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Mechanical and thermal segregation of milli-beads during contact heating in a rotary drum. DEM modeling and simulation.

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Abstract

The flow mechanics and heat transfer phenomena within a bed of milli-metric size spherical beads rotated and heated by contact in a horizontal drum were simulated by means of commercial discrete element software EDEM. Mono-dispersed and bi-dispersed beds (two particle sizes or two particle densities) were considered. The mechanical segregation index (standard deviation of local bed compositions) and the thermal segregation index (standard deviation of beads temperatures) were calculated for the different types of bed and same operating conditions. The thermal segregation was found to be enhanced by mechanical segregation and was much stronger for bi-dispersed beds than for monodispersed one.

Keywords: *rotating drum; particulate solid; segregation; contact heat transfer; DEM simulation.*

1. Introduction

Modeling and simulation of processes involving stirred beds of particulate solids is a difficult task. The classical macroscopic and continuous medium approach gives a global scope of average trends but do not provide the local information which in some high added value processes like the pharmaceutical ones may be critical. In some cases even tiny processing discrepancies between individual particles must be avoided. During drying of granular beds, stirring is very often combined with contact heating and the powder flow mechanics is then coupled with heat transfer. For instance, vacuum contact heating is widely used in the pharmaceutical industry to dry granular products which are sensitive to oxygen and temperature. The vacuum contact drying of powder stirred bed has been firstly investigated in a macroscopic way ("penetration" model) by Schlünder and Mollekopf[1] for a mono-dispersed non sticky granular material. Kwapinska et al.[2] compared results obtained by the "penetration" analytical method with those obtained by numerical DEM.

More recently, several authors have independently investigated the effect of operating conditions on mixing and heating rates of rotated monodispersed granular material. Figueroa et al.[3] have studied various tumbler filling levels and cross-sectional shapes; Chaudhuri et al.[4] various revolution speeds, material types and baffles number and shapes; Gui et al.[5] and Komossa et al.[6] different revolutions speeds; Emady et al.[7] different revolution speeds and material thermal conductivities. However, to our best knowledge, no results were published to date concerning dispersed beds composed of particles of different sizes and materials. This is a major issue because real, industrial materials, even if carefully controlled before processing, are always slightly dispersed.

Rotating mixing of unperfectly monodispersed solid particulate beds unavoidably leads to mechanical segregation, i.e. to accumulation of smaller or/and denser particles in the core of the bed. In the previous study[8], radial and axial segregations were experimentally observed for a bi-dispersed bed with two particle sizes or two particle densities. The radial segregation index was measured for different drum filling ratios and for differnet baffles numbers and heights. The axial segregation index was found to be influenced by the friction coefficient on both drum front and rear walls.

It is thus expected that the bed spatial heterogeneities will lead to thermal heterogeneities because the beads temperature time evolutions depends on their trajectories and especially on their cumulated contact times with the heating wall. The aim of this paper was to investigate the impact of mechanical segregation on the thermal segregation in bi-dispersed beds as compared to a perfectly monodispersed (not mechanically segregated) bed. DEM was applied for modeling and simulation of spherical milli-beads flow and heat transfer in a rotating 'slice' type (nearly bidimensional) drum.

2. Materials and Methods

The simulations of the stirring and contact heating of milli-beads were realized with the commercial software EDEM 2017 (DEM Solutions, Edinburgh, UK). This software is based on the discrete elements method (DEM) which is a very powerfull modern tool to investigate and develop granular solid processes. In the DEM framework, each particle of the granular bed is considered to be distinct and has its own trajectory and speed. The particle-particle and particle-boundary interactions are checked at each time step and the resulting individual particle positions are updated. The main assumption of DEM modeling is that the particles are rigid (nondeformable) solid bodies but have the capability of small interpenetration during their contacts. The resulting decrease of the distance between the centers of two adjoining particles is called the penetration depth (δ) or overlap. The overlap is the fundamental variable which is directly related to the normal contact (interaction) force between the particles and the mechanical stiffness of the particles. This overlap is also the basis for evaluating the heat conductance between the particles as described in the next sections.

2.1 Mechanical DEM modeling

The determination of the position and speed of a given particle (identified by index i) is the time solution of the Newton second law for translational and rotational movement of a solid body. For translation, it writes :

$$\mathrm{m_i}\frac{\mathrm{d^2}\vec{\mathrm{x}}_\mathrm{i}}{\mathrm{dt^2}} = \sum_j \mathrm{F_{ij}} + \mathrm{m_i g} \tag{1}$$

where m_i is the particle mass, x_i its position vector and the right hand side of the equation is the resulting force, cumulating interactions with all adjoining (j) particles (and the wall of the vessel) and gravity. A similar equation can be written for the rotational movement.

