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Discrete particle simulation of a rotary vessel mixer with baffles

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Abstract

The three-dimensional motion of all particles in a rotating mixer with two baffles was calculated using the discrete particle simulation. This simulation dealt with the mixing of single-component spherical particles which fill the mixer half-way. The effect of the baffles on the particles' motion and on particle mixing was studied. It was found that the mixing curve, which shows the relationship between the degree of mixing and time, agreed well qualitatively with previous experimental results. The present simulation predicts that there is an optimal baffle length/height ratio for particle mixing, and that the deformation pattern of the particle bed is affected by the baffles. © 1997 Elsevier Science S.A.

Keywords: Simulation; Discrete element method; Rotary mixers; Baffles; Mixing curve

1. Introduction

Mixing of particles or powder is widely used in various processes such as in the chemical, pharmaceutical and food industries, just to name a few. This is one of the most important operations which controls the quality of products in powder processes. In order to improve the efficiency of mixing, it is important to know how particles behave in an apparatus.

Many experimental studies [1–3] have been directed toward the investigation of particle behavior. However, it is difficult to observe the three-dimensional behavior of particles directly in the experiments, because particles in the bed are invisible. Measurements are generally done by taking samples from the bed [2] or by using probes inserted into the bed [3]. These measurements require much labor and involve sampling errors. Furthermore, the particle bed is inevitably disturbed in these methods. Therefore, it is hard to investigate the detailed behavior of particles experimentally.

On the other hand, numerical simulations of particle mixing have already been done by several researchers. Chan and Fuerstenau [4] studied the simulation of diffusive mixing, using the Monte Carlo method, for axial mixing in an end-loaded barrel mixer. Inoue and Yamaguchi [5] used probabilistic methods to simulate the mixing process in a two-dimensional V-shaped mixer. The simulation of the particle mixing processes was carried out by using the particle transition probability data. These techniques, however, require experimental data such as the main stream pattern of particle flow or the probability of particle transition. Therefore, similar limitations to those in the experiments remained in the previous numerical simulations.

Recently, the discrete element method (DEM) which treats the motion of individual particles has been applied to calculate particulate flows [6–9]. Computers with large storage and high performance processing units incorporate a large number of particles in the simulations. The particle motion is calculated from the equation of motion by taking into account the contact forces. These forces are given by a simple mechanical model. The DEM makes it possible to calculate the particle motion without requiring prior knowledge of experimental data about the particle flow.

In this work, the DEM is applied to simulate the three-dimensional motion of all individual particles in a rotating mixer with two baffles. The present simulation deals with the mixing of spherical monosized particles which fill the mixer half-way. Results of the simulation are evaluated for mixing processes by using mixing curves. The effect of the baffles on the particle mixing and on the motion of particles is studied.

2. Dimensions of the mixer

The tumbling mixer, a type of rotary vessel mixer, used in this work is shown schematically in Fig. 1. This mixer con-

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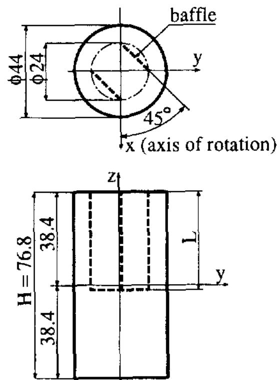

Fig. 1. Configuratoin of the mixer.

sists of a cylindrical vessel, 44 mm in diameter, 76.8 mm in height, with two baffles fixed on one end and making an angle of 45° with the axis of rotation. The axis of rotation coincides with the x-axis.

