Original Paper

Application of DEM Simulation to an Intensive Mixer

Chiharu TOKORO¹, Tatsuya YAMASHITA², Hidetoshi KUBOTA²
and Shuji OWADA¹

¹Department of Resources and Environmental Engineering, School of Creative Science and Engineering,
Faculty of Science and Engineering, Waseda University

²Major in Earth, Resources and Environmental Engineering, Graduate School of Creative Science
and Engineering, Waseda University

Abstract

The discrete element method (DEM) was applied to describe the basic characteristics of particles in an intensive mixer that is expected to grind only the surfaces of particles with a particular agitator and is applied in many industries. Surface grinding experiments using a sample of bauxite particles were also conducted to compare with the simulation. The roles of the pan and agitator were estimated from the DEM simulations and it was revealed that employing only agitator rotation increases the particle mobility in the vertical direction, while employing both pan and agitator rotation increases the mobility in the horizontal direction and stably maintains large mobility in the vertical direction.

We also investigated the correlation between the rates of energy dissipation during interparticle contact calculated from DEM simulation results and the abrasion rate estimated from experimental results. The abrasion rate was estimated from the particle size distribution obtained from the surface grinding experiments using an intensive mixer charged with bauxite particles and a population balance model in which two mechanisms of attrition—abrasion and fracture—are considered. The results show that the abrasion rate decreased with an increase in energy dissipation due to friction, which suggests that the energy dissipation of the friction obtained from the DEM simulation results could be used to estimate the abrasion rate in the surface grinding process.

Key words: Intensive mixer, Discrete element method, Surface grinding, Bauxite, Abrasion rate

1. Introduction

The discrete element method (DEM)¹ is an attractive simulation method for analyzing a non-continuous or nonlinear flow of particles in which multibody interactions are dominant. The DEM has been applied to many granular material systems such as a fluidized bed², solid/liquid or solid/gas multiphase flow³, solid/solid separator⁴, and debris flow⁵. Tumbling mills are an example of the successful application of DEMs in mineral processing or resource recycling research, and application has involved particle behavior prediction, power draft estimation, liner and lifter design, and

micro-scale modeling for calculation of the size distribution^{6–9}.

The objective of this study is an application of a DEM to describe the basic characteristics of particles in an intensive mixer that is expected to grind only the surfaces of particles with a particular agitator and is used in many industries such as chemical, ceramic, and environmental fields. For example, we have demonstrated the effectiveness of an intensive mixer in cleaning shooting range soil contaminated by lead^{10,11}.

An intensive mixer is also effective for the surface grinding of bauxite ore, the raw material in alumina refining¹². In general, the surface of bauxite ore concentrates clays such as kaolinite. These clays result in a residue called red mud after aluminum hydroxide or oxide is produced from bauxite. The annual amount of waste red mud produced in Japan is 0.6 million tons and almost all is dis-

Paper presented at the 6th Japan/Korea International Symposium on Materials Science and Resources Recycling, 20–21 November 2008, Pohang, Korea
Accepted 2 July, 2009

carded into the ocean. Because of the harm caused to the environment, reduction of the amount of red mud is a pressing issue; and because ocean disposal is being increasingly restricted, alternative disposal methods must be implemented. Surface grinding in which Kaolinite is removed selectively from bauxite ore is a possible method for reducing the amount of red mud.

This paper reports detailed DEM simulation results for an intensive mixer to estimate the roles of two rotating parts of the mixer: the pan and agitator. We also investigate the correlation between the rate of energy dissipation during interparticle contact calculated from DEM simulation results and the abrasion rate estimated from experimental results. The abrasion rate is calculated from the particle size distribution obtained in surface grinding experiments using an intensive mixer charged with bauxite and the population balance model in which two mechanisms of attrition—abrasion and fracture—are taken into consideration¹³.

2. Materials and methods

2.1 DEM simulation

In the present work, RFLOW¹⁴ was used as DEM simulation software. DEM modeling used in this study is based on the original DEM concept proposed by Cundall and Strack¹, and contact between a particle and a particle or wall is modeled using a Voigt model consisting of a spring and dashpot in normal and tangential directions. A slip model defined by the friction coefficient is included for the tangential force. A linear contact model is adopted to reduce the computation load.

