

This is the author's manuscript for publication. The publisher-formatted version may be available through the publisher's web site or your institution's library.

## **Applications of discrete element method in modeling of grain postharvest operations**

J. M. Boac, R. P. K. Ambrose, M. E. Casada, R. G. Maghirang, and D. E. Maier

### **How to cite this manuscript**

If you make reference to this version of the manuscript, use the following information:

Boac, J. M., Ambrose, R. P. K., Casada, M. E., Maghirang, R. G., & Maier, D. E. (2014). Applications of discrete element method in modeling of grain postharvest operations. Retrieved from <http://krex.ksu.edu>

### **Published Version Information**

**Citation:** Boac, J. M., Ambrose, R. P. K., Casada, M. E., Maghirang, R. G., & Maier, D. E. (2014). Applications of discrete element method in modeling of grain postharvest operations. *Food Engineering Reviews*, 6(4), 128-149.

**Copyright:** © Springer Science+Business Media New York 2014

**Digital Object Identifier (DOI):** doi:10.1007/s12393-014-9090-y

**Publisher's Link:** <http://link.springer.com/article/10.1007/s12393-014-9090-y>

This item was retrieved from the K-State Research Exchange (K-REx), the institutional repository of Kansas State University. K-REx is available at <http://krex.ksu.edu>

1       **APPLICATIONS OF DISCRETE ELEMENT METHOD IN MODELING OF**  
2       **GRAIN POSTHARVEST OPERATIONS**

3       **J. M. Boac, R. P. K. Ambrose, M. E. Casada, R. G. Maghirang, and D. E. Maier**

4       **Authors:**

5       **Josephine M. Boac, Ph.D.**, Postdoctoral Fellow, Department of Grain Science and Industry,  
6       Kansas State University, Manhattan, Kansas;

7       **R. P. Kingsly Ambrose, Ph.D.**, Assistant Professor, Department of Grain Science and Industry,  
8       Kansas State University, Manhattan, Kansas;

9       **Mark E. Casada, Ph.D.**, Research Agricultural Engineer, USDA-ARS Center for Grain and  
10       Animal Health Research, Engineering and Wind Erosion Research Unit, Manhattan, Kansas;

11       **Ronaldo G. Maghirang, Ph.D.**, Professor, Department of Biological and Agricultural  
12       Engineering, Kansas State University, Manhattan, Kansas; and

13       **Dirk E. Maier, Ph.D.**, Professor and Department Head, Department of Grain Science and  
14       Industry, Kansas State University, Manhattan, Kansas.

15  
16  
17  
18  
19  
20  
21       **Corresponding author:**

22       **R. P. Kingsly Ambrose**, Department of Grain Science and Industry, Kansas State University,  
23       312 Shellenberger Hall, Manhattan, Kansas; phone: 785-532-4091; fax: 785-532-7010; e-mail:  
24       kingsly@ksu.edu.

26       **Abstract.** Grain kernels are finite and discrete materials. Although flowing grain can behave  
27 like a continuum fluid at times, the discontinuous behavior exhibited by grain kernels cannot be  
28 simulated solely with conventional continuum-based computer modeling such as finite-element  
29 or finite-difference methods. The discrete element method (DEM) is a proven numerical method  
30 that can model discrete particles like grain kernels by tracking the motion of individual particles.  
31 DEM has been used extensively in the field of rock mechanics. Its application is gaining  
32 popularity in grain postharvest operations, but it has not been applied widely. This paper reviews  
33 existing applications of DEM in grain postharvest operations. Published literature that uses DEM  
34 to simulate postharvest processing is reviewed, as are applications in handling and processing of  
35 grain such as soybean, corn, wheat, rice, rapeseed, and the grain coproduct distillers dried grains  
36 with solubles (DDGS). Simulations of grain drying that involve particles in both free-flowing  
37 and confined-flow conditions are also included. Review of existing literature indicates that DEM  
38 is a promising approach in the study of the behavior of deformable soft particulates such as grain  
39 and coproducts and it could benefit from the development of improved particle models for these  
40 complex-shaped particles.

41

42       **Keywords** Discrete element method, grain handling, grain processing, free-flowing grain,  
43 confined grain

## 44 **Introduction**

45 Grain kernels are considered finite and discrete materials. At times, flowing grain can behave  
46 like a continuum fluid or a collection of individual interacting particles depending, in large part,  
47 on the energy imparted to the grain kernels (de Bruyn 2012). Granular materials such as cereal  
48 grains that exhibit discontinuous behavior cannot be simulated solely using conventional  
49 continuum-based modeling techniques such as finite-element or finite-difference methods.  
50 Examples of processes dominated by discontinuum behavior include flow of bulk solids in  
51 hoppers, feeders, chutes, screens, crushers, ball mills, mixers, and conveyor systems. Micro-  
52 mechanical behavior of particular media, stability of underground mine openings, stability of  
53 rock slopes, and mineral processing are other solids handling or processing examples in which  
54 continuum theory may be inapplicable (Dewicki 2003).