3. Equations and conditions of calculation

A rotating coordinate system fixed on the mixer is used to describe the particle motion, because it is convenient to express the boundary conditions for the rotating walls. When the mixer rotates at an angular velocity vector $\boldsymbol{\Omega}$, then the equations of translational and rotational particle motion are given by

$$\ddot{\boldsymbol{r}}=\frac{\boldsymbol{F}}{m}-2\boldsymbol{\Omega}\times\dot{\boldsymbol{r}}-\dot{\boldsymbol{\Omega}}\times\boldsymbol{r}-\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{r})+\boldsymbol{g} \quad (1)$$

$$\dot{\boldsymbol{\varphi}}=\frac{\boldsymbol{T}}{I}-\boldsymbol{\Omega}\times\boldsymbol{\varphi}-\dot{\boldsymbol{\Omega}} \quad (2)$$

where $\boldsymbol{r}$ is the particle position vector, m the particle mass, $\boldsymbol{F}$ the sum of the contact forces acting on the particle, $\boldsymbol{g}$ the gravitational acceleration vector, $\boldsymbol{\varphi}$ the angular velocity vector of the particle, $\boldsymbol{T}$ the net torque caused by the contact forces, and I the moment of inertia of the particle.

The contact force between particles is expressed by the contact force model as shown in Fig. 2. Some models [6–8] have been proposed concerning the parameters in the model. The model proposed by Tsuji et al. [8], which gives the Hertzian contact force and a constant coefficient of restitution, is applied to the present simulation.

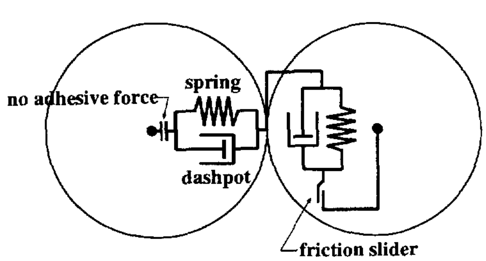

Fig. 2. Model of the contact force.

Table 1
Conditions of simulation

Particle diameter	2.0×10^{-3} m
Particle density	2.7×10^{3} kg/m^3
Young's modulus of elasticity for particles	10^5 Pa
Coefficient of restitution	0.6
Coefficient of friction	0.3
Coefficient of restitution against wall	0.6
Coefficient of friction against wall	0.3
Number of particles	9000
Rotational speed of vessel	30 rpm (3.14 rad/s)
Length/height ratio of mixing baffle, L/H	0.0–1.0

The conditions of the simulation are given in Table 1. The present simulation dealt with the mixing of single-component particles distinguished only by color. The number of particles, 9000, amounts to half the volume of the mixer. The size of the mixer is taken to be much smaller than that of the industrial mixer in order to reduce the number of particles treated in the simulation. The angular velocity of the mixer, $\boldsymbol{\Omega}$, is based on the Froude number Fr, which is defined by

$$Fr=\frac{\Omega^2(H/2)}{g} \quad (3)$$

where H is the height of the mixer. In the rotary mixer, Fr generally takes a value of less than 1.0. If Fr is much bigger than 1.0, the effect of the centrifugal force overcomes the effect of the gravitational force, making all the particles stick to the wall. In this work $Fr=0.4$ is used.

4. Results and discussion

The initial condition was calculated by the following procedure. Particles were placed randomly in the mixer and were allowed to fall freely under gravity inside the mixer. The motion of the particles decayed and finally they came to rest. This condition was used as the initial condition. The non-dimensional time τ is normalized by the period of rotation $2\pi/\Omega$. Snapshots of particle mixing are arranged sequentially from the initial condition to half a revolution in Fig. 3. Though there is no experiment corresponding to the present condition, it can be seen from the figures that the calculated particle motion in the mixer shows realistic patterns.

4.1. Mixing curve

The mixing process of the present simulation was investigated by using the mixing curve which is the relation between the degree of mixing and time. The degree of mixing was evaluated by the following method.

