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Breakage of fractal agglomerates

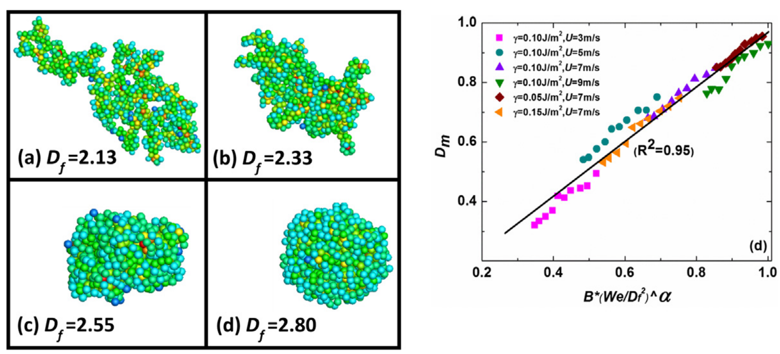
Xiaoliang Deng, Rajesh N. Davé *

New Jersey Institute of Technology, Newark, NJ 07102, USA

HIGHLIGHTS

- A simple method is demonstrated to generate fractal agglomerates.
- The breakage of fractal agglomerates is investigated using discrete element method.
- Damage ratio is influenced by impact speed, surface energy, and fractal dimension.
- Lower fractal dimension leads to lower agglomerate strength and higher damage ratio.
- Previous Thornton scaling law is generalized by incorporating fractal dimension.

GRAPHICAL ABSTRACT



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ABSTRACT

Breakage behavior of fractal agglomerates as a function of impact velocity and surface energy was investigated using discrete element method (DEM). Agglomerates with fractal dimensions (D_f) ranging from about 2.0 to 2.8 were produced by letting primary particles having random initial velocities agglomerate under a centripetal force. The simulation results show that the damage ratio (D_m), defined as the ratio of broken interparticle contacts to the initial total contacts, decreases with increasing fractal dimension in the range between 2.0 and 2.6, which can be explained by the increased mechanical strength with increasing fractal dimension. Previously introduced Weber number (We) based correlation for damage ratio is generalized by incorporating the fractal dimension: $D_m = B\left(\frac{W_e}{D_f^2}\right)^{\alpha}$, where B and α depend exponentially and linearly on Weber number, respectively. Visualization of impact process illustrates the feature of ductile fracture of fractal agglomerates irrespective of fractal dimensions.

1. Introduction

Fine particles have a strong tendency to agglomerate due to the relatively strong interparticle cohesive forces compared with their gravitational forces. In a variety of engineering processes, it is highly desirable to break those agglomerates in order to achieve required properties and improve product performance. For instance, in pharmaceutical industry it is critical to break the irregular agglomerates during the mixing process in order to achieve homogeneity of the mixture at sub-agglomerate scale (Ammendola et al., 2011; Deng et al., 2013). Therefore, breakage of agglomerates is one of the fundamental issues commonly encountered in many industrial processes and has attracted a great deal of research interest (Antonyuk et al., 2006; Golchert et al., 2004; Liu et al., 2016; Moreno et al., 2003; Ning et al., 1997; Spettl et al., 2015; Thornton and Liu, 2004; Thornton et al., 1996; Zheng et al., 2015).

* Corresponding author at: New Jersey Center for Engineered Particulates, New Jersey Institute of Technology, Newark, NJ 07102, USA.

E-mail address: dave@njit.edu (R.N. Davé).

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Nomenclature

Roman

B	fitting parameter
D	diameter of particle, m
D_f	fractal dimension of agglomerate
D_m	damage ratio
F	force, N
g	gravitational acceleration, m/s^2
I	moment of inertia, kg·m^2
k	pre-factor
m	mass of particle, kg
n	shape parameter
N	number of primary particles
r	particle position, m
R_e	equivalent radius of agglomerate, m
R_g	radius of gyration of agglomerate, m
T	torque, N m
U	impact velocity, m/s
v	linear velocity of particle, m/s
V	volume of primary particle, m^3
V_a	volume of agglomerate, m^3
We	Weber number

Greek letters

ρ	density, kg/m^3
ω	rotational velocity of particle, rad/s
γ	surface energy, J/m^2
ε	porosity
σ	strength of agglomerate, Pa
α	fitting parameter
Γ	work of adhesion, J/m^2

