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

V.D. Nguyen^a, C. Cogné^{a,*}, M. Guessasma^a, E. Bellenger^a, J. Fortin^b

^aLaboratoire des Technologies Innovantes, IUT de l'Aisne, 48 rue d'Ostende, 02100 Saint Quentin, FRANCE

^bLaboratoire des Technologies Innovantes, INSSET, 48 rue Raspail, 02100 Saint Quentin, FRANCE

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 1 Introduction

² 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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^{*.} Corresponding author. Email address: claudia.cogne@u-picardie.fr (C. Cogné).

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 12 heat generation, whose distribution between the different bodies is difficult 13 to estimate [5]. Besides, the determination of the contact area, which plays 14 an important role in the value of the transferred heat flow is also difficult 15 to estimate. It depends on various parameters like porosity, particles state, 16 the distribution of contact forces, the nature of each phase and the structure 17 of media. Mechanical engineers are at the origin of the greatest number of 18 works. Slavin et al. [6], Bahrami et al. [7] and Filali [8] have developed mo-19 dels to estimate the effective thermal conductivity of a particles packing, from 20 the intrinsic properties of solids and fluids materials. These models enable 21 to determine the apparent thermal conductivity evolution of a granular me-22 dia depending on the mechanical forces applied to the particle bed. Vargas 23 et al. [9] has studied more particularly the influence of contact pressure on 24 the apparent conductivity of the bed with a small, but finite area of contact. 25 All these models are considering the state surface of the spheres but only the 26 heat transfers by contact are studied. Laguerre et al. [10] have presented a 27 heat transfer model which took into account radiation phenomena in a pa-28 cking so as to simulate the cooling of a fruit pile in a cold chamber. In all the 29 above mentioned works, it is assumed that the study is realized in a static bed. 30 31

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

45 2 Mechanical resolution by DEM

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

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

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

(1)

58

In a system composed of p heterogeneous particles, the critical parameter for 59 the modelling time is the maximum number of interactions between particles. 60 The more the interaction range is important the more we have to test the pos-61 sible interactions between particles. MULTICOR uses the partitioning method 62 coupled to a connectivity table [12]. This technique allows to reduce conside-63 rably the computational time. In that case, the computational time no longer 64 increases like $O(p^2)$ but only like O(p), which is almost optimal. For each 65 couple of particles Ω_i and Ω_j which may enter in contact, is associated with 66 a local reference whose axes are oriented according to the two unit vectors n67 and t, respectively normal and tangential vectors in the contact plan (Fig. 1). 68 The normal n is directed from Ω_i to Ω_i . The variables put in duality are \dot{u}^{ij} . 69 the relative local velocity of Ω_i compared to Ω_j , and the contact reaction r^{ij} 70 of Ω_i on Ω_i . In the local base, they are written by: 71

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

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.

The introduction of Coulomb's friction μ 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:

81

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

(3)

where γ is a numerical parameter and $proj(\tau^{ij}, K_{\mu})$ the projection of Cou-82 lomb's cone which leads, according to the value of τ^{ij} , to one of these states: 83 non contact, contact with adherence or sliding contact. Conventionally, at each 84 time step, the contact forces in the system are determined repeatedly by the 85 method of successive balances based on a Gauss-Seidel algorithm for the 2D86 version. Each contact force is calculated by adopting temporary values over 87 the other contacts. The convergence is obtained when the force confirms the 88 unilateral contact law with dry friction. 89

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 qDetection of the contact number α 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

In general, heat transfer in granular media with a stagnant interstitial fluid is
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.

Radiant heat transfer between the fluid within neighboring voids and radiant heat transfer between the surfaces of neighboring particles. For heat transfer
 by radiation, contact between surfaces is not required. Radiation is linked

- 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.

In frictional granular flow regimes, heat transfer occurs from the phenomenon presented above. In addition, it is necessary to consider the heat generated by friction between two particles Ω_i and Ω_j . Indeed, the sliding contact is an

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



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

(4)

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

115
$$\qquad \frac{\lambda_s s}{\lambda_f a} \gg$$

1

where λ_s and λ_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 $(\lambda_f \to 0)$ [13]. Under these conditions, the heat transfer between two adjacent particles Ω_i and Ω_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).

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):

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

where φ_{ij} is the heat flow transferred between the particles Ω_i and Ω_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 Ω_i and Ω_j with j varies from 1 to

134 the contact number α .