At the initial condition of calculation, the particle bed was divided into two layers of particles as shown in Fig. 3(a) in which particles belonging to the lower layer were colored. The degree of mixing was evaluated by using these two groups of particles at every cycle of revolution from $\tau=1.1$,

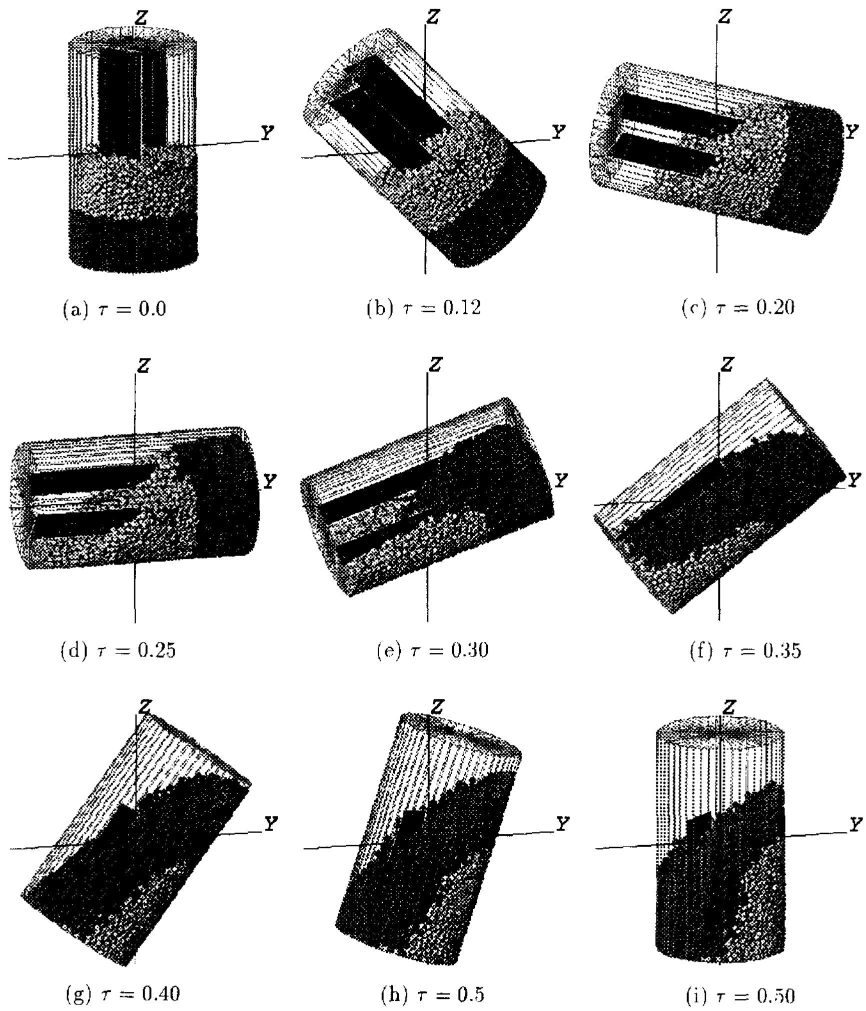

Fig. 3. Snapshots of particle mixing.

when the free surface of the particle bed was nearly parallel to the bottom wall.

To evaluate the degree of mixing, the particle bed was divided into small cells as shown in Fig. 4. Each cell has the same volume. The standard deviation σ for the proportion of colored particles in each cell is given by

$$\sigma = \left[\frac{\sum_{i=1}^{N} (x_i - \bar{x}_c)^2}{N-1} \right]^{1/2} \tag{4}$$

where x_i is the proportion of colored particles in cell i, $\bar{x}_c$ is the overall proportion of colored particles, and N is the number of cells.