For the purpose of this study, default modeling option in EDEM, the Hertz-Mindlin contact model[7] was used. In this model, the particle-particle mechanical interaction involves the normal impact force and the tangential friction force. The normal force is essentially elastic but both normal and tangential forces include damping components. The normal force is thus expressed by means of non linear visco-elastic behavior law :

$$\mathrm{F_{ij}} = \alpha\delta_{ij}^{3/2} - \beta\mathrm{v_{ij}} \tag{2}$$

where α is the elasticity coefficient depending on the material Young's modulus and particles radius, β is the damping coefficient depending on the kinetic energy restitution factor of the particles, δ_{ij} is the overlap between particle i and j and v_{ij} is the relative velocity of the two particles. The maximal tangential friction force is given by the *Coulomb* law which involves a material dependent friction coefficient.

2.2 Thermal DEM modeling

In tumbler systems, several heat-transfer phenomena coexist between neighboring particles and including walls : direct solid-solid heat conduction, conduction and convection through the insterstitial fluid and surface radiation. In this study, convection and radiation are neglected. The direct particle-particle conduction is expected to largely dominate due to the high ratio of conductivity of particles to the conductivity of interstitial gas and due to moderate surface temperatures.

In DEM framework, as already stated in the preceding section, two particles in contact interpenetrate each other at a depth depending on theirs dynamics and mechanical properties. For spherical particles, the contact radius R_c, which is the radius of the circle resulting from the two particles (spheres) overlapping, can be straightly derived from the penetration depth. Approximate analytical solutions of the *Fourier* conduction equation between two smooth, elastic particles with a finite small contact area have been proposed in the literature[5,6,7] and applied to evaluate the thermal conductance K_{ij} between the two particles centers :

$$K_{ij} = 2\lambda_{eff}R_c = 2\lambda_{ij}\sqrt{R_{ij}}\sqrt{\delta_{ij}} \tag{3}$$

where λ_{ij} is the harmonic mean of the thermal conductivities of the two materials, R_{ij} is the harmonic mean of the particles radii. The conductive heat flux between particle i and particle j writes simply :

$$\dot{Q}_{ij} = K_{ij}(T_j - T_i) \tag{4}$$

The total heat flux transferred to or from a given particle (i) is the sum of heat fluxes exchanged with all neighboring (j) particles and the thermal energy balance of a single particle writes :

$$m_i c_{pi} \frac{dT_i}{dt} = \sum_j \dot{Q}_{ij} \tag{5}$$

where c_{pi} is the particle specific heat capacity. The time integration of the above equation provides the thermal history of the considered particle.

2.3 Particulate bed global caracteristics

In order to caracterise globally and macroscopically the geometrical distribution (mechanical segregation) of each kind of beads and their temperature distribution (thermal segregation) within the bed, statistical indexes already introduced in the literature[3] were used. The mechanical segregation index was defined by :

$$MSI' = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(C_i' - \langle C\rangle)^2} \tag{6}$$

where C_i' is the number fraction of one kind of beads (of the considered size or density) in a control volume i among N other control volumes, <C> is the average number fraction of this kind of beads in the entire bed divided in N equal size control volumes. By analogy, the overall thermal segregation index was defined as :

$$\mathrm{TSI} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(T_i - \langle T \rangle)^2} \tag{7}$$

where T_i is the temperature of the bead i among all other beads, <T> is the average temperature of all N beads of the bed. This index represents simply the standard deviation of beads temperatures. However, in case of bi-disperded beds, two beads populations coexist, according to their size or density. These two populations are mechanically separated (segregated) by the drum rotations and this will influence directly their thermal dispersion (segregation). In order to observe separately the thermal evolution of the two populations, a population (density or size) specific thermal segregation index was therefore defined :

$$\mathrm{TSI}' = \sqrt{\frac{1}{M-1}\sum_{j=1}^{M}\left(T_j' - \langle T \rangle\right)^2} \tag{8}$$

where T_j' is the temperature of bead j of a given kind among M other beads of the same kind.

2.4 Solver settings, material properties and process parameters

The simulations were realized on a DELL workstation (T7910) with two 10 cores processors (Intel Xeon E5-2660v3). The maximum processing time step was set at 40 % of the theoretical Rayleigh time step. This is the time taken for a shear wave to propagate through the particle which depends on the particle size and mechanical properties. The adjoining particles numerical search distance was set at 5 fold particle radius. The "Hertz-Mindlin with Heat Conduction model" was selected and a user defined routine called "Heat conduction for Geometry" was incorporated for implementing particles-wall direct heat conduction.

