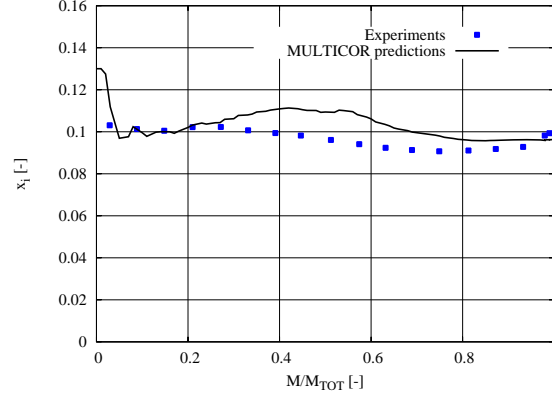


FIG. 7 –. Comparison of experimental and predicted mass fraction of fine particles during the discharge of a well-mixed initial fill.

229 The next example is a layered initial fill. The silo is filled with two horizontal  
 230 layers, one for each of the particles diameter, fine over coarse particles (Fig. 9).  
 231 The initial charge contains 50% of fine particles. Fig. 8 represents the evolution  
 232 of fine particles  $x_i$  versus the normalized discharged mass  $M/M_{TOT}$ .

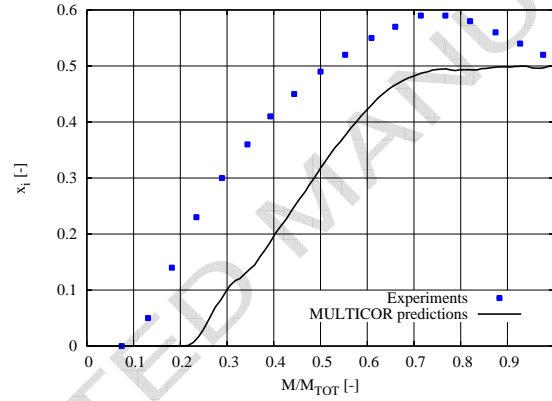


FIG. 8 –. Comparison of experimental and predicted mass fraction of fine particles during the discharge of a layered initial fill.

233 Unlike Fig. 7 that represents an homogenous discharge, three phases may be  
 234 noted during the process (Fig. 8 and Fig. 9):

- 235 – phase 1: at first, only coarse particles are discharged (Fig. 9a).
- 236 – phase 2: as the flow proceeds, the centerline velocities increase and fine  
 237 particles begin to discharge (Fig. 9b).
- 238 – phase 3: at the end of the discharge, the discharge is quite homogenous (Fig.  
 239 9c).

240 As shown in Fig. 8, the experiments and MULTICOR predictions have the  
 241 same shape. However, the MULTICOR software gives lower prediction with

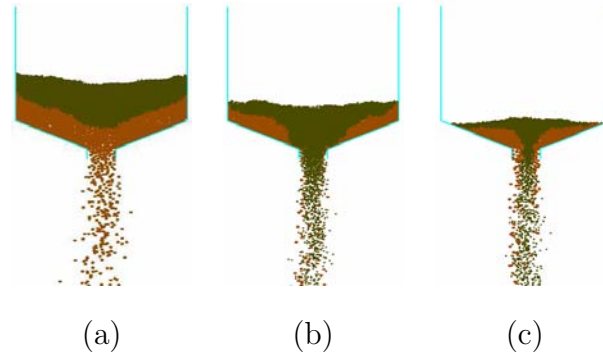


FIG. 9 – The three phases of the hopper discharge filled in double layers.

242 respect to the experimental results. This difference may be due to the 2D plane  
243 modeling which cannot reproduce the same behavior as the experimental test.

244  
245 After the mechanical validation of MULTICOR software for the discharge of  
246 silos, we propose to study heat transfer induced by vault effects during forced  
247 flow of granular media.

#### 248 4.2 Heat generation in forced flow of granular media

249 In this section, MULTICOR software is expanded to include thermal pheno-  
250 mena so that its applications is not limited to isothermal system. Thermal  
251 equations are based on the normal force between two particles in contact (Eq.  
252 6) so heat transfer are directly linked to the force chains. We have studied  
253 the influence of several parameters (friction coefficient, discharge forces) on  
254 the heat generation in granular forced flow. Through this parametric study,  
255 we have shown the influence of vault effects on the heat generation. Theses  
256 phenomena lead to problems for industrial processes such as hopper dischar-  
257 ging [20] or grain conveying in pipes [21]. We precise that in theses works  
258 [20] and [21], the thermal aspects which can be observed for such industrial  
259 applications are not discussed.