The degree of mixing is defined by

$$\sigma / \sigma_0 \tag{5}$$

The suffix 0 denotes the completely unmixed state. σ_0 is given by [1]

$$\sigma_0 = [\bar{x}_c(1-\bar{x}_c)]^{1/2} \tag{6}$$

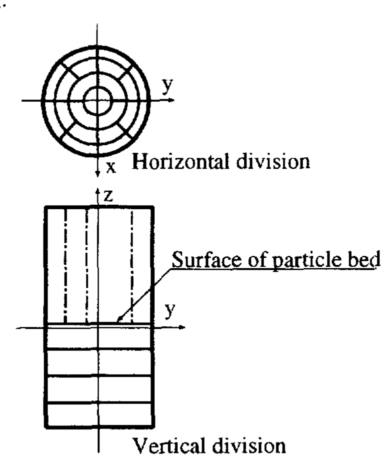

Fig. 4. Division of sampling cells.

On the other hand, for the completely random mixture (indicated by subscript r) it is given by

$$\sigma_r = [\bar{x}_c(1-\bar{x}_c)/n]^{1/2} \tag{7}$$

where n is the average number of particles in each cell. In these equations, N, n and $\bar{x}_c$ take the approximate values of 84, 107 and 0.5, respectively.

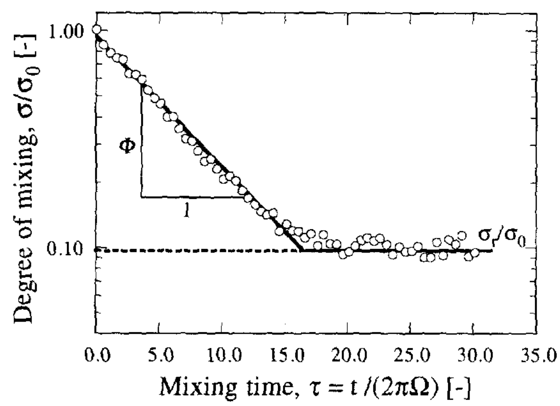

Fig. 5. Mixing curve at $L/H=0.6$.

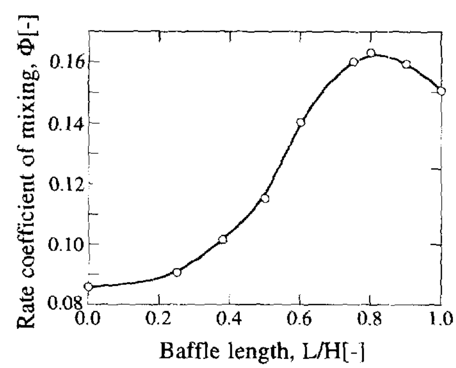

Fig. 6. Relation between the rate coefficient of mixing, Φ, and the baffle length.

Fig. 5 shows an example of the mixing curve predicted by the present simulation. A plot of the degree of mixing on the natural log scale versus time yields straight lines. The mixing process is classified into two stages. In the first stage of the mixing, $\ln(\sigma/\sigma_0)$ decreases with the slope $-\Phi$. In the second stage, $\ln(\sigma/\sigma_0)$ takes the constant value of the random mixture which is given by $\ln(\sigma_r/\sigma_0)$. Previous experimental studies [1,10] revealed that the mixing process which consists of these two stages is typically observed in the mixing of non-adhesive particles. Therefore the results of the present simulation compared qualitatively well with the previous experimental results.

The slope Φ is called the rate coefficient of mixing [1,10]. Φ indicates the effectiveness of a machine as a mixer. The larger the mixing rate, the larger the rate coefficient of mixing.

4.2. *Effect of baffle length*

Since the baffle length is a principal parameter of this type of mixer, the effects of the baffle length on the motion of particles and the mixing rate were studied. Simulations were carried out with the same initial condition for several baffle lengths.

Results of simulations were characterized by the rate coefficient of mixing, Φ. Fig. 6 shows the relationship between the baffle length and Φ. Clearly, the mixing rate is improved by the baffles. Another significant feature of this relation is that Φ takes a maximum value at $L/H=0.8$.

To see the effect of baffles on the particle motion, further deformation patterns of the particle bed per cycle of vessel revolution were visualized.

