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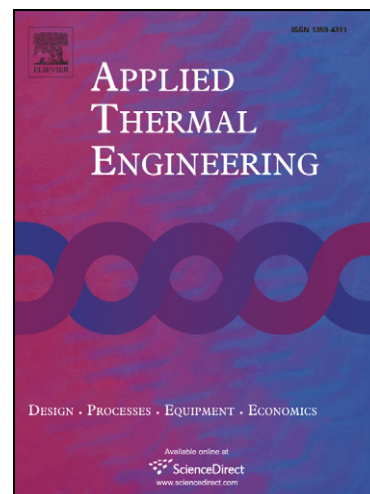
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Discrete modeling of granular flow with thermal transfer: application to the discharge of silos

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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

1 Introduction

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

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

11

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

31

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

45 2 Mechanical resolution by DEM

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

$$54 \quad \underline{M}\ddot{q} = F_{ext}(q, \dot{q}, t) + R^\alpha \quad (1)$$

55 where F_{ext} represents the known external forces and R^α the unknown inter-
 56 ior forces related to contact reactions with α the number of contacts for the
 57 considered particle.

58
 59 In a system composed of p heterogeneous particles, the critical parameter for
 60 the modelling time is the maximum number of interactions between particles.
 61 The more the interaction range is important the more we have to test the pos-
 62 sible interactions between particles. MULTICOR uses the partitioning method
 63 coupled to a connectivity table [12]. This technique allows to reduce consid-
 64 erably the computational time. In that case, the computational time no longer
 65 increases like $O(p^2)$ but only like $O(p)$, which is almost optimal. For each
 66 couple of particles Ω_i and Ω_j which may enter in contact, is associated with
 67 a local reference whose axes are oriented according to the two unit vectors n
 68 and t , respectively normal and tangential vectors in the contact plan (Fig. 1).
 69 The normal n is directed from Ω_j to Ω_i . The variables put in duality are \dot{u}^{ij} ,
 70 the relative local velocity of Ω_i compared to Ω_j , and the contact reaction r^{ij}
 71 of Ω_j on Ω_i . In the local base, they are written by:

$$72 \quad \dot{u}^{ij} = \dot{u}_t^{ij}t + \dot{u}_n^{ij}n, \quad r^{ij} = r_t^{ij}t + r_n^{ij}n, \quad (2)$$

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

75 The introduction of Coulomb's friction μ leads to a non linear problem which
 76 can't be solved by a linear programming method. Unlike the usual approach,
 77 the bipotential method leads to a single variational principle and an inequality
 78 [11]. By using Usawa's algorithm, we obtain a resolution algorithm of the
 79 constitutive law based on the predictive-corrective scheme expressed by Eq.

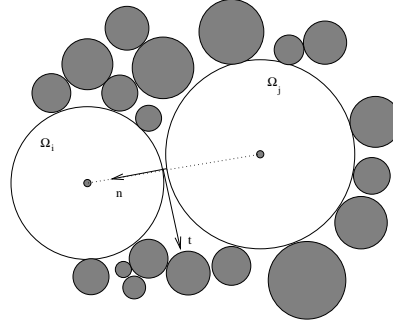


FIG. 1 – A local referential.

80 3:

$$\text{predictor : } \tau^{ij} = r^{ij} - \gamma[\dot{u}_t^{ij} + (\dot{u}_n^{ij} + \mu|| - \dot{u}_t^{ij}||).n],$$

$$81 \quad \text{corrector : } \quad r^{ij} = \text{proj}(\tau^{ij}, K_\mu) \quad (3)$$

82 where γ 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 τ^{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).

