Using DEM to Solve Bulk Material Handling Problems

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The discrete element method (DEM) models the behavior of individual particles to provide insight into the behavior of the bulk material.

Despite the prevalence of processes involving particulate material, or bulk solids, throughout the chemical process industries (CPI), the fundamentals of solids flow in such processes are not widely understood. This lack of widespread understanding can adversely affect process efficiency and product quality, so efforts are underway to develop such an understanding. One approach is the use of first-principles computational methods. With the steadily increasing speed of computer hardware, the virtual design of complex multiphase systems is fast becoming a reality.

The discrete element method (DEM) is a numerical technique developed by Peter Cundall and Otto Strack *(1)* to study problems in rock mechanics that has found wide applicability in many fields where granular materials are processed or handled. DEM is a versatile tool that can enable engineers to better understand particle flow dynamics and that, in time, should lead to more-efficient equipment designs and improved process efficiency and product quality.

The theoretical basis of the method is Sir Isaac Newton's laws of motion. DEM models the total force experienced by individual grains or particles in a granular system and tracks the subsequent accelerations, velocities, and positions over a period of time. The total force is the summation of contact forces (particle/particle and particle/boundary) and body forces (such as gravity, magnetic, and electrostatic forces). The major distinction between DEM and molecular dynamics (MD) is that the finite particle collisions and rotations play a dominant role in DEM.

Unlike continuum methods, such as computational fluid dynamics (CFD) and finite element analysis (FEA) — where specific relationships between stresses and strains (known as constitutive laws) are needed — DEM models the interactions between individual particles to predict the behavior of the bulk material. In other words, DEM requires no constitutive model; rather, the constitutive behavior results from a DEM model. This makes DEM inherently computation intensive, with long run times for systems with large numbers of particles.

Nevertheless, DEM is increasingly being used to study three-phase (gas-liquid-solid) fluid-particle processes, including heat transfer, chemical reaction, and cohesion. The challenge in these simulations is not only the characterization of physics to obtain meaningful results, but also maintaining practical run times. The characterization of material properties to be used as model inputs should not be overlooked, as this could substantially influence the results.

DEM can be coupled with CFD to study fluid-particle systems in which both the solid and fluid phases contribute significantly to the flow dynamics, such as pneumatic conveyors and fluidized beds. In this approach (generally referred to as a Eulerian-Lagrangian method), the solid phase is first modeled discretely using DEM, and those results are coupled with the CFD fluid model. Reference 2 provides an overview of applications in process engineering using coupled fluid-particle simulations.

Although DEM is emerging as a very powerful tool to study bulk materials, significant challenges and common misconceptions remain. This article describes the basic principles, applications, and limitations/challenges of the method.

Model description

DEM is a mesh-free method that models individual particle forces and predicts the dynamic behavior of the bulk (Figure 1). The user first creates the geometry of the system and defines the boundary motion of the moving parts

within that geometry (for example, rotating paddles in a mixer, a vibrating screen in a sorter, etc.). The particles are then generated within the domain and are assigned certain initial grid coordinates. The simulation advances using small incremental time steps, and the total force on each particle is determined at every instant in time. The total force is the sum of all mechanical contact and body forces:

$$F = F_{contact} + F_{body} = ma \tag{1}$$

Although gravity is the major body force, other forces such as fluid drag or cohesion arising from Van der Waals interactions, liquid bridging, or electrostatic or magnetic fields can also be incorporated into a DEM model. Each particle's linear and angular velocities (spin) along with its displacements are calculated using a central-difference integration scheme by time.

Mechanical contact forces

Although many mathematical models have been proposed to approximate the physical behavior of true impacts between solids, the one most commonly used in a DEM simulation is a damped harmonic oscillator (or spring-dashpot) model (Figure 2). For oblique collisions, the force is decomposed into normal and tangential impact directions with separate spring-dashpot elements. A slider element representing Coulomb (*i.e.,* sliding) friction also acts in the tangential direction.