Table 1 gives parameter values used in the DEM simulation. These values are substituted for physical properties of bauxite used in the surface grinding experiments as described later. Although actual bauxite particles have a size distribution and irregular shape, monodispersed spherical particles are used in the simulation to simplify the calculation. A virtual small spring constant was used to reduce the computational load, which has little effect on the DEM simulation results.

Park and Wassgren¹⁵ proposed that the rates of energy dissipation in the normal and tangential dashpots and tangential frictional sliding element are respectively

$$P_{n,dashpot} = \eta_n (\Delta \dot{\mathbf{x}}_{n,ij} \cdot \mathbf{n}_{ij})^2, \quad (1)$$

$$P_{t,dashpot} = \eta_t (\Delta \dot{\mathbf{x}}_{t,ij} \cdot \mathbf{s}_{ij})^2, \quad (2)$$

$$P_{friction} = \mu |\mathbf{F}_{n,ij}| (\Delta \dot{\mathbf{x}}_{n,ij} \cdot \mathbf{s}_{ij})^2, \quad (3)$$

Table 1 Parameter settings for DEM simulation.

Parameter	Value
Pan diameter	0.235 m
Pan height	0.272 m
Pan angle of inclination	30°
Pan rotation speed	900–5000 rpm
Agitator diameter	0.138 m
Agitator height	0.2695 m
Agitator rotation speed	–42 rpm
Number of blades	7
Particle diameter	4.0 mm
Particle density	2580 kg/m ³
Number of particles	53770
Particle/particle and particle/wall spring constant	1.0 × 10 ³ N/m
Particle/particle and particle/wall dashpot coefficient	0.41
Particle/particle friction coefficient	0.72
Particle/wall friction coefficient	0.48
Simulation time step	1.0 × 10 ^{–5} s

where η and μ are the dashpot and friction coefficients respectively, $\Delta \dot{\mathbf{x}}$ is the velocity of particle i relative to particle j at the contact point, and $\mathbf{n}_{ij}$ and $\mathbf{s}_{ij}$ are the unit vectors pointing from the center of particle i to the center of particle j in the normal and tangential directions respectively. Subscripts n and t denote the normal and tangential direction values respectively. We used these equations to calculate the rates of energy dissipation from the DEM simulation results.

2.2 Experimental

2.2.1 Preparation of bauxite particles

The material used in this study was bauxite ore from Gove, Australia. All samples were dried at ambient temperature for more than two days and screened into nine fractions, the smallest fraction being particles smaller than 0.125 mm. This was followed by chemical composition analysis using X-ray fluorescence (PW1480/1404, Philips). The particle distribution and composition of the bauxite are given in Figures 1 and 2. In Figure 2, the vertical and horizontal axes respectively show the weight percentages of minerals and size fractions, with the area of each composition indicating its ratio to the whole sample. These figures show that the weight ratio of kaolinite increased as the particle size decreased and 50 wt.% of kaolinite was found to be in the 0.5–4 mm particle size fraction. The distributions of Si and Al for the bauxite particles 0.5 mm or larger were observed by scanning electron microscopy and energy dispersive X-ray spectroscopy (SEM/EDS, JSM-6360, JEOL), as shown in Figure 3. Al was ubiquitous in the baux-

Fig. 1 Particle size distribution of bauxite particles in the sample used for the surface grinding experiments.

Fig. 2 Chemical compositions of bauxite particles in the sample used for the surface grinding experiments.

ite particle, while Si was on the surface layer and represented a kaolinite-rich layer. These results show that the surface grinding of bauxite in the 0.5–4 mm of size fraction is expected to be an effective method for removing kaolinite selectively from bauxite and hence reducing the amount of red mud.

2.2.2 Surface grinding experiments

An intensive mixer (R02 type, Eirich) with a total volume of 5 L was used for all experiments. A target volume of bauxite sample in the 0.5–4 mm size fraction was added to the mixing vessel so that the total volume of the sample was 3 L. The residence time and rotational speed were respectively adjusted to 1 min and 900–5000 rpm. The bauxite sample after grinding experiments was screened into nine fractions and then its chemical composition was determined by X-ray fluorescence analysis.