146

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

where r_n^{ij} is the normal force, λ_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 ν Poisson's ratio.

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.

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.

154 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:

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

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

$$\beta_{ij} = \frac{\lambda_s^i}{\lambda_s^i + \lambda_s^j} \tag{8}$$

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

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 Δt can be written as follows (Eq. 9):

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

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

180

1

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 Ω_i (conduction) is significantly lower than the contact resistance between two particles Ω_i et

188 Ω_j , proved if:

$$Bi = \frac{H_c^{ij}}{\lambda_s a} \ll 1 \tag{10}$$

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

$$_{192} T_{i}^{t+\Delta t} = T_{i}^{t} + \frac{\Delta t}{m_{i}C_{Pi}} \sum_{j=1}^{\alpha} \left(H_{c}^{ij}(T_{j}^{t} - T_{i}^{t}) + \beta_{ij}E_{\mu_{ij}} \right) (11)$$

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

 $t = t + \triangle t$

Evaluation of the particle positions q

Detection of the contact number α in the system

Evaluation of the particle velocity

(without contact)

$$i = i + 1$$
 (iterations of solver bipotential)

195

 $\alpha = \alpha + 1 \quad \text{(contact loop)}$ Evaluation the contact reaction r^{ij} Indicator of error Evaluation of T_i^t , H_c^{ij} , $E_{\mu_{ij}}$ Evaluation of the temperature $T_i^{t+\Delta t}$ Evaluation of the velocity FIG. 5 –. Algorithm for thermal resolution.

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

Numerical simulation 198

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

202 4.1 Mechanical application

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

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



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

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

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

228



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

The next example is a layered initial fill. The silo is filled with two horizontal layers, one for each of the particles diameter, fine over coarse particles (Fig. 9). The initial charge contains 50% of fine particles. Fig. 8 represents the evolution

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 particles begin to discharge (Fig. 9b).
- $_{238}$ phase 3: at the end of the discharge, the discharge is quite homogenous (Fig. $_{239}$ 9c).
- As shown in Fig. 8, the experiments and MULTICOR predictions have the same shape. However, the MULTICOR software gives lower prediction with



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

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

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

248 4.2 Heat generation in forced flow of granular media

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

260

In MULTICOR, we have assumed that the contact equations and the Hertz theory have been validated with experimental data in a static configuration in a previous work [22]. In the following parts 4.2.2 and 4.2.1, we have focused on the MULTICOR simulations of the forced silo discharging process to investigate the influence of physical phenomena on the temperature increase. The particles properties (steel particles) are summarized in Table 1 and the 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 :

- 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 $M(t)/M_{TOT}$,

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

Тав. 1 –

Particles properties used in MULTICOR simulations.

278 4.2.1 Influence of the discharge velocity

282

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



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

A more striking result is seen in Fig. 12 when we examine the force chains after 0.1 s of discharge for three velocities $(5.10^{-2} m.s^{-1}, 10^{-1} m.s^{-1} \text{ and } 1.5.10^{-1} m.s^{-1})$. For an imposed velocity, the contact distribution is not homogenous, forces and also heat transfer follow preferred paths. And we note that the probability of finding contacts, directly linked to the conductance value, increases as the velocity increases.



FIG. 12 –. Influence of the velocity on the force chains after 0.1 s of discharge; (a) $v_1 = 5.10^{-2} m.s^{-1}$; (b) $v_2 = 10^{-1} m.s^{-1}$; (c) $v_3 = 1.5.10^{-1} m.s^{-1}$.

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

Influence of the friction coefficient particle/particle and particle/wall on heat 296 generation and temperature increase is investigated at constant discharge ve-297 locity (v = 0.1 $m.s^{-1}$). Fig. 14 represents the increase temperature versus the 298 mass discharged for different friction coefficients. As expected, temperature 290 increases significantly in case of large friction coefficients. But the tempera-300 ture increase is not homogenous, steps can be noted in the heat generation 301 especially for an important friction coefficient ($\mu = 0.35$) that could be ex-302 plained with the analyze of the force chains. During the discharging flow for 303 $0.4 < M/M_{TOT} < 0.7$, there is no increase of temperature. In this range, the 304 forces chain represented in Fig. 15a shows low forces chains. On the contrary, 305 for $M/M_{TOT} = 0.7$, there is a gap in the temperature increase. In Fig. 15b, we 306 note large force chains with vault effect at the bottom of the silo, generating 307 heat by friction and temperature increase of the wall. 308



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

309 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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