研 究

DEM Simulation of Mixing and Segregation in High-Shear Mixer

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Received March 11, 2002

SYNOPSIS

A high-shear mixer was used to mix a two-component system different only in the density, which was subjected to DEM (Discrete Element Method) simulation. In the first place, the kinetic motion of particles in an agitating vessel was visualized to obtain the information on how particles different in granular density were mixed and segregated. Then, segregation index was defined to clarify the relationship of segregation index and density ratio with operational conditions. The conditions were also clarified for obtaining favorable mixing conditions while segregation was prevented. In other words, it has been pointed out that DEM simulation could be not only employed to readily understand the mixing and segregation conditions of particles in a mixer but also effective in determining optimal operational conditions for obtaining favorable mixing conditions even when the density ratio is different.

KEY WORDS

discrete element method, high-shear mixer, mixing, segregation, optimization

1 Introduction

Mixing of particles is an important operation used frequently in various industrial fields. Because of a wide variety of particles in their size and shape, which are used in mixing operations, the mixing process and the uniformity of mixtures (products) are influenced by the type of a mixer and the operational conditions¹⁻³⁾. The mixing process of particles consists of two actions, namely, mixing and segregation. It has been reported from mixing experiments⁴⁾ and simulations⁵⁻⁹⁾ that difference in the particle diameter or density of starting materials may result in failure to obtain intended mixing conditions. In these reports, a tumbling mixer was often used. It is known that a vessel-fixed type mixer equipped with ribbons or screws develops segregation less frequently compared with a tumbling mixer⁸⁾. However, at the best of our knowledge, no studies have been reported about the relationship between the properties of starting materials and mixing index, with attention focused on a high-shear mixer (granulator) used in many industrial fields among models of tumbling mixers. And in the experiment, it is very difficult to measure particle flow or to take sample powder for evaluating the mixing future in real time.

The authors conducted simulation in a high-shear mixer, with attention given to DEM simulation^{9,10)}. The simulation

could enable us to understand the kinetic motion and mixing state of particles in a mixer easily and economically. It could also provide copiously visual information, which would be unavailable through experiments¹¹⁾. Thus, we are able to not only surmise the relationship of physical properties of particles such as density with mixing process and mixing index, but also examine optimal operational conditions for obtaining favorable mixture.

In this study, a high-shear mixer was used to mix the two-component system different only in the density, which was subjected to DEM simulation to evaluate the kinetic motion of particles in the mixer and the mixing state. The mixture and segregation state in the mixer were visualized, with attention given to the density ratio of the two-component system, in particular. A convenient segregation index was defined and the relationship between the segregation index and the density ratio was studied as well. Further, discussion was made for the condition wherein segregation was prevented by changing the rotational speed of an agitating blade.

2 Simulation

2.1 Simulation method and conditions

Mixing of particles in a high-shear mixer was carried out in accordance with DEM simulation. The methodology

and calculation were the same as those given in the previous report¹²⁾ and will be described briefly as below here.

The Newton's equation of motion was used to determine behaviors of individual particles in the high-shear mixer.

$$m \frac{dv}{dt} = mg + F_{\text{collision}} + F_{\text{wall}} \quad (1)$$

Wherein m represents mass of a single particle; g , gravitational acceleration; $F_{\text{collision}}$, contact force between particles exerting on a given particle; F_{wall} , contact force exerting on between wall surface/agitating blade and target particles. The contact force model consisting of spring, dashpot and friction slider, as shown in Fig. 1, was used to determine the contact force exerting on between particles. This model is characterized by the contact force expressed by using actions of mechanical physics-related fundamental elements consisting of the spring giving repulsion in proportion to displacement as well as the dashpot and the friction slider for considering energy attenuation on contact.

Fig. 2 shows the schematic diagram of a high-shear mixer.

Fig. 1 Contact force model.

Fig. 2 Schematic diagram of a high-shear mixer.

The mixer is 0.16 m in diameter and $1.5 \times 10^{-3} \text{ m}^3$ in effective capacity, and provided with an agitating blade rotating horizontally on the base.