55 Williams et al. (1985) described the discrete element method (DEM) to numerically solve  
56 problems involving discrete elements like grain kernels. The DEM belongs to a family of  
57 numerical modeling techniques designed to solve problems in engineering and applied science  
58 that display gross discontinuous behavior (Hustrulid and Mustoe 1996; Hustrulid 1998; Dewicki  
59 2003). DEM can analyze multiple, interacting, deformable, discontinuous, or fractured bodies  
60 undergoing rotations and large displacements. The basic assumption in DEM is that every  
61 discrete element has distinct boundaries that physically separate it from every other element in  
62 the analysis. Basic equations of elasticity are written under an inertial frame then transferred to a  
63 non-inertial frame, which is translating and rotating. This is performed so that to an observer in  
64 the non-inertial frame, i.e., the new frame, the object exhibits no mean translation or rotation.  
65 The deformation can then be decoupled from the mean motion and written as the sum of the  
66 bodies' normal modes, which in turn gives a newly derived set of decoupled modal equations.

67 These equations are applied on an element-by-element basis, and the elements communicate  
68 through boundary forces. The decoupled equations are then solved by an explicit central  
69 difference scheme, and the final solution is obtained by means of modal superposition (Williams  
70 et al. 1985).

71 Cundall and Strack (1979), who were the first to publish this technique, defined DEM as a  
72 numerical model capable of describing the mechanical behavior of assemblies of discs and  
73 spheres. The model is based on an explicitly numerical scheme in which the particle interaction  
74 is monitored at each contact, and the particle motion is modeled particle by particle. Figure 1  
75 illustrates a schematic overview of the sequence of calculations involved in DEM simulation  
76 using the central difference, distinct element method proposed by Cundall and Strack (1979). In  
77 DEM modeling, particle interaction is treated as a dynamic process, which assumes that  
78 equilibrium states develop whenever internal forces in the system balance (Theuerkauf et al.  
79 2007). Contact forces and displacements of a stressed particle assembly are obtained by tracking  
80 the motion of individual particles. Motion results from disturbances that propagate through the  
81 assembly. The mechanical behavior of the system is described by the motion of each particle and  
82 the force and moment acting at each contact. Zhu et al. (2007) also mentioned that DEM  
83 simulations can provide dynamic information, such as trajectories of, and transient forces acting  
84 on, individual particles, which is extremely difficult or impossible to obtain by physical  
85 experimentation at this stage of development. Thus, DEM has been used increasingly to study  
86 the particle mechanics in solids handling and processing applications. A complete description of  
87 the DEM can be found in Williams et al. (1985), Cundall (1988b), Hart et al. (1988), and Cundall  
88 and Hart (1989).

89

90 DEM application is gaining popularity in postharvest processing of grain and food products  
91 because of its close characterization of actual conditions in predicting various processes. Unlike  
92 the field of mining and the chemical industry, however, DEM is not being widely applied  
93 because of various particle property issues arising from the biological origins of grain and food  
94 products. The objective of this paper is to review existing published research that used DEM as  
95 the numerical modeling technique in postharvest grain handling and processing. The scope of  
96 this paper is limited to DEM applications on grain and its coproducts.

## 97 **Theoretical Background of DEM**

### 98 ***Approaches in DEM Modeling***

99 Two types of DEM techniques are most common: hard-sphere and soft-sphere approaches.

100 These approaches are differentiated by how the deformation during collision or contact is  
101 represented. The hard-sphere approach does not allow deformation or interpenetration during  
102 impact (Hoomans et al. 1996), whereas the soft-sphere approach does (Zhu et al. 2007;  
103 O’Sullivan 2011a, 2011b). The hard-sphere approach is at the basis of the collisional or event-  
104 driven (ED) models. The ED models are also categorized as non-smooth DEM, which models  
105 the shocks between particles by means of shock laws with restitution coefficient (Fortin et al.  
106 2004). The strategy with ED models is to start with equations governing momentum exchange,  
107 which contrasts with the soft-sphere approach that solve the equations governing the linear and  
108 angular motion of the colliding or contacting particles (O’Sullivan 2011b). With the hard-sphere  
109 approach the time step interval for the numerical solution varies with the time between each  
110 collision. In contrast, the soft-sphere approach uses a constant time step interval in the solutions.