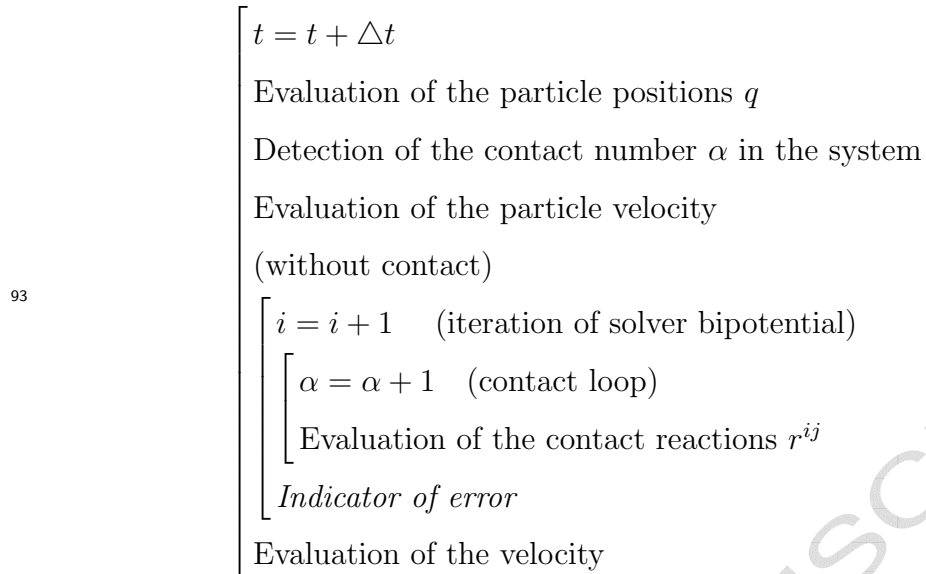


FIG. 2 –. Algorithm for mechanical resolution.

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 Ω_i and Ω_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 Ω_i and Ω_j . Indeed, the sliding contact is an

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

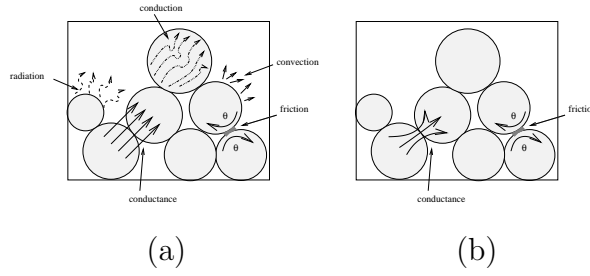


FIG. 3 –. (a) Heat transfer mechanisms in granular media (b) Heat transfer in MULTICOR software.

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

$$115 \quad \frac{\lambda_s s}{\lambda_f a} \gg 1 \quad (4)$$

116 where λ_s and λ_f are respectively the conductivities of the particles and the
 117 fluid, a and s are respectively the radius of the particle and the contact area.
 118

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

125 3.1 Heat transfer by conductance

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

$$130 \quad \varphi_{ij} = H_c^{ij}(T_j - T_i) \quad (5)$$

131 where φ_{ij} is the heat flow transferred between the particles Ω_i and Ω_j , $T_j - T_i$
 132 the temperature difference between the mid-planes of the spheres and H_c^{ij} the
 133 contact conductance between the particles Ω_i and Ω_j with j varies from 1 to

134 the contact number α .

135

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

$$140 \quad H_c^{ij} = 2\lambda_s a_H = 2\lambda_s \left(\frac{3r_n^{ij} a^*}{4E^*} \right)^{1/3} \quad (6)$$

141 where r_n^{ij} is the normal force, λ_s the thermal conductivity of the particle, a_H
 142 hertzian contact radius and a^* is the equivalent radius expressed by $\frac{1}{a^*} =$
 143 $\frac{1}{a_i} + \frac{1}{a_j}$, $\frac{1}{E^*} = \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j}$ the effective Young's modulus (E^* expresses an
 144 equivalent Young's modulus between the particles in contact) and ν Poisson's
 145 ratio.

146

147 The contact between two adjacent particles is assumed to be smooth and
 148 sliding. The contact conductance is calculated dynamically at each time step
 149 and for all contacts of a particle Ω_i .

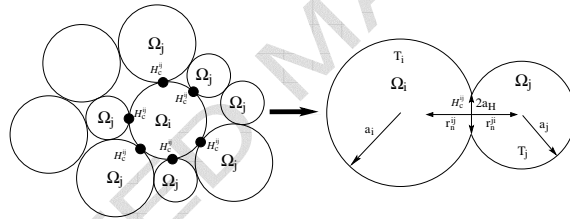


FIG. 4 – Schematic representation of heat transfer by conductance.