In this study, simulation was carried out for the two-component system different only in the density. The simulation conditions were shown in Table 1. Major particles were allowed to change in the density at 1,500, and 5,000 then 7,800 kg/m^3 , with minor particles kept constant at 2,500 kg/m^3 . Thus, these particles were identical in their particle properties except the density. Although, about real material, the difference of particle density may cause difference in the value of Restitution Coefficient and Friction Coefficient, in this study, this matter was ignored for making calculation faster. Another mixing simulation was conducted where the density of the major particles was kept equal with that of minor particles (2,500 kg/m^3) for grasping the state of mixture and segregation more precisely.

About 30,000 particles were charged into the agitating vessel, which resulted in about 50% charged level. The simulation was conducted at a fixed ratio of the major particles number to minor particles at 1:9. Initial charge was carried out so that the major particles constituted a top layer and minor particles constituted a bottom layer. In this state, the particle was spherical and 3 mm in diameter. The simulation was conducted by changing the rotational speed and total revolution of the agitating blade. The simulation was conducted throughout the processes in a three-dimensional model.

A personal computer with Pentium III 800 MHz and 256 MB memory was used to calculate this simulation. The calculation time per second obtained in the study corresponded to about 7.5 hours in terms of CPU time. Flow and heat analysis software for particle dispersion system (RFLOW Corp.) was adopted.

Table 1 Conditions of simulation.

Model	DEM (soft sphere model) mixing of dissimilar particles
Particle diameter (m)	3×10^{-3}
Particle density (kg/m^3)	1500, 2500, 5000, 7800
Spring constant (N/m)	1200
Restitution coefficient (-)	0.9
Friction coefficient (-)	0.3
Time step (s)	1.0×10^{-4}
Rotational speed of the agitating blade (rps)	4, 8
Number of particles	approx. 30,000
Initial charged state	Top-bottom loading

2.2 Segregation index I

Segregation index I was defined as a convenient way to obtain a quantitative determination of mixture and segregation state in a process of mixing a two-component system with different density. The segregation index I was calculated in the following procedures. A section extending from the rotational axis of the agitating blade to the wall of the vessel (6 mm wide, about 100 mm high and 80 mm long) was designated as shown in Fig. 3. Then, the section was subdivided in some cubic cells to define boundaries present in particles. Thereafter, occupied area fraction of particles in each lattice and the number of major particles were studied on the assumption that in fully randomized mixture (hereinafter pseudo-fully randomized mixture) the major particles present in the section would be homogeneously distributed in particle occupied regime. Namely, we conducted the study, assuming that the number of major particles would be equal per unit area (unit lattice). The following equation was used to quantify the difference between the pseudo-fully randomized mixture and the distribution of major particles, thus obtaining the segregation index I . The segregation index I was convenient and considered appropriate as an index showing the mixture and segregation state of major particles in the agitating vessel.

$$n_i = \sum_{j=1}^k n_{ij} \quad (2)$$

n_i : number of major particles in particle occupied regime

n_{ij} : number of major particles in a cell

k : number of lattice where particles are present

Fig.3 Computation of segregation index.

$$S = \sum_{i=1}^k s_i \quad (3)$$

s_i : area fraction of particles in unit cell, which is assumed to be unity

S : area of particle occupied regime

$$n^* = n_i / S \quad (4)$$

n^* : number of major particles in unit cell in pseudo-fully randomized mixing state

$$\sigma^2 = \frac{\sum_{i=1}^k (n_i - s_i n^*)^2}{k} \quad (5)$$

σ^2 : variance of sample concentration, pseudo-fully randomized mixture

$$I = \frac{1}{N} \sum_{j=1}^N \sigma \quad (6)$$

I : segregation index

σ : standard deviation of sample concentration, pseudo-fully randomized mixture

N : number of sample (number of section)

In order to further clarify the segregated structure, two-component system equal in the density was used to conduct mixing simulation to determine segregation index I_0 and to define segregation index I' from the following equation.

$$I' = I - I_0 \quad (7)$$

Namely, a greater segregation index I' would represent a poorer mixing state, resulting in a marked density-driven segregation.