A general force-displacement law *(3)* is given as:

$$F_{contact} = -K\delta^n - D\delta^l \delta'^m \tag{2}$$

where δ is the overlap between the particles, δ' is the relative impact velocity (the prime indicates the time derivative of the overlap), and K and D are the spring stiffness and damping constant, respectively. By setting the exponents $l = 0$, $m = 1$, and $n = 1$ or 1.5, a damped Hookean ($n = 1$) or damped Hertzian ($n = 1.5$) spring force is obtained. A non-zero value of the exponent l results in a variety of energy dissipation behaviors *(3)*. For example, setting $l = 0.25$ produces a constant coefficient of restitution (ratio of rebound to incident velocity of impact) that does not vary with the impact velocity. This is not representative of true impact behavior, where the coefficient of restitution decreases with the impact velocity. Setting $l \geq 1$ (typically $l = 1$) produces a velocity-dependent coefficient of restitution that is consistent with experimental observations.

Material properties

The spring stiffness, K, is a function of particle size and material properties, such as Young's modulus (tensile modulus) and Poisson's ratio. The damping constant, D, is related to the coefficient of restitution, which is a measure of the energy lost during a collision. The coefficient of dynamic friction, μ, is a measure of the surface roughness.

The choice of the contact model and the determination of material properties and contact interaction parameters are pivotal, and depend on the system and measurements of interest. For example, in slow moving quasi-static systems such as shear cells, where particles experience multiple enduring contacts, the simulations are sensitive to the stiffness and the coefficients of friction. In contrast, rapid-flow systems such as transfer chutes and fluidized beds are more sensitive to the collision energy losses characterized by the coefficient of restitution.

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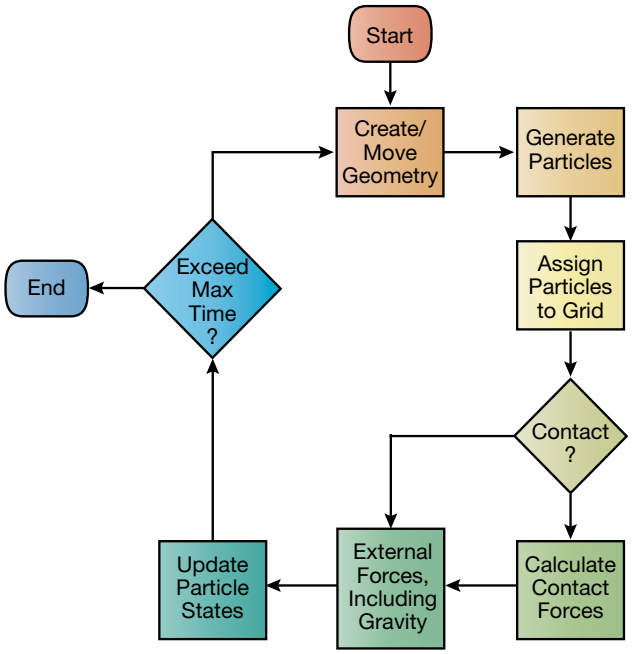
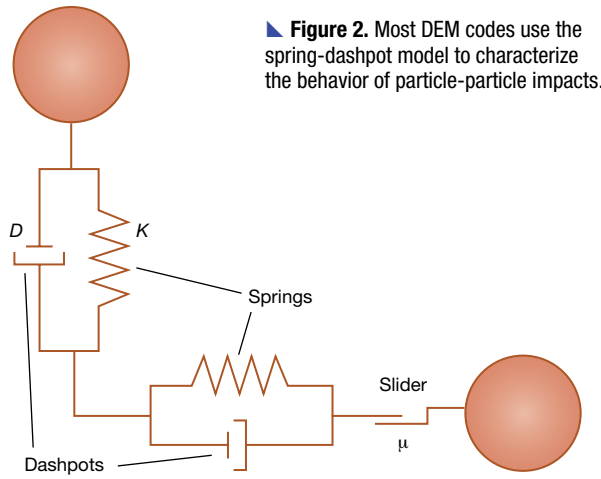
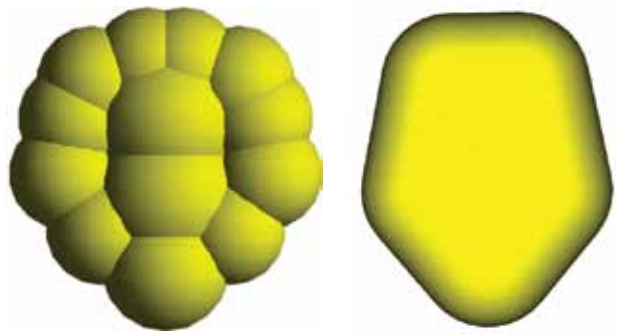