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

154 3.2 Heat generated by friction

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

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

$$161 \quad E_{\mu_{ij}} = \mu \dot{u}_t^{ij} r_n^{ij} \quad (7)$$

162 The modeling of the energy generated by friction requires to share the heat bet-
 163 ween particles in sliding contact. Therefore, we define the partition coefficient
 164 of generated heat flow β_{ij} . This coefficient depends on different microscopic
 165 parameters like the thermal properties, the sliding velocity, heat generation
 166 parameters and the surface roughness if the contact is not perfect [16]. Re-
 167 search in this area has shown different equations to estimate this coefficient
 168 [17] [18]. In our study, this coefficient is obtained from the analytical solution
 169 of Varadi *et al.* [19] defined as the ratio of the conductivities:

$$170 \quad \beta_{ij} = \frac{\lambda_s^i}{\lambda_s^i + \lambda_s^j} \quad (8)$$

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

173 3.3 Thermomechanical resolution

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

$$177 \quad m_i C_{P_i} \frac{\Delta T_i}{\Delta t} = \sum_{j=1}^{\alpha} \left(H_c^{ij} (T_j - T_i) + \beta_{ij} E_{\mu_{ij}} \right) \quad (9)$$

178 where m_i and C_{P_i} are the mass and the heat capacity for Ω_i respectively, α
 179 the contact number.

180
 181 The temperature evolution between two bodies in contact is governed by the
 182 equation (9), representing the balance of the heat energy. This equation is
 183 solved with a low time step ($\Delta t = 10^{-3} s$) to assume that the temperature
 184 of each particle changes slowly that thermal perturbations do not propagate
 185 further than its immediate neighbors during one time step. The second requi-
 186 rement is that the heat transfer resistance through a particle Ω_i (conduction)
 187 is significantly lower than the contact resistance between two particles Ω_i et

188 Ω_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).

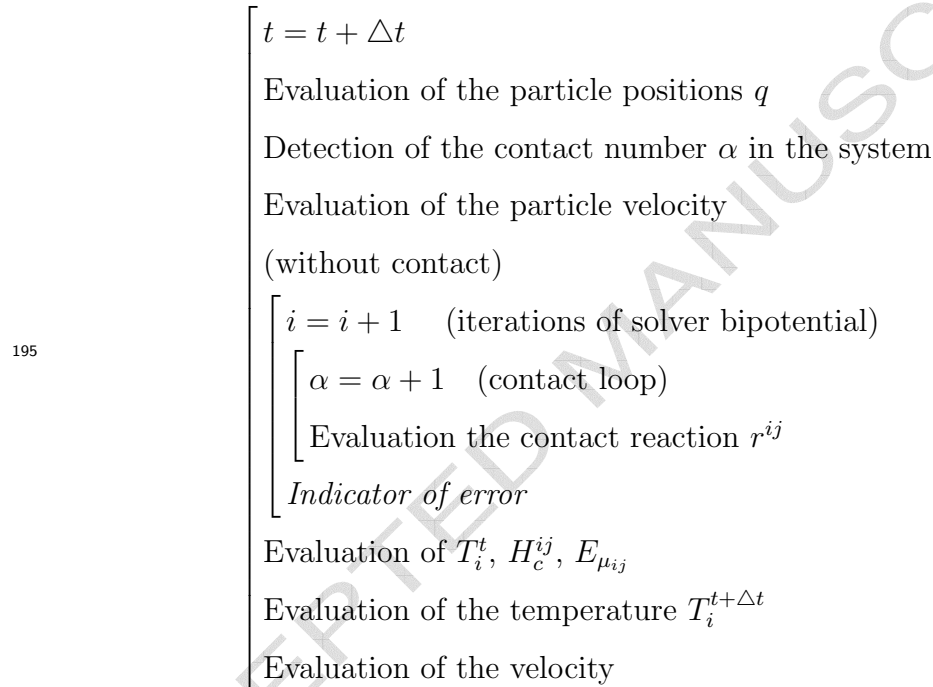


FIG. 5 –. Algorithm for thermal resolution.

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.