3 Results and discussion in simulation

3.1 Mixture of particles having different density

Particles greater in the density, those lower in the density and those equal in the density were used to conduct mixing simulation on the basis of particles having 2,500 kg/m³ density for the purpose of studying the mixing state of a two-component system. Major particles on cross section of the agitating vessel were distributed in space to effect visualization, some results of which were exemplified in Figs. 4(a) to (c). In these Figures, black particles (●) represented major particles, with the particle density representing 7,800, 1,500 and 2,500 kg/m³ respectively. On the other hand, white particles (○) represented minor particles having 2,500 kg/m³ density. These Figures showed the results obtained at the rotational speed of the agitating blade $N=8$ rps and total revolution of the agitation blade

Fig.4 Mixed state for 2,500–2,500, 7,800–2,500 and 1,500–2,500 kg/m³ particle system at 8 rps.

$N\theta$ (N , rotational speed of the agitating blade; θ , mixing time)=48. We have confirmed that at this total revolution, the particle motion in the mixer attained a steady state.

Fig. 4(a) confirmed that particles having a greater density (7,800 kg/m³) were more easily susceptible to centrifugal action resulting from the agitating blade rotating at a high speed and intensely segregated around the wall of the agitating vessel. On the other hand, Fig. 4(b) demonstrated that particles having a lower density (1,500 kg/m³) were segregated in the particle bed, in particular, they were segregated locally around upper part in the particle bed. It was considered that particles having a lower density were severely affected by vibration in the agitation vessel to cause this phenomenon. More particularly, it was interpreted as follows: The particles rose upward due to agitation by the agitating blade and then descended due to free-fall to receive the agitation again, the repletion of which causes tapped action, thus forming up and down movement among particles, or vibration field, in the agitation vessel, and this vibration caused the particles having a lower density to rise upward, resulting in segregation.

The segregation process was to be observed from the results obtained by animating the kinetic motion of particles in the agitation vessel over the time. In the first place, the particles having a greater density moved toward the wall of the agitating vessel due to centrifugal action. Since the nearer the particles moved to the wall, or closer to the tip of the agitating blade, the more potent became the agitating action, the particles having a greater density were most susceptible to the agitating action resulting from the blade. As the result, the particles having a greater density were segregated on the wall of the agitating vessel but also observed around the center of particle bed. On the other hand, since particles having a lower density were brought in the particle bed and also segregated to the upper part of the particle bed, they were less susceptible to the agitation

due to the agitating blade. Therefore, the particles having a lower density were hardly observed around the center of the particle bed. The results obtained from observation of the animated kinetic motion of particles have demonstrated that the magnitude of the agitation exerting on segregated particles may be attributable to a more marked segregation found in the particles having a lower density than in those having a greater density.

On the contrary, the two-component system equal in the density did not cause segregation (Fig. 4(c)), namely, mixing two components having an equal density resulted in favorable mixing operation. Difference in the density between two particles to be mixed could result in a poor mixing condition.

Further, the segregation provided by the above-mentioned simulation was in agreement with the experimental results¹¹⁾.

Most mixing operations are to obtain a homogenous mixture. However, segregation makes it difficult to obtain favorable mixture. Thus, procedures are needed, which provide a favorable mixture, while preventing segregation.

Hence, we noticed the rotational speed of an agitating blade and total revolution of an agitating blade $N\theta$ (=time sequence) as a method for preventing segregation resulting from difference in density. Discussion was made for the results obtained by switching the rotational speed of the agitating blade from 8 rps to 4 rps to change the total revolution of the agitating blade $N\theta$. Fig. 5 shows an example of the simulation results obtained for 7,800–2,500 kg/m³ particle system (density ratio $H=3.12$). When the total revolution of the agitating blade was $N\theta=4$, the particles having a greater density (●), which were charged to the upper layer at an initial mixing state were not adequately mixed. It was, however, found that when the total revolution of the agitating blade was $N\theta=12$, those having a greater density were dispersed throughout the

Fig.5 Time sequence of mixed state for 7,800–2,500 kg/m³ particle system at 4 rps.

