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NUMERICAL ASSESSMENT OF A STATIC MIXER DESIGN FOR MIXING FREE FLOWING GRANULAR MATERIALS USING THE DISCRETE ELEMENT METHOD

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Abstract— Mixing is a process of a vital importance in agricultural, chemical and pharmaceutical manufacturing industries, however the behavior of particles during the mixing process still not fully understood as it is related to many physical and process parameters (material type, friction, mixer velocity, etc.). Understanding the flow patterns of granular solids during mixing is a complex and difficult task, therefore deliberating mixing of solid ingredients is a crucial maneuver in the production of powder products. In this work, a static mixer is designed which has no moving parts, causing mixing by simply filling solid granules. EDEM® software based on Discrete Element Method (DEM) has been utilized to conduct the numerical experiments. Recorded screens of mixing states are used for qualitative assessments, and the Lacey index of mixing has been calculated for every experiment. Particles inhomogeneity is at its minimum when both particles coefficient of restitution and kinetic energy are at their maximum.

I. Introduction

Lack of knowledge and unpredictability in such a mixing device lead to a huge loss in energy and manpower, also it leads to a huge loss of materials when it comes to a production of expensive products. The design of a mixer and the selection of mixing parameters are of key importance in order to obtain the desired end-product. With that goal in mind, in this paper, we introduced a novel concept of a mixer device that has no moving parts. Numerical experiments based on discrete element method were conducted to investigate the particles flow inside the mixer and assess their uniformity.

The mixing of granular materials could reduce the returns of any related industry as it plays an indispensable role in ensuring the end-product efficiency in many industries including pharmaceutical and agricultural. For instance, the approximate amount lost per annum due to inefficient mixed products for pharmacy in the US is about $1 trillion [1]. Scarcity of scale up rules, range of particles size, size distribution, shape and/or chemical constitution convolute the understanding of internal behavior, hence it could overcomplicate mixer design [2]. Mixing homogeneity is the key to obtain an efficient product and avoid detrimental effects, it is achieved by together convective and dispersive mechanisms [3] [4]. Segregation is the opposite term of mixing which could show up during a mixing process which complicates understanding the flow pattern of particles [5], and describing particles rheology still challenging [6]. Therefore, optimal mixer parameters should be set in advance such as; mixer vessel/rotor velocity, mixing time, etc. As for example, Uchida and Okamoto showed that increasing the pitch length of a screw in a screw auger mixer improves the mixture homogeneity [7]. Milada et al. showed that discrete element modelling and simulation helped to optimize a revolving static mixer by the selection of appropriate geometrical parameters [8].

Usually, a mixture is performed by either the rotation of mixing element(s) (e.g., screw mixer) or the rotation of mixer frame (e.g., drum mixer). However, Static mixers have no moving parts. The last has many advantages over mobile mixers: one, fast and continuous process, two reduced manufacturing and maintenances costs, three, easy to clean, and so on [9] [10].

Commonly, the optimal mixing algorithm is obtained by the trial and error method which is time consuming and expensive. Therefore, Scientists and engineers created and developed new experimental and computational methods either to find more efficient design of mixers or optimize existing mixers by conducting relatively less experiments. Moreover, these techniques brought lights on the selection of optimal physical and process mixing parameters and the assessment of the mixture uniformity. For instance, the discrete element method was capable to investigate the motion of particles in a screw conveyor and assess its performance [11]. Others, investigated the flow of wheat grains in a hopper bottom lab-scale mixer by discrete element simulations [12].

In the present work, DEM simulations of a static mixer were carried out using EDEM®. Two different configurations of blending elements were examined. The impact of particles kinetic energy and particles coefficient of restitution were also investigated. This work provides the very first basic knowledge for designing static mixers for granular materials.

II. The Discrete Element Method

The discrete element methods are currently used for modeling the mechanical behavior of granular media (powders, sand, rocks, etc.). It encompasses a range of problems of different scales: tribological interfaces [13], geophysics [14], masonry [15], blending [16], etc.

Many discrete element methods are available in the literature; we can identify a general strategy working for any simulation of discrete elements. The fundamental steps are then: contact detection, calculation of contact forces and time evolution (prediction and correction) of the media (Figure 1).