111 The ED method is limited to circular or spherical particles, takes into account collisions or  
112 shocks between two colliding particles only, and does not consider multiple contacts (Fortin et

113 al. 2004). A sequence of instantaneous collisions is processed, one collision at a time, and the  
114 forces between particles often are not explicitly considered (Zhu et al. 2007); therefore, the hard-  
115 sphere approach or the ED method is typically most useful in rapid granular flow simulations,  
116 where the granular material is not dense because it has been partially or completely fluidized  
117 (O’Sullivan 2011b). The hard-sphere approach is computationally cheap and, therefore, may be  
118 preferred for non-dense flow. However, Delaney et al. (2007) argued that this approach, although  
119 computationally faster, falls short in describing the details of the dense material’s response  
120 involving multiple simultaneous contacts.

121 Fortin et al. (2004) developed an improved non-smooth DEM based on non-smooth contact  
122 dynamics (NSCD). The NSCD method models the contact between particles with the Coulomb  
123 unilateral contact law with dry friction and takes into account multiple contacts and shocks  
124 between particles (Jean and Moreau 1991). Fortin et al. (2004) improved the NSCD by  
125 overcoming the difficulties that arise in using the dry friction modeled by Coulomb’s law, which  
126 is typically non-associated (i.e., during the contact, the sliding vector is not normal to the friction  
127 cone). They used bi-potential theory, which leads to a fast predictor-corrector scheme involving  
128 just an orthogonal projection onto the friction cone and allows using a convergence criterion  
129 based on an error estimator in the constitutive law. According to O’Sullivan (2011b), the contact  
130 dynamics method is not strictly under the hard- or soft-sphere approaches; they are sometimes  
131 referred to as rigid body dynamics.

132 Cundall and Strack (1979) originally developed the soft-sphere method, which was the first  
133 discrete numerical modeling technique published in the literature. Particles in the soft-sphere  
134 approach are also rigid but they are permitted to overlap at the contact points as a representation  
135 of the deformation that occurs at the contacts (Zhu et al. 2007; O’Sullivan 2011a, 2011b). These

136 deformations are used to calculate elastic, plastic, and frictional forces between particles; the  
137 motion of particles is described by Newton's laws of motion. The major advantage of soft-sphere  
138 models is that they are capable of handling multiple particle contacts, which is important when  
139 modeling quasi-static systems (Zhu et al. 2007).

140 Advantages of the soft-sphere approach in modeling dense-phase bulk granular materials were  
141 also highlighted by Campbell (2006). He emphasized that dense granular materials (as opposed  
142 to those fluidized or in dilute phase) in bulk are soft because their sound speed is approximately  
143 50 times slower than those of their constituent solid materials and the bulk has an apparent  
144 elastic modulus more than three orders of magnitude smaller than its constituent solid. He added  
145 that dense systems interact by force chains (which are quasi-linear structures that support the bulk  
146 of the internal stress within the material) and transmit force along the chain by elastically  
147 deforming the interparticle contacts. Modeling such systems as rigid spheres and any other  
148 model would miss essential physics (Campbell 2006). He also mentioned that particle surface  
149 friction is essential to modeling dense systems because removing it can cause transition between  
150 an elastic and inertial flow regime. Surface friction is important to the strength of the force  
151 chains and force chains are vital to the elastic flow regimes, thus, friction is also essential physics  
152 required in the simulation to avoid erroneous behavior.

153 The soft-sphere approach, with the advantages listed above for describing the bulk material  
154 physics, is most commonly used in the grain and food-processing industries. Thus, soft-sphere  
155 DEM modeling is the focus of this review.

### 156 ***Governing Equations of Motion***

157 In soft-sphere DEM, contact forces and displacements of the particle assembly are computed  
158 by tracking the motion of each individual particle using an explicit numerical scheme and a very



159 small time step (Cundall and Strack, 1979). The process uses Newton's laws of motion that gives  
 160 the relationship between the particle motion and forces acting on each particle. Translational and  
 161 rotational motions of a particle are defined as (Remy et al. 2009):

$$162 \quad m_i \frac{dv_i}{dt} = \sum_j (F_{n_{ij}} + F_{t_{ij}}) + m_i g \quad (1)$$

$$163 \quad I_i \frac{d\omega_i}{dt} = \sum_j (R_i \times F_{t_{ij}}) + \tau_{ij} \quad (2)$$

164 where  $m_i$ ,  $R_i$ ,  $v_i$ ,  $\omega_i$ , and  $I_i$  are the mass, radius, linear velocity, angular velocity, and moment of  
 165 inertia of particle  $i$ , respectively;  $F_{n_{ij}}$ ,  $F_{t_{ij}}$ , and  $\tau_{ij}$  are the normal force, tangential force, and  
 166 torque acting on particles  $i$  and  $j$  at contact points, respectively;  $g$  is the acceleration due to  
 167 gravity; and  $t$  is the time.