2.2.3 Population balance model

The kinetic theory of grinding, which involves integral and differential equations and a particle selection function and particle breakage function, was reviewed by Austin¹⁶. The population balance

Fig. 3 SEM/EDS images of bauxite particles: (a) SEM image of the particle, (b) Al elemental analysis, (c) Si elemental analysis.

equation in a particle size fraction D is given by

$$\frac{\partial P(D,t)}{\partial t} = \int_D^{D_{\max}} S(d)B(D,d)\frac{\partial P(d,t)}{\partial d}dd, \quad (4)$$

where d and D are the particle sizes, $D_{\max}$ is the maximum size of the particles, t is the grinding time, $P(D, t)$ is the undersize distribution, $S(d)$ is the selection function, and $B(D, d)$ is the breakage function. Ouchiyama, et al.¹³ proposed a model in which two mechanisms of attrition were considered, namely abrasion and fracture, and the mechanisms were combined with a population balance equation. In their model, the population balance equation is

$$\begin{aligned} \frac{\partial P(D,t)}{\partial t} = & \int_D^{D_{\max}} S_a(d)B_a(D,d)\frac{\partial P(d,t)}{\partial d}dd \\ & + \int_D^{D_{\max}} S_f(d)B_f(D,d)\frac{\partial P(d,t)}{\partial d}dd, \end{aligned} \quad (5)$$

where subscripts a and f denote the abrasion and fracture respectively. The abrasion mechanism was simplified so that degradation of a particle is linear relative to grinding time, and a large number of extremely small daughter particles are produced. The population balance equation thus becomes

$$\begin{aligned} \frac{\partial P(D,t)}{\partial t} = & 3 \int_D^{D_{\max}} \frac{K_a}{d} \frac{\partial P(d,t)}{\partial d}dd \\ & + K_a \frac{\partial P(D,t)}{\partial D}, \end{aligned} \quad (6)$$

where K_a is the abrasion rate. The following simple mathematical models were assumed for the selective and breakage functions of particle degradation due to the mechanism of fracture.

$$S_f(d) = K_f d^n, \quad (7)$$

$$B_f(D, d) = \left(\frac{D}{d}\right)^m, \quad (8)$$

where K_f , n , and m are taken as constants independent of both size and time. Substituting Eqs. (7) and (8) into Eq. (4) gives an expression for the mechanism of fracture alone:

$$\frac{\partial P(D, t)}{\partial t} = K_f D^m \int_D^{D_{\max}} \frac{\partial P(d, t)}{\partial d} \cdot \frac{1}{d^{m-n}} dd. \quad (9)$$

Degradation by the combined mechanisms of abrasion and fracture can be described by combining Eqs. (6) and (9), giving

$$\begin{aligned} \frac{\partial P(D, t)}{\partial t} = & 3 K_a \int_D^{D_{\max}} \frac{\partial P(d, t)}{\partial d} \cdot \frac{1}{d} dd \\ & + K_a \cdot \frac{\partial P(D, t)}{\partial D} \\ & + K_f D^m \int_D^{D_{\max}} \frac{\partial P(d, t)}{\partial d} \cdot \frac{1}{d^{m-n}} dd. \end{aligned} \quad (10)$$

The distribution function in Eq. (10) can be substituted with dimensionless sizes and time, giving

$$\begin{aligned} \frac{\partial P(x, T)}{\partial T} = & 3 \alpha \int_x^1 \frac{\partial P(y, T)}{\partial y} \cdot \frac{1}{y} dy \\ & + \alpha \frac{\partial P(x, T)}{\partial x} \\ & + (1 - \alpha) x^m \int_x^1 \frac{\partial P(y, T)}{\partial y} \cdot \frac{1}{y^{m-n}} dy. \end{aligned} \quad (11)$$

where x and y are the dimensionless size of a particle and T is the dimensionless grinding time, which are defined as

$$x = \frac{D}{D_{\max}}, \quad y = \frac{d}{D_{\max}}, \quad (12)$$

$$T = \left(\frac{K_a}{D_{\max}} + K_f D_{\max}^n \right) t. \quad (13)$$

The parameter α depends upon the prevailing mechanism of degradation, such that $\alpha = 1$ for abrasion and $\alpha = 0$ for fracture, and it is defined as

$$\alpha = \frac{K_a / D_{\max}}{K_a / D_{\max} + K_f D_{\max}^n}. \quad (14)$$

Fig. 4 DEM simulation snapshots of the intensive mixer for pan rotation only.

