



národní
úložiště
šedé
literatury

Modelling of Mechanical Interactions of Particles in Disperse Solid-Fluid Systems

Barczy, T.
2012

Dostupný z <http://www.nusl.cz/ntk/nusl-126621>

Dílo je chráněno podle autorského zákona č. 121/2000 Sb.

Tento dokument byl stažen z Národního úložiště šedé literatury (NUŠL).

Datum stažení: 24.07.2024

Další dokumenty můžete najít prostřednictvím vyhledávacího rozhraní [nusl.cz](http://www.nusl.cz) .

Modelling of mechanical interactions of particles in disperse solid-fluid systems

T. Barczy¹, M. Kohout¹, O. Hadač¹, J. Havlica²

¹ Department of Chemical Engineering, Institute of Chemical Technology; Technická 5, 166 28 Prague, Czech Republic; tel. +420 2 2044 3168, e-mail: martin.kohout@vscht.cz

² Institute of Chemical Process Fundamentals of the ASCR, v. v. i.; Rozvojova 2/135, 165 02 Prague, Czech Republic

Granular materials (porous structures, packed beds, etc.) present a unique state of matter and are currently in the urgent need of developing the proper theoretical basis for its basic aspects. A number of attempts have been made to find a way how to characterize the forces between the granular particles, in both the dry and partially wet states (moisture). Despite this, the present state of affairs is rather unsatisfactory.

One of the possible ways for mathematical modelling of mechanical interactions of particles in disperse solid-fluid systems is based on ballistic deposition methods and discrete element methods. In this contribution both of these approaches are examined and discussed their advantages and disadvantages in more detail.

Several algorithms based on methods simulating ballistic deposition for random close packing have been described in the literature [1,2] whereby particles are inserted into the simulation unit cell one at a time. Starting from random initial position (in case of a packed bed at the top of the box), they follow a trajectory under the action of two forces in a direction given by the sum of 'attractive' and a repulsive 'collision' forces. If there is no collision, there is no repulsive vector and the particle moves freely towards the center of gravity. The movement of the particle stops when the repulsive contact forces (usually three contacts for a stable position) exactly offset the attractive force or when the particle reaches the bottom of the box. The collision force is proportional to the inter-particle overlap by an 'elasticity' constant which determines the final degree of overlap between the particles.

Another possible approach for describing complex solid phase behavior is method based on discrete element models (DEM) [3]. Each particle consists of several spherical elements whose positions are fixed relative to positions of other elements within the particle. The state of each particle is characterized by the position of centre of mass, by the translational and the angular velocities and by the Euler angles, respectively. The translational and the angular velocities characterize the movement of the particle and the Euler angles describe its orientation.

Acknowledgments: This work has been supported by the grant No. P105/12/0664 of the Czech Grant Agency.

Literature:

- [1] D. Coelho, J. F. Thovert, P.M. Adler, *Geometrical and transport properties of random packings of spheres and aspherical particles*, Physical Review E 55, p. 1959 – 1977, 1997.
- [2] M. Kohout, A.P. Collier, F. Štěpánek, *Microstructure and transport properties of wet poly-disperse particle assemblies*, Powder Technol. 156, p. 120 – 128, 2005.
- [3] J.F. Favier, M.H. Abbaspour-Fard, M. Kremmer, A.O. Raji, *Shape representation of axisymmetrical, non-spherical particles in discrete element simulation using multi-element model particles*, Engineering Computations 16, p. 467 – 480, 1999.