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Simulation and calibration of granules using the discrete element method

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ABSTRACT

The discrete element method (DEM), developed by Cundall and Strack (1979) to solve geomechanical problems, is used to simulate the mechanical behavior of granules. According to the DEM, an individual granule can be modeled as a realistic mechanical system consisting of primary particles bonded by interaction forces.

Granulometric properties of the model material, zeolite 4A, have been measured to determine their macro properties. To investigate the compression behavior, a compression test was performed using a strength tester on single granules between two pistons. A modeled granule consisting of more than 22,000 primary particles was generated. The micro properties of the modeled granule have been precisely set to allow its macro properties to be equivalent to the macro properties of zeolite 4A granules. To calibrate the mechanical properties, diametrical compression was simulated using two rigid walls stressed at a constant stressing velocity. The force–displacement curve of the modeled granule at compression has been calibrated by the experimental curve of zeolite 4A.

1. Introduction

During processing and transportation, granules are stressed by compression, impact, friction, and attrition, especially in fluidized beds and in pneumatic conveying. As a consequence, breakage and/or abrasion can be generated depending on the stress intensity. Damaged granules can result in a change of the size distribution. The physical product properties can also be deteriorated and the resulting product quality affected. Therefore, an understanding of the mechanical properties of the granules is useful.

Compared with experimental investigations, numerical simulations offer the chance to observe process dynamics in given time and spatial coordinates. Relevant process parameters such as spatial force distribution, stress and particle velocity distribution can be investigated. Detailed micro- and macro-scale information can also be recorded.

Reruns of the numerical simulations using different material and process parameters become possible for optimization. Significantly more information can be obtained from this model than by experiments. Increasing computing power and memory further allow for more complex and realistic modeling of physical processes than previously possible.

Several authors have conducted several experimental studies concerning the compression, impact, and fracture behavior of granules (Schönert, 2004; Subero & Ghadiri, 2001; Wu, Chau, & Yu, 2004). Numerical studies using the discrete element method (DEM) have also been carried out (Carmona, Wittel, Kun, & Herrmann, 2008; Kafui & Thornton, 2000; Thornton & Liu, 2004).

The current work is about the generation and calibration of a granule used for investigation of the compression, impact, and breakage behavior and to receive new insights into the micro-macro-interactions of the modeled material.

2. Discrete element method

The DEM simulations are based on commercial software PFC^{3D} (Itasca, 2005) that has been described by Potyondy and Cundall (2004).

The dynamics of discrete, stable, and mechanically easily computable elements that have three degrees of freedom of both translation and rotation is described by the DEM by Bicanic (2004). The elements of the DEM model involve the particles and the surrounding walls of a process chamber. The particles are represented

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Nomenclature

Symbols

d_{50}	mean diameter, mm
E	modulus of elasticity, MPa
$\vec{F}$	force, N
k	stiffness, N/m
n	number
$\vec{n}$, $\vec{t}$	normal, tangential vector
p	pressure, MPa
R	radius, mm
s	overlap, displacement, mm
X_W	moisture content, kg_{H2O}/kg_{TS}
$\vec{v}$	velocity, m/s
ε	porosity
η	damping coefficient, kg/s
μ	friction coefficient
ρ_g, ρ_s	granule, solid density, kg/m^3
σ_B	fracture strength, MPa
$\vec{\varpi}$	angular velocity, rad/s

Subscripts

B	breakage
el	elastic
F	yield
i, j	particle i, j
max	maximum
min	minimum
n, t	normal, tangential direction
p	particle
PB	parallel bond
w	wall

as spheres with a symmetric shape. The walls can be used to model moving stress tools of machines and the fixed walls of apparatuses.

At the start of the simulations, the discrete elements are placed in an individually defined configuration and are ascribed material properties such as solid density ρ_s, contact stiffness k, friction and damping coefficients, μ and η, and initial velocities, $\vec{v}$. All primary particles are defined as rigid and non-deformable. The contact area between the two elements is comparatively small, i.e. the model assumes "stiff particles with soft contact" (Tomas, 2007). To model the contact behavior, an approach is used whereby the rigid spheres can overlap within the contacts.

The material behavior is determined by classical contact models, i.e. elastic contact laws, coulomb friction, and viscous damping. Fig. 1 presents the contact model of particle–particle contact in the normal and tangential directions.