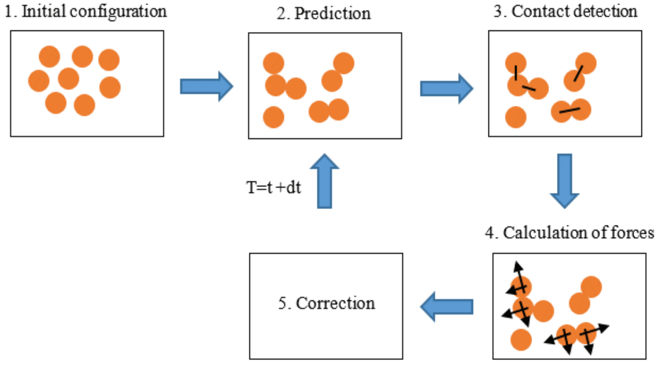

Figure 1: Description of the sequence steps of the discrete element method

The classic schematic is naturally broken down according to the following steps:

1. The initial configuration t_0 or the set of positions, accelerations and velocities of known elements.
2. Determination of particles motions on a time interval [t_i, t_i^*] by performing a prediction of the system configuration ($t_i^* < t_{i+1}$).
3. Searching contacts in the whole domain without any prior knowledge of the contact forces.
4. Calculation of interaction forces between elements.

5. Correction of the system configuration taking into account the contact forces calculated previously.

Spherical or a clump of spherical discrete elements could be used. In the present work, spherical non-cohesive particles have been used. Elasticity, friction, and coefficient of restitution were pre-processed in EDEM® discrete element software to represent the model of a particle interaction.

Currently, the discrete element method is the best used tool to forecast particles flow and distribution by calculating the normal and tangential forces of each particle. The equations are the following:

$$F_n = \frac{4}{3}E_0\delta^{\frac{3}{2}}\sqrt{R_0} - 2\sqrt{\frac{5}{6}}\frac{\ln C_r}{\sqrt{\ln^2 C_r+\pi^2}} + \sqrt{2E_0}\sqrt[4]{R_0\delta}\sqrt{m_0}\vartheta_{nrel} \quad (1)$$

The equivalent young's modulus E_0 of two intermingling particles is obtained by the ensuing formula: $1/E_0 = (1-\vartheta_1^2)/E_1 + (1-\vartheta_2^2)/E_2$. Represents the amount when those two particles overlap and C_r is the coefficient of restitution (defined in EDEM® as the ratio of speed of separation to speed of approach in a collision). The normal overlap δ characterizes the normal deformation of particles.

$$F_t = -8G_0\sqrt{R_0\delta}\delta_t - 2\sqrt{\frac{5}{6}}\frac{\ln C_r}{\sqrt{\ln^2 C_r + \pi^2}} + \sqrt{2G_0}\sqrt[4]{R_0\delta}\sqrt{m_0}\vartheta_{trel} \quad (2)$$

The equivalent shear modulus G_0 of two intermingling particles is obtained by the ensuing formula: $1/G_0 = (2-\vartheta_1)/G_1 + (2-\vartheta_2)/G_2$. δ_t Characterizes the tangential overlap between two particles which in turns represents the tangential deformation and ϑ_{trel} is the tangential constituent of the relative velocity of particles. The tangential overlap is the tangential movement from the first to last contact between two particles, either when one particle begins to roll or slip against another.

A large number of time steps is required to solve the differential equations of the individual particles motions resulting from the theorems of linear and angular momentum. However, the setting of time step has a great impact on the simulation results [17]. In our simulations we fixed the time step at 25% of Rayleigh time step for all the runs.

III. Lacey mixing index

This method is established following some statistical analysis, more precisely via the calculation of the variance of particles concentration. Many studies were conducted using this index and it was revealed to be reliable [18] [19].The following three equations have to be calculated in order to find the index.

$$S^2 = \frac{1}{N-1}\sum_{i=1}^{n}(x_i - x_m) \qquad (3)$$

$$S_0^2 = x_m(1 - x_m) \qquad (4)$$

$$S_R^2 = \frac{x_m(1-x_m)}{n} \qquad (5)$$

Finally, the mixing index is calculated as following:

$$M = \frac{S^2 - S_0^2}{S_R^2 - S_0^2} \qquad (6)$$

where:

S^2 = Variance of the number fraction of white particles in every cell

S_0^2 = Variance of fully unmixed structure

S_R^2 = Variance of fully mixed structure

N = Number of cells

n = Average number of particles in each cell

x_m = average number (concentration) of white particles fraction

x_i = Number of white particles fraction in each cell

IV. Discrete element testing model of the mixer

As shown in Figure 1, due the conjecture that the vertical movement of particles has the highest effect on the mixture, in addition to the long simulation time, only a slice representing the static mixer composed of a rectangular prism chamber and three cylindrical bars which are fixed in the upper part is used for testing. Two configurations of the bars were considered in this study. Dimensions of the testing model of the static mixer and blending elements are listed in Table 1.