### 168 **Modeling of Contact Forces**

169 Force-displacement laws at contact points can be represented by different contact models. The  
 170 wide range of contact models and their corresponding equations are not discussed in detail in this  
 171 review. Zhu et al.'s (2007) summarizes various contact force models as well as non-contact force  
 172 models used in discrete particle simulations. O'Sullivan (2011b) also gives detailed discussions  
 173 of contact models in her book.

174 The simplest contact model commonly used is the linear spring-dashpot model (Cundall and  
 175 Strack 1979), in which the spring stiffness is assumed to be constant (Mishra 2003). An  
 176 improvement to the linear contact model employs the Hertz theory to obtain the force  
 177 deformation relation for the contact (e.g., nonlinear-spring dashpot model). Unlike the linear  
 178 contact model, the Hertzian contact law considers that normal stiffness varies with the amount of  
 179 overlap. This approach has been extended to cases in which colliding bodies tend to deform  
 180 (constrained plastic deformation). Numerical models of interaction at the contact involve the

181 force-deformation equation, which is augmented with a damping term to reflect dissipation in the  
182 contact area.

183 One model to represent the force-displacement laws at the contacts is the Hertz-Mindlin  
184 contact model (Mindlin 1949; Mindlin and Deresiewicz 1953; Tsuji et al. 1992; Di Renzo and Di  
185 Maio 2004, 2005). This non-linear model features both the accuracy and simplicity derived from  
186 combining the Hertz theory in the normal direction and the Mindlin model in the tangential  
187 direction (Tsuji et al. 1992; Remy et al. 2009). Forces on the particles at contact points include  
188 contact force and viscous contact damping force (Zhou et al. 2001). These forces were calculated  
189 by assuming the presence of elastic springs and dashpots in the normal (n) and tangential (t)  
190 directions (Figure 2).

191 The normal force,  $F_n$ , is given as follows (Tsuji et al. 1992; Remy et al. 2009):

$$192 \quad F_n = -K_n \delta_n^{3/2} - \eta_n \dot{\delta}_n \delta_n^{1/4} \quad (3)$$

193 where  $K_n$  is the normal stiffness coefficient;  $\delta_n$  is the normal overlap or displacement;  $\dot{\delta}_n$  is the  
194 normal velocity; and  $\eta_n$  is the normal damping coefficient.

195 The tangential force,  $F_t$ , is governed by the following equation (Tsuji et al. 1992; Remy et al.  
196 2009):

$$197 \quad F_t = -K_t \delta_t - \eta_t \dot{\delta}_t \delta_t^{1/4} \quad (4)$$

198 where  $K_t$  is the tangential stiffness coefficient;  $\delta_t$  is the tangential overlap;  $\dot{\delta}_t$  is the tangential  
199 velocity; and  $\eta_t$  is the tangential damping coefficient. The tangential overlap is calculated by  
200 (Remy et al 2009):

$$201 \quad \delta_t = \int v_{rel}^t dt \quad (5)$$

202 where  $v_{rel}^t$  is the relative tangential velocity of colliding particles and is defined by (Remy et al.  
203 2009):

$$204 \quad v_{rel}^t = (v_i - v_j) \cdot s + \omega_i R_i + \omega_j R_j \quad (6)$$

205 where  $s$  is the tangential decomposition of the unit vector connecting the center of the particle.

206 In addition, a tangential force is limited by Coulomb friction ( $\mu_s F_n$ ), where  $\mu_s$  is the coefficient  
207 of static friction. When necessary, rolling friction can be accounted for by applying a torque to  
208 contacting surfaces. The rolling friction torque,  $\tau_i$ , is given by (DEM Solutions 2013; Remy et al.  
209 2009):

$$210 \quad \tau_i = -\mu_r F_n R_0 \omega_0 \quad (7)$$

211 where  $\mu_r$  is the coefficient of rolling friction,  $R_0$  is the distance of the contact point from the  
212 center of the mass, and  $\omega_0$  is the unit angular velocity vector of the object at the contact point  
213 (Tsuiji et al. 1992; Di Renzo and Di Maio 2004; Li et al. 2005; DEM Solutions 2013; Remy et al.  
214 2009).

### 215 ***Stiffness and Damping Coefficient***

216 After modeling the contact forces, the next step is to determine the values of stiffness,  $K$ ,  
217 damping coefficient,  $\eta$ , and friction coefficient,  $\mu$ . The friction coefficient is measurable and  
218 considered a parameter obtained empirically. The damping coefficient can be computed from  
219 stiffness. Thus, the stiffness is the parameter which must be determined first and can be  
220 computed by Hertzian contact theory when the physical properties such as Young's modulus and  
221 Poisson ration are known (Tsuiji et al. 1992).