▲ **Figure 1.** DEM calculates the forces acting on every particle in a system at specified increments of time to predict the dynamic behavior of the bulk material.



◣ **Figure 2.** Most DEM codes use the spring-dashpot model to characterize the behavior of particle-particle impacts.



▲ **Figure 3.** Left: The glued-sphere method approximates a real particle shape as a cluster of spheres bonded together. Right: Nonspherical particles can also be represented as superquadrics (image of rounded polygon courtesy of Conveyor Dynamics, Inc., Rocky DEM).

Particle shapes

The most common particle shape used in DEM computer codes is a sphere. The benefits of straightforward contact detection and overlap (used to calculate contact force) make spheres the ideal choice. However, this ideal shape representation fails to accurately model most phenomena exhibited by real granular materials, such as mechanical interlocking.

Several other methods have been proposed to represent nonspherical shapes. The simplest and most prevalent is the glued-sphere or multi-sphere method *(4, 5).* In this approach, the shape is approximated by rigidly bonding a cluster of spheres that may or may not overlap (Figure 3, left). An advantage of this technique is that it retains the simplicity of contact detection associated with spheres. However, it requires more computational bookkeeping. Although any arbitrary shape can be modeled by this technique, a significant drawback is the difficulty in approximating shapes that have sharp edges and large aspect ratios.

Nonspherical particles can also be represented by mathematical approximation of their shape using continuous functions, *e.g.,* superquadrics (Figure 3, right) *(6, 7).* This approach can algebraically model a wider variety of shapes than the glued-sphere method, and do so more accurately. However, for these shapes, contact detection is computationally expensive and prohibitively slow for practical applications.

Although particle shape plays an important role in granular flow dynamics, the user needs to assess the benefits of improving a DEM model (to account for the nonspherical shape) against the added complexity of such changes as they relate to contact detection and computational efficiency. References 6 and 8 discuss the implications and issues of different shape representations in DEM models.

Applications

DEM is currently being used to study such processes as mixing, segregation, separation, storage, handling, transport, and flow of fluid-particle systems. It is used primarily as a research and development tool in many applications (with the exception of transfer chutes for mining and mineral processing). It is ideal for situations where large-scale, parametric experimental studies are difficult to perform or prohibitively expensive.

A DEM simulation can be used to predict several key characteristics and quantities, such as:

- flow patterns
- flowrates
- force, torque, and power consumption of equipment
- impact forces
- abrasive forces
- wear and stress patterns on surfaces
- breakage rates
- velocity profiles and dead zones
- mixing and segregation
- residence time of particles in certain regions.

A few examples of DEM applications include *(2, 9, 10):*

- predicting flow patterns and surface wear during the design of transfer chutes for mining operations (Figure 4)
- evaluating the performance of screw auger conveyers (torque and power consumption) for a variety of material characteristics
- evaluating the separation and sorting performance of various sieves
- predicting mixing and segregation patterns in pharmaceutical blending operations and other rotating devices
- scaling up mixers and granulators based on mixing efficiency predictions
- understanding grinding mechanisms in milling operations.