The mixing progresses rapidly in the first stage in which Φ is estimated. Since large-scale mixing is driven by the convective motion of the particle bed [1,10], it is important to see the convection pattern. The deformation pattern of the particle bed represents the convection. To visualize the deformation pattern, the particles were divided into five vertical layers and colored as shown in Fig. 7. Pattern (a) was used to see the deformation in the x–z plane, with pattern (b) in the y–z plane.

Deformation patterns are shown in Fig. 8 for six values of the baffle length/height ratio. A distinct change in the defor-

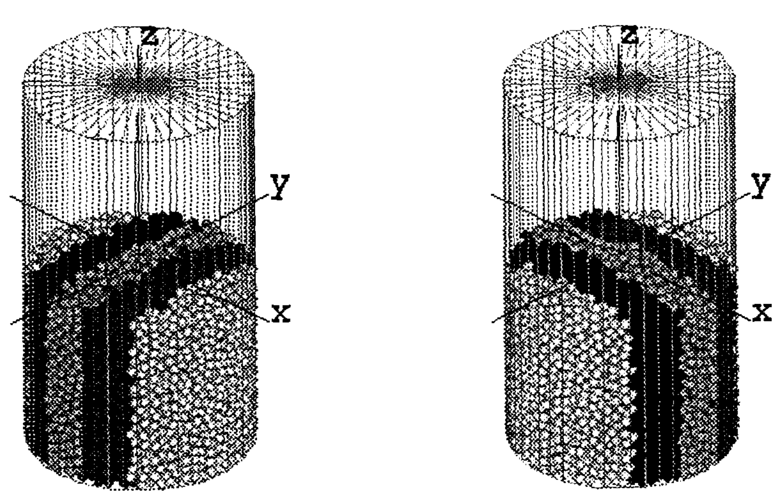

Fig. 7. Initial conditions for observation of the deformation of the particle bed.