260  
261 In MULTICOR, we have assumed that the contact equations and the Hertz  
262 theory have been validated with experimental data in a static configuration  
263 in a previous work [22]. In the following parts 4.2.2 and 4.2.1, we have focu-  
264 sed on the MULTICOR simulations of the forced silo discharging process to  
265 investigate the influence of physical phenomena on the temperature increase.  
266 The particles properties (steel particles) are summarized in Table 1 and the  
267 silo geometry is represented on Fig. 10.

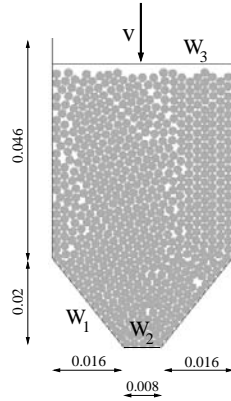


FIG. 10 –. Scheme of the silo.

After sedimentation in a closed silo, the wall W2 is opened allowing the beginning of the discharge. The discharging flow is controlled by the velocity  $v$  of the superior mobile wall W3. The initial temperature of the system is  $T_{ini} = 25^\circ C$ . We have considered that the silo walls do not transfer heat with the exterior atmosphere. For each application, we have studied two parameters :

- the percent of the temperature increase on the wall W1 due to friction between particles:  $100 \times (T(t) - T_{ini})/T_{ini}$ ,
- the normalized mass discharged  $M(t)/M_{TOT}$ ,

where  $T$  is the averaged temperature of the wall W1,  $t$  the time,  $M$  is the mass discharged and  $M_{TOT}$  the total mass of particles initially in the silo.

Parameter	Value
Density	$7800 \text{ kg.m}^{-3}$
Poisson ratio	0.29
Young's modulus	193 GPa
Particle radius	$10^{-3} \text{ m}$
Thermal conductivity	$15 \text{ W.m}^{-1} \text{ K}^{-1}$
Number of particle	600
Heat capacity	$444 \text{ J.kg}^{-1} \text{ .K}^{-1}$

TAB. 1 –  
Particles properties used in MULTICOR simulations.

#### 278 4.2.1 Influence of the discharge velocity

279 In this part, the friction coefficient is constant ( $\mu = 0.3$ ) and the influence of  
280 discharging velocity is explored. Fig. 11 shows the impact of the velocity on  
281 the temperature increase inside the silo.

282

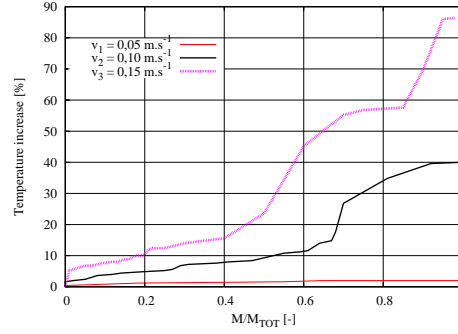


FIG. 11 –. Influence of the discharge velocity on the temperature increase.

283 A more striking result is seen in Fig. 12 when we examine the force chains after  
284 0.1 s of discharge for three velocities ( $5 \cdot 10^{-2} \text{ m.s}^{-1}$ ,  $10^{-1} \text{ m.s}^{-1}$  and  $1.5 \cdot 10^{-1}$   
285  $\text{m.s}^{-1}$ ). For an imposed velocity, the contact distribution is not homogenous,  
286 forces and also heat transfer follow preferred paths. And we note that the prob-  
287 ability of finding contacts, directly linked to the conductance value, increases  
288 as the velocity increases.

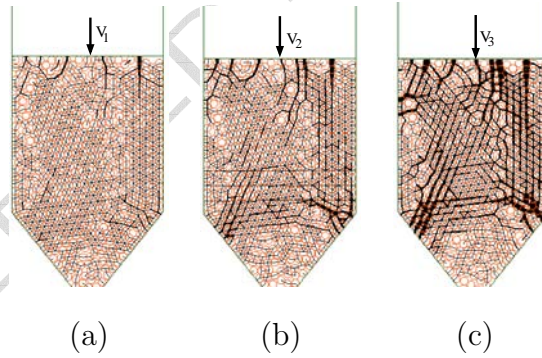


FIG. 12 –. Influence of the velocity on the force chains after 0.1 s of discharge; (a)  $v_1 = 5 \cdot 10^{-2} \text{ m.s}^{-1}$ ; (b)  $v_2 = 10^{-1} \text{ m.s}^{-1}$ ; (c)  $v_3 = 1.5 \cdot 10^{-1} \text{ m.s}^{-1}$ .