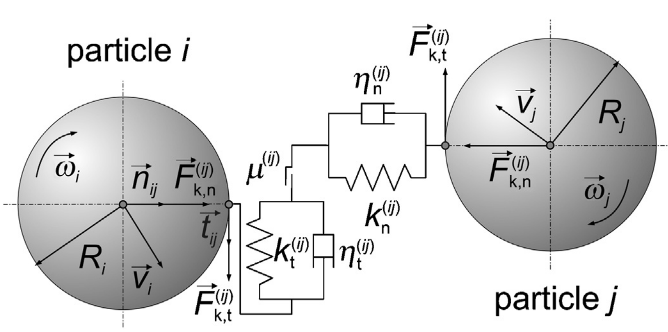

Fig. 1. Schematic representation of particle–particle contact in the normal and tangential directions.

Using the simplest approach, the acting contact force, $\vec{F}^{(ij)}_{k,n}$, is assumed to be proportional to the overlap $s_n^{(ij)}$. The contact force in the normal direction is shown in Eq. (1) and is modeled as a parallel arrangement of an elastic spring and a viscous dashpot (Kelvin-Voigt body), as shown in Fig. 1.

$$\vec{F}^{(ij)}_{k,n} = (k_n^{(ij)} s_n^{(ij)} + \eta_n^{(ij)} v._n^{(ij)})\vec{n}_{ij}. \quad (1)$$

The spring provides an elastic repulsion or restitution force, while the dashpot dissipates energy during contact. As a result, the effective coefficient of restitution is less than one. The contact force in the tangential direction, shown in Eq. (2), also results in a parallel arrangement of an elastic spring and a viscous dashpot, which are additionally connected in series with a friction limit (slider), as shown in Eq. (3).

$$\vec{F}^{(ij)}_{k,t} = (k_t^{(ij)} s_t^{(ij)} + \eta_t^{(ij)} v._t^{(ij)})\vec{t}_{ij} \quad (2)$$

$$\vec{F}^{(ij)}_{k,t,\max} = \mu_{ij} F^{(ij)}_{k,n} \vec{t}_{ij} \quad (3)$$

If the tangential contact force, $\vec{F}^{(ij)}_{k,t}$, is equal to or slightly larger than the maximum tangential contact force, $\vec{F}^{(ij)}_{k,t,\max}$, then the relationship shown in Eq. (4) applies. The force is set to this friction limit and sliding occurs within the contact area between the elements.

$$\vec{F}^{(ij)}_{k,t} \geq \vec{F}^{(ij)}_{k,t,\max}. \quad (4)$$

Fig. 1 shows the contact model of particle–particle contact (Antonyuk, 2006) consisting of simplified mechanical elements, i.e., elastic springs with stiffness $k_n^{(ij)}$ and $k_t^{(ij)}$, viscous dashpots with damping coefficients $\eta_n^{(ij)}$ and $\eta_t^{(ij)}$, and a slider with friction coefficient μ_{ij}.

The primary particles are bonded by additional adhesion forces like solid bridge bonds (Tomas, 2007) and the so-called parallel bonds (PFC3D Manual) (Itasca, 2005) were introduced by Potyondy (2007). Agglomerates can be generated as brittle or ductile solids of arbitrary shape. These parallel bonds are modeled as elastic springs connected in parallel and uniformly distributed around the contact center. The friction element of the contact model between the particles is not influenced by a parallel bond. If a parallel bond is unloaded, the bridge is elongated and the distance between the particles increases, the additional contact forces are set to zero (Antonyuk, 2006).

3. Granule sample

Zeolite 4A granules were selected as the model material. The non-water soluble, spherical, and highly hygroscopic granules are produced from zeolite powder with a mineral binder such as clay. They have a regular microporous structure and a pore size of 4 Å (0.4 nm). Zeolite 4A granules are easy to handle, relatively cheap, produced industrially, and can be used for different applications, e.g. adsorbents, molecular sieves, and for drying of organic liquids, air, and inert gases. Granulometric properties have been measured to determine the macro properties and are presented in Table 1.

4. Compression tests

To investigate compression behavior, a strength tester has been used. The compression test of single granules is performed between two pistons. The granule is stressed at a constant stressing velocity of v_B = 0.02 mm/s (i.e. strain driven) until breakage. The force is recorded as a function of displacement. To obtain representative results, the tests were repeated 100 times. Fig. 2 shows a representative force–displacement curve of the compression tests. The