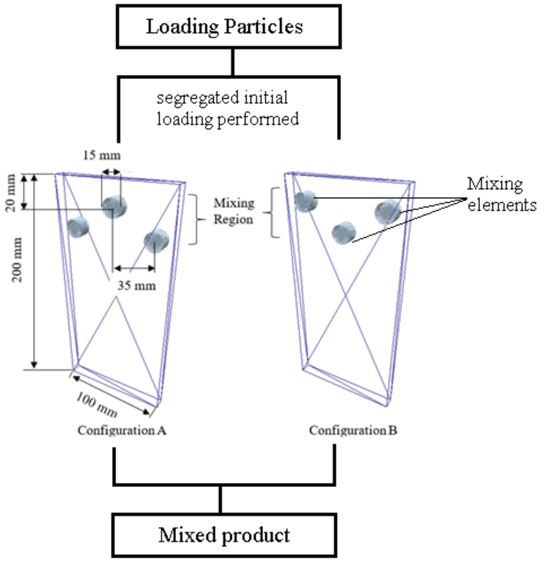

Figure 2: Mixing diagram including the geometry of the static mixer model setup with different configurations of mixing elements

Table 1: Geometrical parameters of the testing models of the static mixer

Parameter	Value (mm)
Static mixer cuboid	
Length	200
Width	100
Thickness	10
Mixing bars	
Diameter	15
Length	10

In this static mixer, the mixing zone consists of three cylindrical bars, the lateral distance between each of the bars was fixed. The three parameters: vertical distance between bars, particles kinetic energy (by giving particles an initial velocity), and particles coefficient of restitution were varied in the numerical experiments. Table 3 shows the simulation cases that were performed in order to investigate the effects of the three forementioned parameters on the mixing efficiency in the static mixer.

Monosized spherical bead particles of diameter 2mm were utilized as granular material. Initially, particles were filled separately through two inlets and the mixed number of particles was kept constant in all simulations to 2000 particles for each group, corresponding to a total number of 4000 particles. The micro-mechanical parameters used for the particles and the mixer are presented in Table 2.

Table 2: Micro-mechanical parameters of the mixer and particles used in simulations

Properties	Particles	Wall	Particle-Wall
Density, ρ (kg/m^3)	2500	2500	-
Young's modulus, E (MPa)	1e6	1e6	-
Coefficient of restitution	0.1, 0.3 and 0.7	-	0.1
Poisson's ratio, υ	0.25	0.25	-
Coefficient of friction, μ	0.5	-	0.5

V. Results and discussions

A. Design of numerical simulations and parameters analysis

In total, 54 simulations were carried out, 27 simulations for each bars configuration to study the mixing efficiency in the static mixer. A full factorial design of experiments has been generated based on the 3 factors, each factor has 3 levels (Table 3).

Table 3: Simulations conducted and their obtained Lacey indices

Run order	Vertical distance between bars (mm)	Particles coefficient of restitution	Particles initial velocity (m/s)	Lacey mixing index (configuration A)	Lacey mixing index (configuration B)
1	40	0.7	5	0.474	0.325
2	60	0.3	2	0.209	0.115
3	60	0.3	5	0.392	0.331
4	40	0.3	0	0.012	0.015
5	20	0.3	2	0.277	0.195
6	20	0.3	5	0.44	0.356
7	60	0.1	0	0.015	0.004
8	40	0.3	2	0.225	0.135