222 Following the Hertz-Mindlin contact model above, the normal stiffness and normal damping  
223 coefficients are (Tsuiji et al. 1992; Remy et al. 2009):

224 
$$K_n = \frac{4}{3} E^* \sqrt{R^*} \quad (8)$$

225 
$$\eta_n = \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \sqrt{m^* K_n} \quad (9)$$

226 where  $E^*$  is the equivalent Young's modulus,  $R^*$  is the equivalent radius,  $m^*$  is the equivalent  
 227 mass, and  $e$  is the coefficient of restitution. Equivalent properties ( $R^*$ ,  $m^*$ , and  $E^*$ ) during  
 228 collision of particles with different materials such as particles  $i$  and  $j$  are defined as (Di Renzo  
 229 and Di Maio 2004; DEM Solutions 2013):

230 
$$R^* = \left( \frac{1}{R_i} + \frac{1}{R_j} \right)^{-1} \quad (10)$$

231 
$$E^* = \left( \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j} \right)^{-1} \quad (11)$$

232 
$$m^* = \left( \frac{1}{m_i} + \frac{1}{m_j} \right)^{-1} \quad (12)$$

233 where  $\nu$  is the Poisson's ratio (Di Renzo and Di Maio 2004; DEM Solutions 2013). Similarly, for  
 234 a collision of a sphere  $i$  with a wall  $j$ , the same relations apply for Young's modulus  $E^*$ , whereas  
 235  $R^* = R_i$  and  $m^* = m_i$ .

236 Tangential stiffness and tangential damping coefficients are defined as follows (Tsuji et al.  
 237 1992; DEM Solutions 2013; Remy et al. 2009):

238 
$$K_t = 8G^* \sqrt{R^* \delta_n} \quad (13)$$

239 
$$\eta_t = \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \sqrt{m^* K_t} \quad (14)$$

240 where  $G^*$  is the equivalent shear modulus defined by (Li et al. 2005):

241 
$$G^* = \left( \frac{2-\nu_i}{G_i} + \frac{2-\nu_j}{G_j} \right)^{-1} \quad (15)$$

242  $G_i$  and  $G_j$  are shear moduli of particles  $i$  and  $j$ , respectively.

243 **Critical Time Step**

244 For dynamic processes, important factors to consider are the propagation of elastic waves  
245 across the particles, the time for load transfer from one particle to adjacent contacting particles,  
246 and the energy transmission across a system that should not be faster than in nature (Li et al.  
247 2005). In the non-linear contact model (e.g., Hertzian), the critical time increment or critical time  
248 step cannot be calculated beforehand, unlike the linear contact model in which the critical time  
249 step is related to the ratio of contact stiffness to particle density. Miller and Pursey (1955),  
250 however, showed that Rayleigh waves or surface waves account for 67% of the radiated energy,  
251 whereas dilational or pressure waves and distortional or shear waves are 7% and 26%,  
252 respectively, of the radiated energy. Thus, it is assumed that all of the energy is transferred by the  
253 Rayleigh waves because the speed difference between the Rayleigh wave and the distortional  
254 wave is small, and the energy transferred by the dilational wave is negligible (Li et al. 2005).  
255 Moreover, the average time of arrival of the Rayleigh wave at any contact remains the same  
256 irrespective of the contact point location. For simplicity, the critical time step is based on the  
257 average particle size, and a fraction of this is used in the simulations (Li et al. 2005; DEM  
258 Solutions 2013). The critical time step is given by the following equation (Li et al. 2005; DEM  
259 Solutions 2013):

260 
$$t_c = \frac{\pi \bar{R}}{\beta} \sqrt{\frac{\rho_p}{G}} \quad (16)$$

261 where  $\bar{R}$  is the average particle radius,  $\rho_p$  is the particle density,  $G$  is the particle shear modulus,  
262 and  $\beta$  can be approximated by (Li et al. 2005):

263 
$$\beta = 0.8766 + 0.163\nu \quad (17)$$

264 A major concern in using the DEM is the computational time because of the calculation of  
265 particle interactions and spatial movement at very small time steps. Boukouvala et al. (2013)

266 developed the Discrete Element- Reduced- Order Modeling (DE-ROM) approach to reduce  
267 computational time. The authors used principal component analysis (PCA) based on the data  
268 decomposition approach for discrete simulation and validated the new approach by studying a  
269 mixing process. Although this approach is encouraging, it requires data pre-processing to  
270 identify the optimal discretization based on the geometry and the state variable variability. This  
271 recently published work has not been adapted in grain postharvest operation modeling.