289 In this configuration, it is necessary to determine the better conditions of  
290 discharge. As represented in Fig. 13, increasing the discharge velocity means  
291 a lower discharge time, but in the same time it generates a larger increase  
292 of the wall temperature by friction at the end of the discharging process. So  
293 depending on the material properties of particles, the discharging flow should  
294 be optimized to control the heat generation.



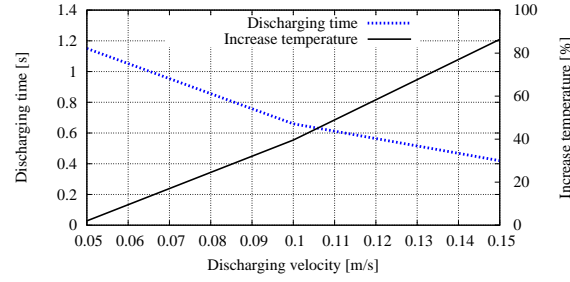


FIG. 13 – Discharging time and increase temperature versus the discharging velocity

#### 4.2.2 Influence of the friction coefficient $\mu$

Influence of the friction coefficient particle/particle and particle/wall on heat generation and temperature increase is investigated at constant discharge velocity ( $v = 0.1 \text{ m.s}^{-1}$ ). Fig. 14 represents the increase temperature versus the mass discharged for different friction coefficients. As expected, temperature increases significantly in case of large friction coefficients. But the temperature increase is not homogenous, steps can be noted in the heat generation especially for an important friction coefficient ( $\mu = 0.35$ ) that could be explained with the analyze of the force chains. During the discharging flow for  $0.4 < M/M_{TOT} < 0.7$ , there is no increase of temperature. In this range, the forces chain represented in Fig. 15a shows low forces chains. On the contrary, for  $M/M_{TOT} = 0.7$ , there is a gap in the temperature increase. In Fig. 15b, we note large force chains with vault effect at the bottom of the silo, generating heat by friction and temperature increase of the wall.

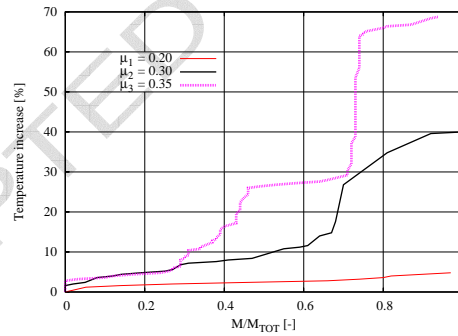


FIG. 14 – Influence of the friction coefficient on the temperature increase.

## 5 Conclusion

The present work focuses on the extend of MULTICOR software, a computational code using discrete elements method, to incorporate heat transfer and heat generation from dissipation of mechanical energy. The results mentioned

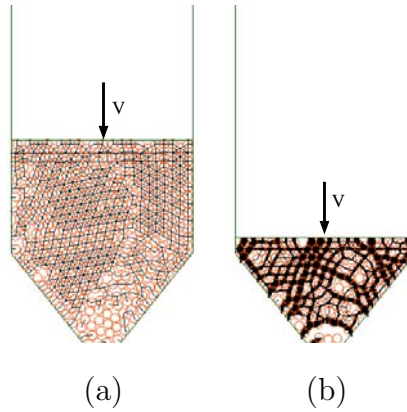


FIG. 15 –. Force chains; (a) low temperature increase; (b) large temperature increase.

here show a good adequation with experimental results from the literature, which allows us to validate our assumptions especially in the mechanical field. MULTICOR software also provides good qualitative agreements concerning the influence of the friction coefficient and the discharge velocity on the increase temperature in a silo.

The next step will consist in the incorporation of the other heat transfer phenomena like convection or radiation. Moreover, further studies will focus on the dynamic friction coefficient and its changes with the temperature and the wear in the contact area. An experimental campaign is also planned with our industrial partner INERIS, a French National Institute that has controlled risks for sustainable development, to validate our thermal assumptions in dynamic behavior.

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