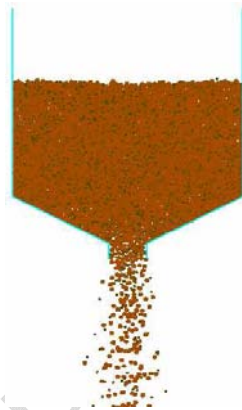


FIG. 6 –. Hopper discharge of a well-mixed initial fill.

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

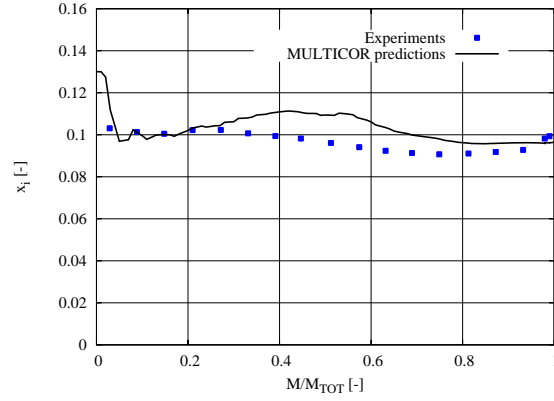


FIG. 7 – Comparison of experimental and predicted mass fraction of fine particles during the discharge of a well-mixed initial fill.

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} .

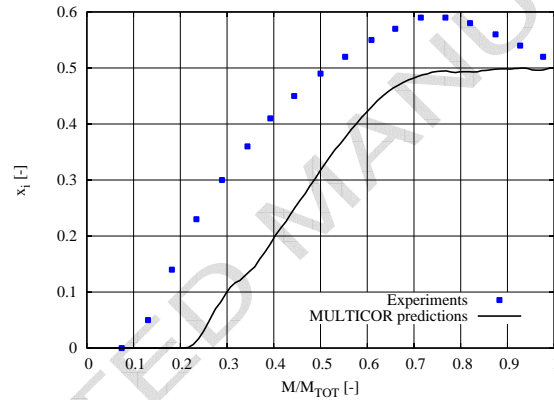


FIG. 8 – Comparison of experimental and predicted mass fraction of fine particles during the discharge of a layered initial fill.

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

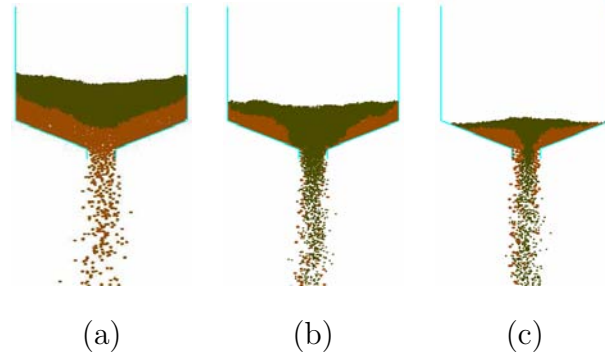


FIG. 9 – The three phases of the hopper discharge filled in double layers.

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.

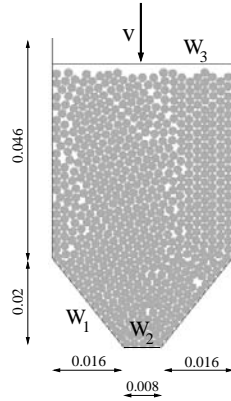


FIG. 10 –. Scheme of the silo.

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

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

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

Parameter	Value
Density	7800 kg.m^{-3}
Poisson ratio	0.29
Young's modulus	193 GPa
Particle radius	10^{-3} 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

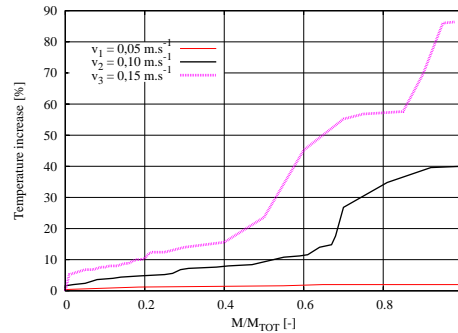


FIG. 11 –. Influence of the discharge velocity on the temperature increase.