## 272 **Particle Models – Grain and its Coproducts**

273 The choice of shape representation for modeling particles is critical to the accuracy of real  
274 particle behavior during simulation, contact detection, and computation for contact forces  
275 determination (Hogue 1998; Favier et al. 1999). The earliest particle models were two-  
276 dimensional (2-D) and of circular (Cundall and Strack 1979) or polygonal shapes (Walton 1983).  
277 Later developments extended representations to three-dimensional (3-D) shapes, using spheres  
278 (Cundall 1988a), polyhedra (Cundall 1988b; Hocking 1992), ellipses (Ting et al. 1993),  
279 ellipsoids (Lin and Ng 1997), superquadric functions (Williams and Pentland 1989; Hogue  
280 1998), multi-element axi-symmetrical non-spherical particles (Favier et al. 1999), and bonded  
281 particles (Potyondy and Cundall 2004; Metzger and Glasser 2013). Although contact detection  
282 and computation time are very important, the critical objective in DEM modeling is accurate  
283 simulation of the behavior of an assembly of real particles (Favier et al. 1999). Favier et al.  
284 (1999) also mentioned that the influence of particle shape on predicted behavior is less  
285 documented than the relationship between shape and the efficiency of contact detection, with the  
286 exception of particle models that used polyhedral shapes (Hart et al., 1988; Ghaboussi and  
287 Barbosa, 1990). In the following sections, the particle models developed and used for predicting

288 handling and processing behavior of cereal grains, oilseeds, and their coproducts are explored  
289 and summarized in Table 1.

### 290 ***Soybeans***

291 Soybean is one of the major oilseeds produced around the world. Like any other agricultural  
292 grain, the physico-chemical properties of soybeans and their products depend on the place of  
293 origin and processing methods. Soybean-handling systems and processing operations have been  
294 simulated for the past 20 years in an effort to optimize processes. LoCurto et al. (1997) used a  
295 particle model for soybeans consisting of a cluster of four spheres of equal radius, with centers  
296 lying on a plane. This was similar to Favier et al.'s (1999) representation of non-spherical  
297 particles comprising overlapping spheres with centers fixed in a position relative to each other  
298 along the major axis of the particle's symmetry. The 3-D four-sphere particle model was used to  
299 simulate the behavior of a single soybean kernel bouncing in aluminum, glass, and acrylic  
300 surfaces to measure the coefficient of restitution. The simulations predicted the coefficient of  
301 restitution with reasonable accuracy. Vu-Quoc et al. (2000) created a soybean particle model  
302 based on the multi-sphere method developed by Favier et al. (1999) to predict the dry granular  
303 flow of soybean in a chute.

304 Soybean kernels resemble a sphere with high average sphericity values of above 0.8 (Isik  
305 2007); thus, to reduce computation times, single spheres were used by most researchers to  
306 simulate bulk soybean characteristics. Li et al. (2002) simulated the separation of soybeans and  
307 mustard seeds in a sieve using 2-D DEM and modeling soybeans as circular discs. They used a  
308 linear spring model and modified their codes by conducting trial runs to select the appropriate  
309 time step for the simulations. Both kernels (soybeans and mustard seeds) were assumed to have  
310 uniform particle size. The screen wire was also modeled in DEM using a group of circular

311 particles that had the properties of the screen wires, and these particles were vibrated to simulate  
312 the movement of a mechanically agitated screen. The authors found that the two spherical  
313 particle models representing soybeans and mustard seeds in a screening process were adequate  
314 and that the DEM simulation can provide the critical feeding rate for the most effective screening  
315 operation. Boac et al. (2010) used a single sphere particle model to simulate bulk soybean  
316 property testing using EDEM (DEM Solutions, Ltd., Edinburgh, UK), a commercial DEM code.  
317 The researchers used a no-slip Hertz-Mindlin contact to simulate and model the bulk density and  
318 angle of repose measurement tests. They conducted this simulation to develop a particle model  
319 with appropriate parameter combinations of coefficients of restitution, static friction, rolling  
320 friction, particle size distribution, and particle shear modulus that best matched the property  
321 values available in the literature. The developed soybean particle model was then used to  
322 simulate the commingling of two soybean lots, with different intrinsic properties, in a bucket-  
323 type grain elevator boot system (Boac et al. 2012).

### 324 ***Corn***

325 Corn is a cereal grain that is grown widely throughout the world and is a major food grain in  
326 Africa and Latin America, with the United States as its largest producer. In the U.S., almost 85%  
327 of corn produced is used as livestock feed and as a raw material for industrial products (FAO,  
328 2013). The design and development of processing and handling equipment for corn is a mature  
329 area, but because of the volume of grain handled and the new varieties that are being developed  
330 and to mitigate dust issues, particle modeling is being used to improve the design of equipment.  
331 Chung and Ooi (2006, 2008a, 2008b) modeled corn kernels using overlapping spheres to match  
332 the measured average major, intermediate, and minor dimensions. They used Particle Flow Code  
333 (PFC) 3D (Itasca Consulting Group, Inc., Minneapolis, MN), a commercial DEM code, to



334 simulate a confined compression and rod penetration in a dense granular medium (Chung and  
335 Ooi 2006; 2008a) and silo discharging (Chung and Ooi 2008b). The authors used a four-sphere  
336 particle representation for corn because increasing the number of spheres in a single particle  
337 leads to additional computational cost (Chung and Ooi 2006). Measured material properties  
338 (Chung et al. 2004) were used for simulation purposes.