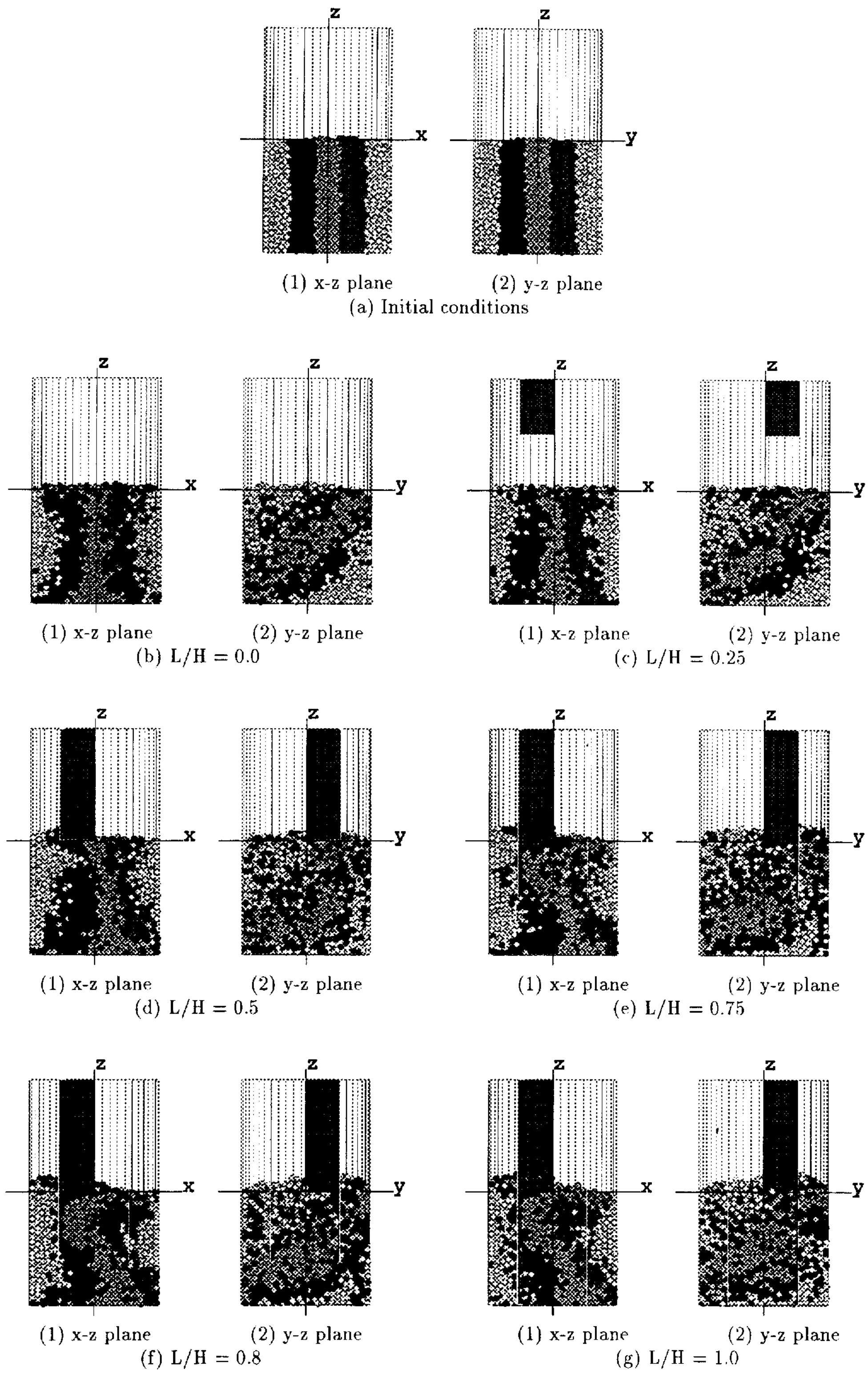

Fig. 8. Cross-section of the particle bed.

mation pattern is observed in the x–z plane, but not in the y–z plane. This result shows that the baffles make a contribution to the particle convection in the x–z plane which involves the rotating axis. Thus, attention is focused on the deformation in the x–z plane. In the case of $L/H<0.8$, the deformation increases with increasing baffle length. When L/H is larger than 0.5, large shear occurs around the end of the baffles. This effect causes a large increase in mixing rate as shown in Fig. 6. In the case of $L/H>0.8$, the clearance between the end of the baffles and the bottom of the vessel is so narrow that the shear becomes smaller as the baffle length increases. This tendency in the deformation pattern is consistent with the change in the rate coefficient of mixing.

5. Conclusions

The three-dimensional motion of all individual particles in a rotating mixer with baffles was calculated using the discrete particle simulation. The principal results are as follows.

1. The mixing curves obtained by the present simulation depict well the two distinct stages which are the typical characteristics observed in the experiments.

2. The present simulation predicts that the mixing rate is improved by the baffles, and there is an optimal length/height ratio of the baffles.

3. The deformation patterns of the particle bed have been visualized. The effect of baffles on the deformation pattern is consistent with the result of the particle mixing rate.

6. List of symbols

$\boldsymbol{F}$	contact force vector
Fr	Froude number of mixing
$\boldsymbol{g}$	gravity acceleration vector
H	height of mixer
I	moment of inertia of particle
L	length of baffles
m	particle mass
n	average number of particles in sample
N	number of samples
$\boldsymbol{r}$	particle position vector
$\boldsymbol{T}$	torque
x_i	proportion of colored particles in sample i
$\bar{x}_c$	overall proportion of colored particles

Greek letters

σ	standard deviation of samples
σ_0	standard deviation for unmixed material
σ_r	standard deviation for completely randomized mix
τ	non-dimensional time
$\boldsymbol{\varphi}$	angular velocity vector of particle
Φ	rate coefficient of mixing
$\boldsymbol{\Omega}$	angular velocity vector of mixer

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