Although DEM is still in its early stages, its use in studies involving heat transfer and/or reaction chemistry in chemical engineering processes (*e.g.,* drying, coal combustion in gas-fluidized beds, rotating drums, scale-up of fluidized-bed granulators [Figure 5]) has been explored.

Limitations and challenges

Although DEM can be used as an efficient design tool, considerable limitations and challenges exist.

The primary limitation is its inherent computational intensity. Since the technique tracks each individual particle and its interactions over time, an increase in the number of particles (N) increases the computational time, which typically scales linearly in direct proportion to N. This limits the number of particles, and thus the particle size (N scales as approximately d^{-3} for the same volume, where d is the particle diameter), that can be practically modeled. Current models are typically restricted to modeling on the order of 10^6 particles.

Secondary forces (*e.g.,* cohesion) and technical complexities such as nonspherical particle shapes, moving

boundaries, and contact force models also influence computational time. Coupling DEM with CFD or FEA increases the computational time as well.

Another major concern is validation of the DEM model results. DEM is ideal for systems where experimental measurements are difficult or extremely costly. However, in such situations, validating model results is also difficult and costly.

The most common way to validate or calibrate a model is by qualitative visualization of flow profiles or quantitative measurement of macroscopic quantities, such as discharge rates, forces, etc. These methods typically test the sensitivity of outputs to inputs such as friction, coefficient of restitution, particle size and shape, etc. This requires large numbers of simulations to check the sensitivity of each parameter individually and in combination, which can quickly become resource intensive, cost prohibitive, and beyond the time constraints of most projects.

This simple sensitivity analysis approach (known as the material model of a DEM simulation) is based on the principle that bulk behavior can be reasonably represented by a combination of various inputs to the DEM model. Much caution must be used when performing this kind of calibration because various combinations of material inputs can produce similar bulk behavior *(11),* and significant insight is required to determine which factors are truly responsible. Furthermore, a particular material input combination might not work for all processes.

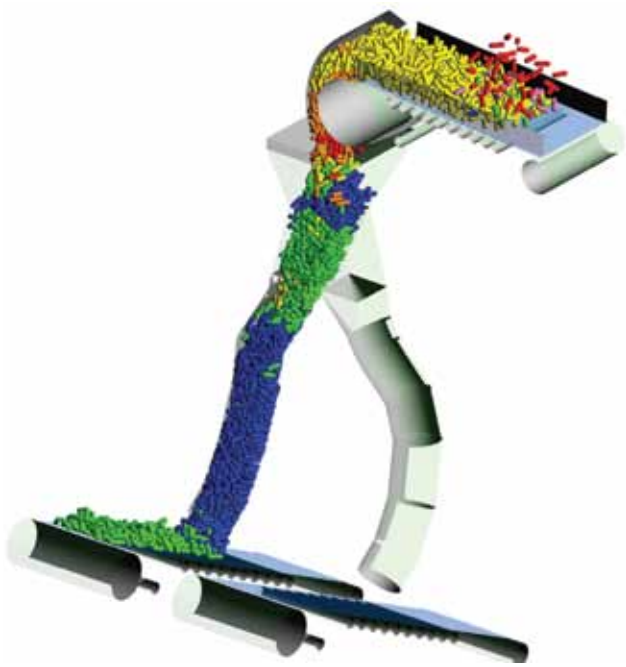
Yet another concern is the representation of nonspherical particle shapes as perfect spheres. Although it is quite tempting to use spheres for computational efficiency and simplicity of model development, studies have shown that most applications are very sensitive to mechanical interlocking of particles. This makes accurate representation of particle shape in a DEM model essential. Examples of applications where this is particularly important include the modeling of mixing and segregation in blenders, and the prediction of the performance of vibratory screen separators and sorters.

DEM codes

Many open source and commercial DEM and coupled (DEM-CFD and DEM-FEA) computer codes are available (Table 1). Although all DEM software uses the same basic method, their implementation details differ, and the accuracy of the results produced by different codes can vary *(12)*. Thus, every code needs to be validated independently.