Fig.6 Time sequence of mixed state for 1,500–2,500 kg/m³ particle system at 4 rps.

particle bed to provide a relatively favorable mixing state. It was also observed that when the mixing was conducted up to $N\theta=48$ (steady state) the particles having a greater density segregated and sank on the base of the vessel. Thus, it was revealed that when the particle system having 7,800–2,500 kg/m³ was mixed at the rotational speed of the agitating blade 4 rps, the major particles, which were perfectly segregated at an initial charge, were then adequately distributed by the agitating blade to segregate and sink on the base of the agitating vessel in association with increase in the total revolution $N\theta$ (longer mixing operation).

Fig. 6 shows another example of the simulation results obtained for 1,500–2,500 kg/m³ particle system. This Figure shows the time sequence of mixed state (total revolution $N\theta$) at the rotational speed of $N=4$ rps. It was observed from the Figure that the particles having a lower density (●) were distributed locally at the upper layer of the particle bed at the total revolution $N\theta \leq 12$. It was, however, found that when steady state $N\theta=48$ was attained, the particles having a lower density were uniformly distributed all over the particle bed to provide a favorable mixture.

Thus, the particle system having 1,500–2,500 kg/m³ (density ratio $H=0.6$) was expected to provide a favorable mixture when the rotational speed of the agitating blade N was changed from 8 rps to 4 rps to reduce the influence resulting from difference in density.

As explained above, DEM simulation conducted for mixing the two-component system different in density enabled us to visualize the mixed/segregated state on the basis of difference in the density. It was also suggested that segregation could be prevented when the rotational speed or total revolution of the agitating speed was taken into account. Then, the next chapter will deal with a quantitative examination on the mixed/segregated state when the previously mentioned segregation index I is used.

Hereinafter, $N=8$ rps is called high rotational speed; $N=4$ rps, low rotational speed; $N\theta=24$, short mixing operation and $N\theta=48$, long mixing operation, respectively in a convenient way.

3.2 Relationship between segregation index, total revolution of an agitating blade and density ratio

Fig. 7 shows the relationship between segregation index I and density ratio H (=density of major particles/density

Fig.7 Relationship between segregation index I and ratio of particle density H .

of minor particles). This Figure also covers the results obtained for the total revolutions, $N\theta = 24$ and 48, at the rotational speeds, $N = 4$ rps and 8 rps. Here, the result of $H = 1$ shows mixed state for the particle system equal in density ($2,500\text{--}2,500\text{ kg/m}^3$). Thus, a greater difference in the segregation index I at $H = 1$ would cause the density-driven segregation and result in a poorer mixing state accordingly.

We noticed the result of $N\theta = 48$ (◆) at the high rotational speed of an agitating blade, $N = 8$ rps. The segregation index I showed greater values as the density ratio increased from $H = 1$ to $H = 2$ ($5,000\text{--}2,500\text{ kg/m}^3$ system) and to $H = 3.12$ ($7,800\text{--}2,500\text{ kg/m}^3$ system), and resulted in apparently poor mixture. As shown from the result of Fig. 4(a), it was interpreted that the particles having a greater density were more susceptible to centrifugal effect and segregated around the sidewall of the agitating vessel. It was also found that the segregation index at the density ratio $H = 0.6$ was greater than that at the density ratio $H = 3.12$. This was considered due to the fact that in the two-component system at $H = 0.6$ ($1,500\text{--}2,500\text{ kg/m}^3$ system), particles with a lower density were segregated intensely around the upper part in the particle bed, as given in Fig. 4(b). It was, thus, found that when a high-shear mixer was used to mix two-component system different in the density at the high rotational speed of $N = 8$ rps, particles with a lower density showed more intense segregation as compared with those having a greater density. The result quantitatively represented the visualized state.

It was found that the segregation index I at the rotational speed $N = 8$ rps provided a slightly greater value when the total rotation was conducted at $N\theta = 48$ (◆) than when at $N\theta = 24$ (◇) at any density ratio ($H = 0.6, 2$, or 3.12). Animated observation results also confirmed that a marked segregation emerged very soon after agitation at the high rotational speed of 8 rps.