339 Modeling corn particles using overlapping discs called clumps in PFC 2D also has been  
340 employed in the development of particle models (Coetzee and Els (2009a, 2009b, 2009c). A  
341 clump is a single entity composed of two or more overlapping spheres (in 3-D) and discs (in 2-  
342 D) to form one rigid particle. Internal contact forces between the overlapping spheres or discs are  
343 ignored in calculations (Lu and McDowell 2007). Clumps do not break during simulations  
344 regardless of the forces acting upon them (Itasca 2008; Ferrellec and McDowell 2010). Coetzee  
345 and Els (2009a, 2009b, 2009c) used this 2-D-clump corn particle model to calibrate material  
346 parameters such as the particle internal friction angle using laboratory shear tests and particle  
347 stiffness using compression tests. They validated the calibration process by modeling silo  
348 discharge and bucket filling. Coetzee et al. (2010) extended these studies to DEM modeling of  
349 dragline bucket filling using particle models comprising two to four overlapping spheres that  
350 represent crushed rocks.

351 The highest number of spheres used to develop a corn particle model was simulated by  
352 Gonzalez-Montellano et al. (2011, 2012a, 2012b). They modeled corn kernels consisting of six  
353 spheres using the multi-spheres method (Favier et al. 1999) and experimentally derived material  
354 property values (Gonzalez-Montellano et al. 2012c). The authors indicated that using more than  
355 six spheres to construct one corn particle would have slowed their simulation significantly, thus  
356 increasing computation time. The friction coefficients of this corn particle model were used to

357 predict the flow patterns of the discharging particles from a silo (Gonzalez-Montellano et al.  
358 2011). Then, they applied this modified corn particle model to study the pressure distributions,  
359 bulk density distributions, and flow properties during filling and emptying of silos (Gonzalez-  
360 Montellano et al. 2012a, 2012b).

### 361 ***Wheat***

362 Wheat is a highly irregularly shaped kernel whose shape representation for simulation  
363 purposes is challenging; the presence of a crease makes it difficult to develop a particle with  
364 identical spheres. Studies have reported using wheat kernels in 2-D to investigate the flow of  
365 wheat in a mixed-flow grain dryer (Iroba et al. 2011a; 2011b; Mellman et al. 2011; Weigler et al.  
366 2012). Monosized spherical particles were used to model the grain dryer in 2D using PFC 2D  
367 software. Iroba et al. (2011a) indicated that using multiple spheres would make the simulation  
368 time longer, whereas using non-spherical particles would be more difficult to model and would  
369 require more advanced algorithms. Because of the disc shape of the 2-D particles in the  
370 simulation, however, bridging between particles occurred at the bottom discharge device of the  
371 grain dryer, which did not happen during experiments. Iroba et al. (2011a, 2011b) explained that  
372 because the long and ellipsoidal shape of wheat kernels can orient in different directions during  
373 discharge, flow can be enhanced, and bridging did not occur in the experiment. Spherical  
374 particles (discs) tend to form bridges even though orientation is the same in all directions. To  
375 overcome bridging of particles during simulation, the fixed part of the discharge device was  
376 vibrated. In the subsequent simulations, the authors used non-spherical particles represented by a  
377 2-D ellipsoidal clump consisting of five circular elements (Weigler et al. 2012). The clumps were  
378 assumed to have the same material properties as wheat, which were adapted from Markauskas et  
379 al. (2010). The DEM model indicated that using non-spherical particles (2-D ellipsoidal clumps)

380 can predict the real flow pattern, but disc-shaped particles did not produce the expected dynamic  
381 angle of repose that typically formed under the air ducts.