In this study, Eqs. (11)–(14) were numerically solved using the trapezoidal method for the integral equation and the finite difference method for the differential equation, and the abrasion rate K_a was estimated from the fitting the results to the experimental results for the size distribution.

3. Results and discussion

3.1 Effects of the pan and agitator

Simulation snapshots are presented in Figures 4–6 for only pan rotation, only agitator rotation, and both pan and agitator rotations respectively. Particles in the intensive mixer are given one of three colors according to their initial horizontal positions. Particles are well mixed for the case in which both the pan and agitator rotate while they are not mixed so well for the case of only pan or agitator rotation.

For more quantitative investigation, normalized particle mobility in the vertical and horizontal directions is introduced using

$$M_h = \frac{\sum_i |\Delta r_i|}{NR}, \quad M_v = \frac{\sum_i |\Delta h_i|}{NH}, \quad (15)$$

Fig. 5 DEM simulation snapshots of the intensive mixer for agitator rotation only.

Fig. 6 DEM simulation snapshots of the intensive mixer for both pan and agitator rotations.

where M_h and M_v are the normalized particle mobility in the horizontal and vertical directions respectively, Δr_i and Δh_i are the mobility of particle i in the horizontal and vertical directions respectively, R and H are the diameter and height of the intensive mixer respectively, and N is the number of particles. The normalized particle mobility calculated for each case shows that agitator rotation increases the particle mobility in the vertical direction, as shown in Table 2. For the case of both pan and agitator rotations, the mobility in the horizontal direction increases and that in the vertical direction maintains a large value.

3.2 Correlation between calculated energy dissipation and the experimental abrasion rate

Figure 7 shows that particle size distribution of grinding products for a rotation speed of 900–5000 rpm. In these graphs, the particle size indicated by the Fig. 7 horizontal axis was made dimensionless by dividing by the maximum particle size (4 mm). The gray line shows the size distribution of the feed. From the results for 900–3000 rpm shown in Figure 7, the shape of the particle size distribution for the coarser particles

hardly changed, while the amount of fine particles increased. This means that there was mostly effective surface grinding (i.e., abrasion) in which the coarser bauxite particles were not broken down but only had their surfaces removed and ground into fine particle fractions. In the case of a rotation speed of 5000 rpm, the coarser particle fractions increased, indicating that particle degradation by the mechanism of fracture was mainly occurring. Figure 7 also shows the results from simulation using the population balance model of abrasion described by Eqs. (11)–(14), where the abrasion rate K_a and fracture rate K_f were treated as parameters for fitting to the experimental results of the size distribution. In this study, the constants m and n in Eqs. (7) and (8) were 1 and 0.5 respectively as determined from earlier experimental investigations. Good agreement between experimental and simulation results was achieved for all rotation speeds.

Figure 8 shows the abrasion rate K_a obtained from the fitting results shown in Figure 7 and energy dissipation due to friction calculated using Eq. (3). In this graph, energy dissipation was made

Table 2 Normalized particle mobility calculated from DEM simulation results

	Vertical	Horizontal
Only pan rotation	0.50	0.12
Only agitator rotation	0.47	0.33
Both pan and agitator rotations	0.57	0.28

Fig. 7 Experimental and simulation results for the particle size distribution; rotating speed of 900–5000 rpm.

dimensionless by dividing by the maximum energy dissipation for 5000 rpm rotation speed. An increase in the abrasion rate was associated with a decrease in energy dissipation due to friction. This result shows that too great a frictional force results in particle degradation by the mechanism of fracture rather than abrasion. We also investigated the relationship between the abrasion rate and energy dissipation of the dashpot as calculated using Eq. (1); however, there was not a good correlation between them. Hence, the energy dissipation of the friction obtained from DEM simulation results could be used estimate the abrasion rate.