Then, we noticed the results obtained for the low rotational speed of an agitating blade, $N = 4$ rps, (○, ●). It was apparent that the segregation index I changed greatly as the total revolution (mixing time) increased. More particularly, $1,500\text{--}2,500\text{ kg/m}^3$ system at $H = 0.6$ showed a segregation tendency (○) at $N\theta = 24$ but showed the similar value as with the two-component system equal in the density when it was further agitated to attain $N\theta = 48$ (●, long time mixing). $N\theta = 48$ prevented density-driven segregation and successfully provided a mixture similar to that obtained for the two-component system equal in the density.

The segregation index I for $7,800\text{--}2,500\text{ kg/m}^3$ particle system at $H = 3.12$ provided a greater value when the total rotation $N\theta = 24$ (○ short mixing operation) was switched to $N\theta = 48$ (●), which was reverse to the result obtained at $H = 0.6$. This was due to the fact that the particles having a greater density segregated and sank on the base of the agitating vessel more intensely as the mixing operation proceeded. Therefore, it would be advisable to stop the agitating operation prior to the process where the particles having a greater density segregated and sank at the low rotational speed when the $7,800\text{--}2,500\text{ kg/m}^3$ particle system having a greater density was mixed.

3.3 Relationship between segregation index I and Froude number Fr

Froude number represents the ratio of the centrifugal force to the gravity force and is used as a criterion for the mixing performance of a mixer and scale-up. Figs. 8 and 9 show the relationship between segregation index I and Froude number $Fr (= R_{\max} \omega^2 / g; R_{\max}$: diameter in the vessel, ω : angular velocity, g : gravitational acceleration).

Figs. 8 and 9 show the results obtained at the total revolutions, $N\theta = 24$ and 48, respectively. In the Figures, segregation index I' obtained from equation (6) was indicated by arrow. It was apparent from Fig. 8 that I' s obtained from $1,500\text{--}2,500\text{ kg/m}^3$ particle system ($H = 0.6$, ■) and $7,800\text{--}2,500\text{ kg/m}^3$ particle system ($H = 3.12$, ▲) became smaller as $Fr = 132 \times 10^{-3}$ (rotational speed of an agitating blade, $N = 8$ rps) was lowered to $Fr = 33 \times 10^{-3}$ (4 rps). It was confirmed that I' obtained from $1,500\text{--}2,500\text{ kg/m}^3$ particle system, in particular, was clearly decreased.

Fig. 8 Relationship between segregation index and Froude number after 24 revolutions.

Fig. 9 Relationship between segregation index and Froude number after 48 revolutions.

Therefore, it was demonstrated that short mixing operation at low rotational speed of an agitating blade could effectively prevent segregation even when the density was different to some extent.

I' obtained from the 1,500–2,500 kg/m³ particle system (▲), as shown in Fig. 9, was found clearly decreased in comparison with $Fr = 132 \times 10^{-3}$ (8 rps) when mixing operation was conducted at $Fr = 33 \times 10^{-3}$ (4 rps). It was reconfirmed that mixing operation at around $Fr = 33 \times 10^{-3}$ could provide favorable mixing state similar to that obtained

for the system equal in the density (◆). On the contrary, it was found that I' obtained for 7,800–2,500 kg/m³ particle system (■) became greater when the number was changed from $Fr = 132 \times 10^{-3}$ to $Fr = 33 \times 10^{-3}$, which was reverse to the result obtained for the 1,500–2,500 kg/m³ particle system, showing a greater segregation tendency.

4 Conclusions

A high-shear mixer was used to mix two-component system different in the density, which was subjected to discrete element method simulation. In the first place, the kinetic motion of particles in the agitating vessel was visualized to obtain the information on how particles with different granular size were mixed and segregated. Then, the relationship of the segregation index and density ratio with operational conditions was clarified. Further, conditions were examined where favorable mixing state was obtained while segregation was prevented. The results and discussion so far obtained from the simulation have confirmed that adjustment of the rotational speed and the total revolution of an agitating blade $N\theta$ (agitating time θ) can prevent segregation and provide favorable mixture when a high-shear mixer is used to mix the two-component system different only in the density.

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