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} m.s^{-1} and $1.5 \cdot 10^{-1}$
 285 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.

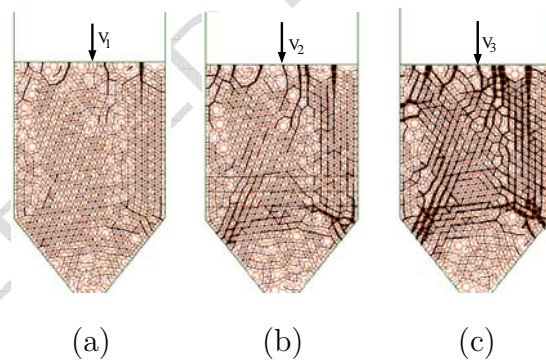


FIG. 12 –. Influence of the velocity on the force chains after 0.1 s of discharge; (a) $v_1 = 5 \cdot 10^{-2} \text{ m.s}^{-1}$; (b) $v_2 = 10^{-1} \text{ m.s}^{-1}$; (c) $v_3 = 1.5 \cdot 10^{-1} \text{ m.s}^{-1}$.

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.

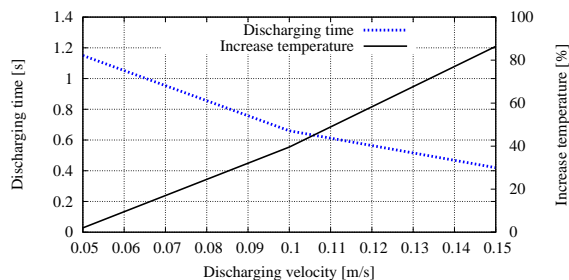


FIG. 13 – Discharging time and increase temperature versus the discharging velocity

295 4.2.2 Influence of the friction coefficient μ

296 Influence of the friction coefficient particle/particle and particle/wall on heat
 297 generation and temperature increase is investigated at constant discharge ve-
 298 locity ($v = 0.1 \text{ m.s}^{-1}$). Fig. 14 represents the increase temperature versus the
 299 mass discharged for different friction coefficients. As expected, temperature
 300 increases significantly in case of large friction coefficients. But the tempera-
 301 ture increase is not homogenous, steps can be noted in the heat generation
 302 especially for an important friction coefficient ($\mu = 0.35$) that could be ex-
 303 plained with the analyze of the force chains. During the discharging flow for
 304 $0.4 < M/M_{TOT} < 0.7$, there is no increase of temperature. In this range, the
 305 forces chain represented in Fig. 15a shows low forces chains. On the contrary,
 306 for $M/M_{TOT} = 0.7$, there is a gap in the temperature increase. In Fig. 15b, we
 307 note large force chains with vault effect at the bottom of the silo, generating
 308 heat by friction and temperature increase of the wall.

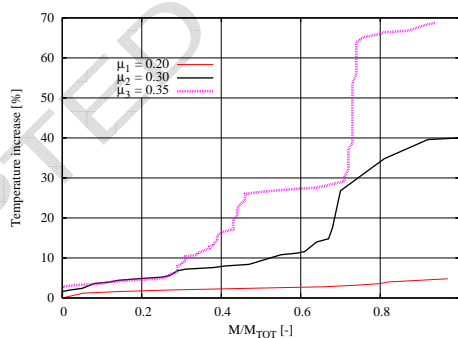


FIG. 14 – Influence of the friction coefficient on the temperature increase.

309 5 Conclusion

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

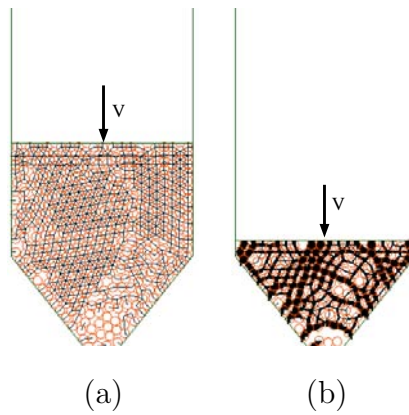


FIG. 15 –. Force chains; (a) low temperature increase; (b) large temperature increase.

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

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

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