Table 1. Beads number for different bed types.

	Mono-dispersed	Bi-density	Bi-size
CA-2	-	-	27905
CA-3	16366	8183	8183
PP-3	-	8055	-

Polypropylene (PP) and cellulose acetate (CA) spherical beads of millimetric size (2 mm and 3 mm diameter) were used. The compositions of the three studied particulate beds are shown in Table 1. All materials mechanical and thermophysical properties needed for EDEM simulations are given in Table 2. The friction coefficients for pairs of materials were obtained by model identification (fitting experimental data) and are given in Table 3. The drum used in this study was a 'slice' type one with a large diameter to depth ratio. It had an internal diameter of 300 mm and an internal depth of 42 mm.

Table 2. Materials thermal and mechanical properties

BEADS	**Property**	**Units**	**CA**	**PP**
	Density [a]	[kg/m^3]	1280	910
	Poisson's ratio [a]	[-]	0.4	0.42
	Elastic modulus [a]	[MPa]	1.0	1.0
	Shear modulus [a]	[MPa]	2.8	2.8
	Thermal conductivity [a]	[W/(m.K)]	0.36	0.22
	Specific heat capacity [b]	[J/(kg.K)]	1200	1700
	Coefficient of rolling friction [c]	[-]	0.01	0.01
	Coefficient of restitution [c]	[-]	0.3	0.3
DRUM			**Steel**	**Glass**
	Density [b]	[kg/m^3]	7800	2500
	Poisson's ratio [b]	[-]	0.3	0.21
	Elastic modulus [b]	[GPa]	182	94.3
	Shear modulus [b]	[GPa]	70	39
	Thermal conductivity [b]	[W/(m.K)]	15	0.93
	Specific heat capacity [b]	[J/(kg.K)]	502	/
	Coefficient of rolling friction [c]	[-]	0	0.01
	Coefficient of restitution [c]	[-]	0.3	0.3

a - manufacturers data (M&L, CIPAM and other), b - web data (Azom, Engineers Edge)], c - data from this study

The front panel was made of glass, the rear one and the peripheral wall were made of stainless steel. The drum was equipped with 4 equidistant straight baffles with a height of 15 mm. All these dimensions corresponds to the set-up used in the previous experimental study[8]. The default revolution speed was 3 rpm which corresponds to very slow rotations often encountered for drying of pharmaceuticals. The initial beads temperature was 25 °C and the peripheral heating wall temperature was 50 °C.

Table 3. Solid-solid static friction coefficients

	Bead-Steel	**Bead-Glass**	**Bead-Bead**	
			CA	**PP**
CA	0.3	0.2	0.3	0.6
PP	0.3	0.2	0.6	0.6

3. Results and discussion

The simulations were realized for the 3 types of bed presented in Table 1. The mechanical segregation index (MSI) and the thermal segregation index (TSI), as defined in section 2.3, were calculated with MATLAB from EDEM data extracted for each simulation and were plotted as function of time on Figures 1 and 2.

According to Figure 1, except for a very short initial period, thermal segregation was the most important for the bi-density bed. Moreover, from the moment the bi-size bed MSI approached the bi-density MSI, the bi-size TSI fell below the mono-dispersed TSI. The bi-density bed TSI was significantly higher than the bi-size TSI, while the the MSI for both bi-dispersed beds were rather close to each other near the simulation end. The correlation between MSI and TSI is thus not straightforward and must be further investigated.