Subscript

i	particle index

Discrete element method (DEM) simulations have access to particle scale information on the coordinates and velocities of all the constituted primary particles within agglomerates, which is crucial for better mechanistic understanding of agglomerate breakage dynamics. As a consequence, DEM simulations have been widely used to investigate the breakage of agglomerates, particularly in identifying broken interparticle contacts induced by impact (Kafui and Thornton, 2000; Liu et al., 2010, 2016; Moreno-Atanasio, 2012; Moreno-Atanasio and Ghadiri, 2006; Moreno et al., 2003; Thornton et al., 1996, 1999; Thornton and Liu, 2004.). In previous literature, the breakage behavior of agglomerates resulting from impact has been comprehensively investigated with the focus on the effect of impact velocity, impact angle, and surface energy (Kafui and Thornton, 2000; Mishra and Thornton, 2001; Moreno-Atanasio and Ghadiri, 2006; Samimi et al., 2004; Thornton et al., 1996, 1999). To quantify the extent of breakage suffered by agglomerate under impact, the concept of damage ratio has been introduced by Thornton et al. (1996). It is a dimensionless number of broken contacts divided by the initial number of contacts within the agglomerate. The damage ratio has been correlated with the Weber number $W_e = \frac{\rho D U^2}{\Gamma}$, where ρ, D, U, and Γ are the particle density, particle diameter, impact velocity, and work of adhesion, respectively (Kafui and Thornton, 2000; Moreno-Atanasio and Ghadiri, 2006; Subero et al., 1999). Later, Thornton et al. modified the Weber number by introducing a critical impact velocity (Thornton et al., 1996).

An important point to note is that the agglomerate models used in previous research are characterized by generally round, regular shape and compact structure, perhaps stemming from particular interest in the granulation process (Kafui and Thornton, 2000; Liu et al., 2010; Reynolds et al., 2005). However, some other applications such as mixing and fluidization of nanoparticles (Chen et al., 2008; Deng et al., 2013; Scicolone et al., 2011) and dry coating (Pfeffer et al., 2001; Yang et al., 2005) require handling and processing the agglomerates formed by dry fine particles, characterized by irregular shapes and more open structures (Froeschke et al., 2003; Kanniah et al., 2012). Therefore, the crucial missing information is the detailed understanding of how the morphological features of agglomerates impact their breakage behavior. There has been several recent DEM simulation studies intended to help better understand the effect of not only the shape but also morphological properties of agglomerates on breakage behavior. For instance, DEM simulation results have shown that the breakage behaviors of spherical, cuboidal, and cylindrical agglomerates differ from each other, depending on impact orientations (Liu et al., 2010). The effect of the internal microstructure of agglomerates on their breakage characteristics has been examined as well, focusing on the role of primary particle size distribution (Spettl et al., 2015). Some experimental results also have shown that the local structure can impact the pattern of agglomerate breakage due to its effect on stress transmission during the impact process (Subero and Ghadiri, 2001). Overall, such results have indicated that the morphological parameters of agglomerates may play a significant role in their breakage behavior, together with other parameters, such as impact velocity and surface energy.

In order to fully characterize the breakage behavior of agglomerates, it is therefore necessary to elucidate the role of agglomerate morphology during the process of breakage. Fractal dimension, an exponent that relates the mass of an agglomerate to its length scale, is an important parameter characterizing the morphological features of agglomerates (Meakin, 1987). However, the effect of fractal dimension on breakage behavior of agglomerates under impact loading has not been well explored. At present, to the best of our knowledge, there is no empirical or theoretical model that is able to assess, even at a qualitative level, how the fractal dimension affects the breakage behavior of agglomerates.

In this paper, first, the original method to form spherical agglomerates is extended to achieve agglomerates of different fractal dimensions. Such agglomerates are used in DEM simulations to examine the effect of fractal dimension on the breakage behavior of agglomerates composed of uniform-sized spheres. Statistical analysis is used to determine the damage ratio as a function of fractal dimension for various impact velocities and surface energies. The goal of the present work is to provide the foundation for the development of a fundamental agglomerate breakage model incorporating realistic morphological information.

2. Simulation model

2.1. Discrete element method

DEM is a commonly used computational tool for simulating the properties of particle assembly. It is able to describe complex temporal evolution of particle system using basic input parameters representing physical properties of particle material without making oversimplifying assumptions. In this method, each particle interacts with its neighbors through contacts which can be dynam-