Figure 9 shows the fracture rate K_f obtained from the fitting results and energy dissipation of the dashpot in normal and tangential directions calculated from Eqs. (1) and (2). In this graph, energy dissipation was made dimensionless by dividing by the maximum energy dissipation for 5000 rpm rotation speed as in Figure 8. The fracture rate increased with an increase in energy dissipation of the dashpot, as described by Park and Wassgren¹⁵.

4. Conclusion

Application of DEM simulation to the surface grinding of bauxite particles using an intensive mixer and a comparison of DEM simulation results and experimental results were presented. The

Fig. 8 Correlation between the abrasion rate and energy dissipation of friction. **Fig. 9** Correlation between the fracture rate and energy dissipation of the dashpot.

roles of the pan and agitator were estimated from the DEM simulations and it was revealed that employing only agitator rotation increases the particle mobility in the vertical direction, while employing both pan and agitator rotations increases the mobility in the horizontal direction and stably maintains large mobility in the vertical direction. We also investigated the correlation between the rates of energy dissipation during interparticle contact calculated from DEM simulation results and the abrasion rate estimated from experimental results. The abrasion rate was estimated from the particle size distribution obtained from the surface grinding experiments using an intensive mixer charged with bauxite particles and a population balance model in which two mechanisms of attrition—abrasion and fracture—are taken into consideration. The results show that the abrasion rate decreases with an increase in energy dissipation due to friction, which suggests that energy dissipation due to friction obtained from the DEM simulation results could be used to estimate the abrasion rate in the surface grinding process.

Acknowledgment

The authors thank Dr. Takeda and Dr. Rong of RFLOW Co., Ltd. for their advice on our DEM simulation.

References

1. P.A. Cundall and O.D.L. Strack: *Geotechnique*, **29**, 1, pp. 47–65 (1979)
2. Y. Tsuji, T. Kawaguchi, T. Tanaka: *Powder Technology*, **77**, pp. 79–87 (1993)
3. T. Tanaka and T. Ishida: *Transactions of the Japan Society of Mechanical Engineers, Series B*, **57**, 534, pp. 60–67 (1991)
4. C. Tokoro, K. Torigoe, T. Yamashita, S. Owada: *Proc. MMIJ Annual Meeting*, **Vol. II**, pp. 177–178 (2009)
5. M. Hakuno: *Hakai no simulation* Morikita publishing, (Tokyo), (1997)
6. T. Inoue and K. Okaya: *Mineral Processing*, **43**, pp. 1–10 (1995)
7. B.K. Mishra: *Int. J. Miner. Process.*, **71**, 73–93 (2003)
8. B.K. Mishra: *Int. J. Miner. Process.*, **71**, 95–112 (2003)
9. R. Soda, A. Sato, J. Kano, E. Kasai, F. Saito, M. Hara, T. Kawaguchi: *ISIJ International*, **49**, 645–649 (2009)
10. C. Tokoro, S. Owada, T. Shiozawa, S. Yuki: *Proc. of the 16th Nisshin engineering particle technology international seminar (NEPTIS-16, Matsushima, December 9-11)*, pp. 13–20 (2007)
11. C. Tokoro and S. Owada: *Dojyo chikasui osen no joka oyobi shufuku gijutsu* NTS, (Tokyo), pp. 285–291 (2008)
12. S. Owada, C. Tokoro, A. Otsuki, H. Kubota, T. Yamashita: *Proc. MMIJ Annual Meeting*, **Vol. II**, pp. 101–102 (2008)
13. N. Ouchiyama, S.L. Rough, J. Bridgwater: *Chemical Engineering Science*, **60**, pp. 1429–1440 (2005)
14. <http://www.rflow.co.jp/rflow.htm>
15. J. Park and C.R. Wassgren: *Particulate Science and Technology*, **21**, pp.157–175 (2003)
16. L.G. Austin: *Powder Technology*, **5**, pp. 1–17 (1971/1972)