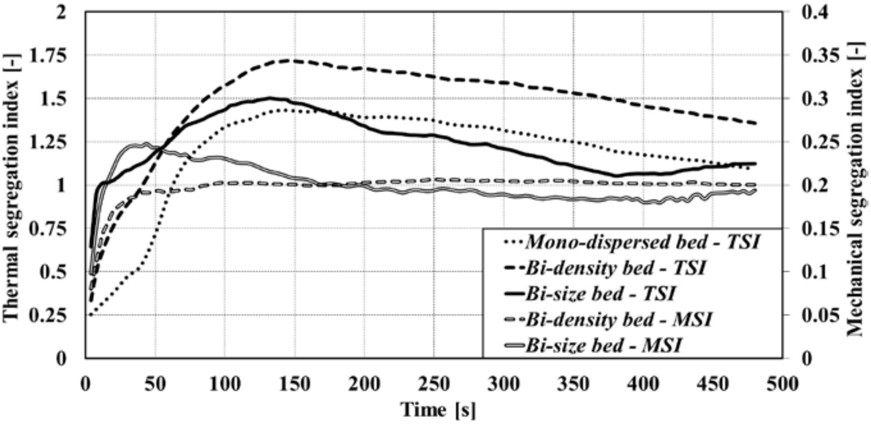

Fig. 1 ***Mechanical and thermal segregation indexes for different bed types.***

As observed on Figure 2, the small beads specific TSI followed closely the overall TSI. The reason could be that the bi-size bed contained much more small than big beads (see bed compositions in Table 1). Therefore small beads thermal dispersion would have a much larger impact than the dispersion of big beads.

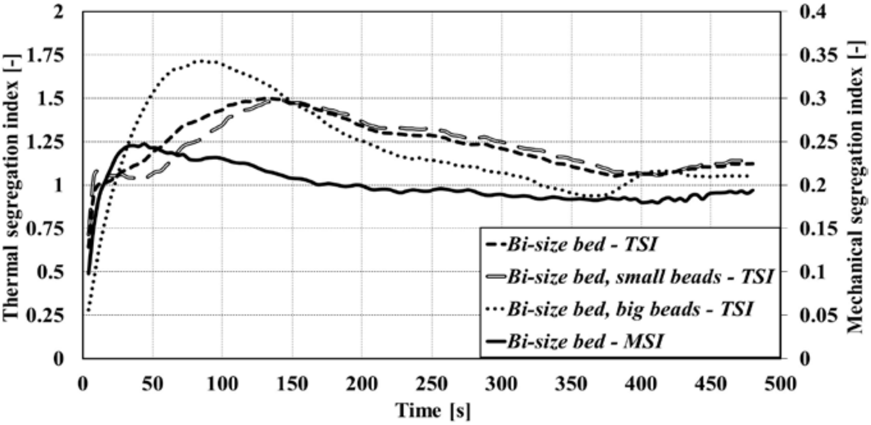

Fig. 2 Mechanical and thermal segregation indexes for the bi-size bed.

For the bi-density bed, the overall TSI was practically the average of the two specific TSIs (Figure not shown) because there was an equal number of light and heavy beads. As concerns average bed temperatures, plotted on Figure 3, the heating rate (curve slope) was stronger for the bi-size bed than for bi-density and mono-disperded beds and this deviation increased with time. This seemed rather odd because for the bi-size bed the small beads were in the core and the big ones at the periphery.

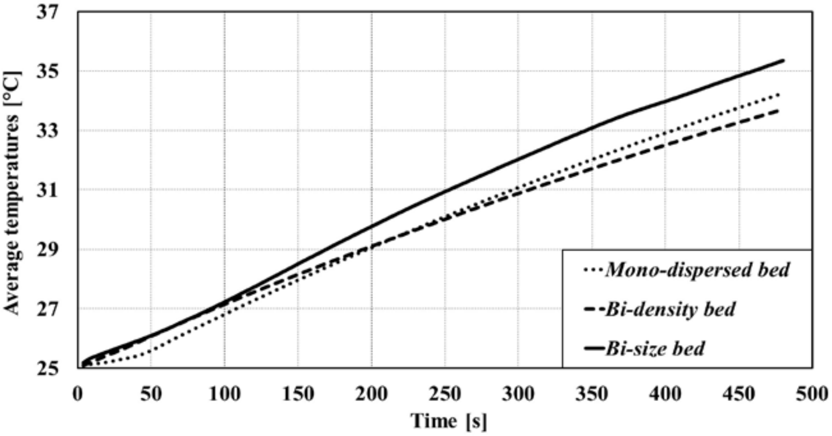

Fig. 3 Average temperatures for different bed types.

As there was much more small beads than big ones in the whole bed, one could expect that the average bed temperature would rather follow the temperature of the small ones which were colder and that the overall heating rate would be slower than for a bi-density bed. These results must be confirmed by carrying out the simulations for much longer times.

4. Conclusion

The mechanical segregation index (standard deviation of local bed compositions) and the thermal segregation index (standard deviation of beads temperatures) were calculated for mono-dispersed, bi-size and bi-density beds of spherical milli-beads submitted to same operating conditions. The thermal segregation was found to be enhanced by mechanical segregation and was much stronger for bi-dispersed beds than for monodispersed one. The bi-density bed exhibited unexpectedly stronger thermal segregation than the bi-size one.

5. References

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