9	60	0.7	0	0.036	0.023
10	20	0.1	0	0	0.007
11	60	0.1	2	0.2	0.123
12	20	0.7	0	0.013	0.004
13	40	0.3	5	0.458	0.309
14	20	0.7	5	0.461	0.385
15	20	0.3	0	0.003	0.013
16	60	0.7	5	0.42	0.361
17	40	0.1	5	0.434	0.299
18	20	0.7	2	0.281	0.202
19	60	0.1	5	0.394	0.339
20	60	0.3	0	0.026	0.007
21	40	0.7	0	0.024	0.019
22	40	0.1	2	0.197	0.117
23	40	0.1	0	0.011	0.022
24	20	0.1	5	0.445	0.369
25	60	0.7	2	0.268	0.151
26	40	0.7	2	0.274	0.169
27	20	0.1	2	0.231	0.172

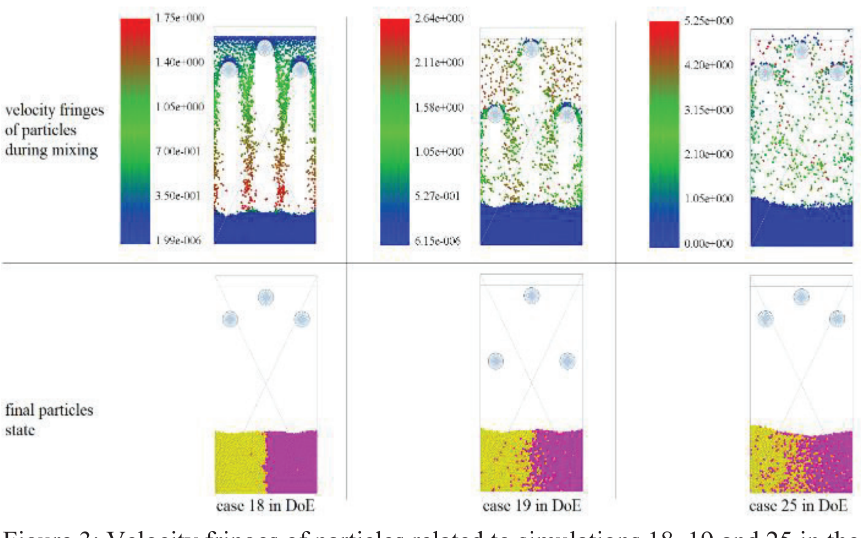

Figure 3: Velocity fringes of particles related to simulations 18, 19 and 25 in the DoE at $t = t_{mixing}/2$ and their related mixture state at the end of the process

Reading the velocity fringes of particles reveals that a higher velocity of particles during mixing gives a better mixture state as in case 25 in DoE.

To make the reading of the DoE results simple, we have calculated the average lacey index in function of every variable. Graphs in Figures 4, 5 and 6 showed that a better mixture could be obtained when the distance between mixing parts is at its minimum and the particles initial velocity and particles coefficient of restitution are at their maximum.

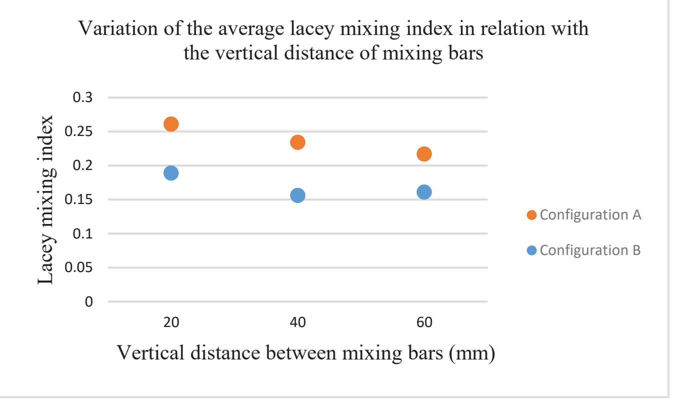

Figure 4: Variation of average mixing index in function of longitudinal distance between mixing bars

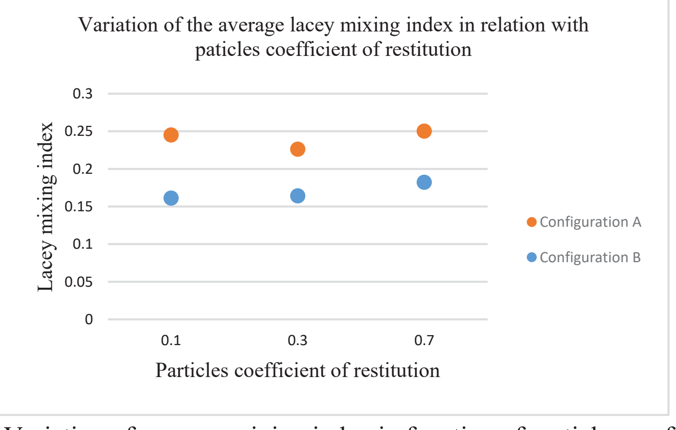

Figure 5: Variation of average mixing index in function of particles coefficient of restitution