When choosing a DEM simulation over other tools to solve a problem, consider:

• *cost and manpower.* How many licenses are needed



▲ **Figure 4.** DEM prediction of the velocities of nonspherical particles shows blockages (blue) in a transfer chute.

▼ **Figure 5.** A DEM-CFD coupled simulation predicts particle velocities and positions in an air suspension coater. Source: *(13).*

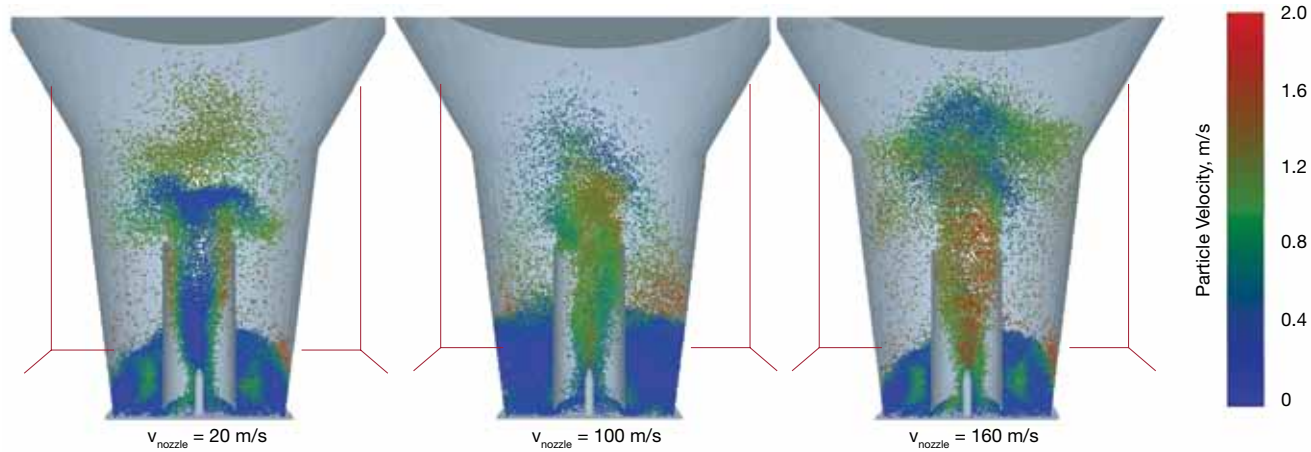


Table 1. Engineers can choose from among a variety of open source and commercial DEM codes.

Pros	Cons
Open Source (*e.g.,* LIGGGHTS, YADE-OPEN, ESys-Particle, LMGC90)	
No license cost Full control of source code implementation Multiple users and simulations Cost-effective scaling for large organizations	Programming and DEM expertise needed Support group needed for multiple users XML-based inputs/outputs
Commercial (*e.g.,* Rocky DEM, PFC3D, EDEM, Chute Maven, Chute Analyst, PASSAGE DEM)	
No programming experience needed Better graphical user interface Support and training available	Expensive license cost, especially for multiple users and multi-core processor licenses No control over implementation Custom user-defined force models and measurements might not be easy to implement

and what is their cost? What are the costs associated with the required hardware? What are the costs associated with hiring experienced personnel?

• *return on investment.* What will the DEM results predict? Will this lead to significant process understanding and an efficient design? How many simulations (and hence licenses) will be needed to obtain reliable results?

• *physics.* Are the physics of the process modeled accurately? Can custom force laws be added with flexibility? Are the geometry and boundary conditions of the process modeled accurately? How accurate is the particle shape representation?

Closing thoughts

DEM is a rapidly developing tool to predict bulk material behavior. With the exception of transfer chute design, it is still used mostly in research and development applications.

Nevertheless, DEM can provide significant insight into processes where plant-scale experiments are not possible or practical. Increasing computer speeds will help to lessen some of the major limitations of DEM. CEP

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