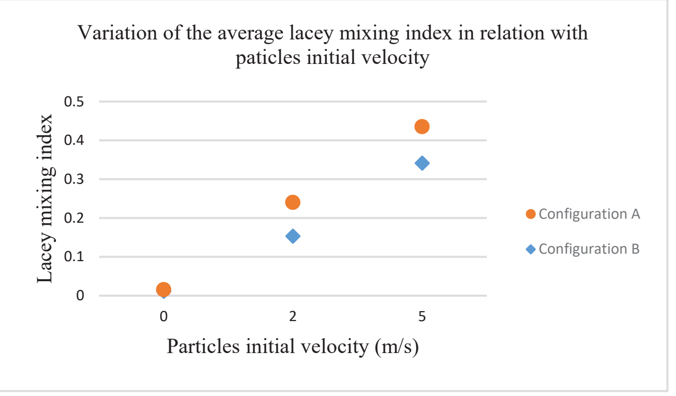

Figure 6: Variation of average mixing index in function of particles initial velocity

B. Optimized discrete element model

The previously conducted testing simulations were used to identify the best parameters that should be considered to get a better mixing quality. Based on that, we created a scaled-up optimized mixer model in this section. A cylindrical mixer having a 100mm radius, the mixer length, mixing bars radii, distance between mixing bars, and particles radii were scaled-up by 1:2. Also, a larger number of particles (50000 particles per group) were mixed as this makes the mixing more challenging.

The homogeneity of the mixture was determined by calculating the Lacey index (section 3), therefore 16 cubic cells resized to the mixture bed were considered. The value of the Lacey mixing index obtained is 0.75. Figure 7 represents the mixture state of particles.

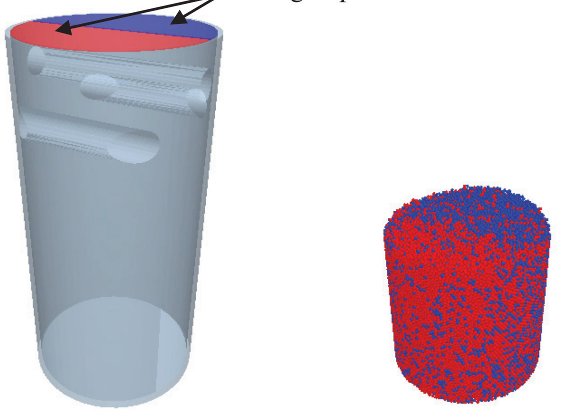

Figure 7: Mixture state obtained by the optimized discrete element model

VI. Conclusions and recommendations

Discrete element simulations were performed in this work. Evaluation of the effects of longitudinal distance between mixing bars, particles kinetic energy and particles coefficient of restitution have been studied for mixing spherical beads in the static mixer. Two configurations of the mixing elements were utilized in the mixer. The following conclusions can be drawn from this study:

- The mixer was shown to be more efficient in mixing the granular bed if particles having higher kinetic energy are considered.
- Particles with higher coefficient of restitution gives a better mixing state.
- A better mixing quality has been achieved when a lesser longitudinal distance between mixing bars is set for all the configurations.
- Mixing elements in "Configurations A" showed a relatively better performance than "Configuration B" in term of mixing efficiency.
- It was revealed by reading fringes post-processed by DEM experiments that particles velocity inside the mixer and mixture state are proportional. Finally, the optimized mixer model

showed a good homogeneity state as the mixing index of Lacey calculated was 0.75.

As for recommendations, more parameters should be studied to improve the efficiency of the mixer. For instance, the number of mixing elements and their configuration inside the mixer could be evaluated. Investigation of the mixed product by letting particles passing through an outlet would be significant as to investigate the mixing uniformity continuously along a process, this could be a case study of this mixer as a continuous mixer. Furthermore, mixing of multicomponent and polydisperse material is of great significance.

VII. Acknowledgement

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