382       Keppler et al. (2012) predicted the velocity distribution of wheat kernels in a mixed-flow dryer  
383 with 3-D wheat kernels using EDEM software. The wheat particle was represented by a clump of  
384 three spheres. Although the particles used in EDEM were slightly bigger than actual particles,  
385 the velocity prediction was nearly accurate. To compare the performance of different particle  
386 models, Sarnavi et al. (2013) simulated 3-D wheat kernels using three types of particle models:  
387 (1) spherical, (2) 4-spheres, and (3) 8-spheres using the PFC3D software. They compared the  
388 performance of the particle models with two contact models (linear vs. nonlinear) in predicting  
389 the angle of internal friction and cohesion of wheat. They found that the single spherical particle  
390 model, using both linear and nonlinear contact models, performed better in the simulations than  
391 the multi-sphere models. Although different particle models have been used to simulate wheat  
392 kernels, the studies clearly demonstrate that 3-D particle models have higher accuracy in  
393 predicting the bulk behavior of wheat than a 2-D approach. The results do not, however, confirm  
394 the best number of spheres to use to represent a single wheat kernel. This could be because of the  
395 complicated shape of wheat kernels; the number of spheres should be approximated by trials  
396 depending on the computation time and prediction accuracy required.

### 397 ***Rice***

398       Rice's ellipsoidal shape is similar to wheat, but the absence of a crease in rice makes it easier  
399 to approximate the rice particle shape. A 2-D circular disc approach was used by Sakaguchi et al.  
400 (2001) to model rice kernels in the shaking separation process using their own DEM codes  
401 (Sakaguchi et al. 1994). The authors obtained good agreement between the simulation and  
402 experiment with respect to the wave-like behavior of the grain assembly and the macroscopic

403 separation behavior of rice. Markauskas and Kačianauskas (2011) modeled rice kernels by  
404 creating an ellipsoid using 11 spheres. They compared two rice particle models, with rolling  
405 friction coefficients of zero and 0.3, using their own DEM code (Kačianauskas et al. 2010).  
406 These particle models were used to simulate the filling and discharge flow and piling of the  
407 kernels. The particle model with rolling friction produced a pile shape that better corresponded to  
408 the actual pile. On the other hand, the particle model without rolling friction showed higher  
409 particle mobility, resulting in a spread of particles rather than a pile. A 7-sphere particle model  
410 was used by Jiang and Qiu (2011) to simulate the impact behavior of rice kernels. The rice  
411 particle modeled was an ellipsoid with a 3.5-mm half major axis and a 1.8-mm half minor axis.  
412 The authors implemented this rice model in EDEM software and studied the impact of rice  
413 particles on the impact board of an inclined elevator head. Simulations predicted the  
414 experimental results with high accuracy up to a certain mass of rice that impacts the board. A 3-  
415 D rice model was also used by Li et al. (2012) to simulate the material motion in an air-and-  
416 screen cleaning device. The authors separated rice kernels and straws using a coupled DEM and  
417 computational fluid dynamics (CFD) model. The rice grain was represented in EDEM by a  
418 spheroid that is 6 mm long with a 1.6-mm radius of rotation. The short straw was represented by  
419 a cylinder 30 mm long by 4 mm diameter. These models were used to study the effect of inlet  
420 airflow velocity in terms of the longitudinal velocity, vertical height, and cleaning loss of rice  
421 kernels and short straws. The coupled CFD-DEM model predicted the air-screen cleaning  
422 process by describing the movement of particles on the screen surface. Coupling CFD with DEM  
423 is a recent advancement in particle modeling that will be useful in the grain processing industry  
424 for prediction of various handling and processing operations.

425 **Rapeseed**

426 Rapeseed is the second leading source of vegetable oil and protein meal in the world next to  
427 soybean (USDA ERS 2013); thus, its processing and handling optimization are important to the  
428 industry. Bulk compressive loading of rapeseeds was modeled by Raji and Favier (2004a) using  
429 a single sphere particle model. They found a slight difference in the initial particle positions  
430 between the experiment and simulation, although strain intervals were calculated at the same  
431 porosity values. This was an early attempt to model rapeseeds, and the authors extended the use  
432 of this single sphere particle model to simulate rapeseed, soybean, and palm-kernel for bulk  
433 compression (Raji and Favier 2004b). Later, other researchers also modeled rapeseed using a  
434 single sphere particle model to simulate the free fall and impact of rapeseeds against a flat  
435 surface (Wojtkowski et al. 2010). The authors used two different contact models, an elastoplastic  
436 contact model for dry seeds by Thornton and Ning (1998) and a viscoelastic contact model for  
437 wet seeds by Kuwabara and Kono (1987). Parafiniuk et al. (2013) simulated rapeseeds as single  
438 spheres to predict flow through a horizontal orifice. The experimental mean radii and standard  
439 deviation values were used to develop the single sphere model. The authors used EDEM  
440 software and applied the contact models used by Wojtkowski et al. (2010) for dry and wet  
441 rapeseeds. Parafiniuk et al. (2013) concluded that the contact models reproduced experimental  
442 results for slow particle flow but needed the improvement of including dissipation for higher  
443 particle flow rates. Wiącek and Molenda (2011) studied the influence of the moisture content of  
444 rapeseeds on the physical properties of grain bedding during uniaxial compression testing using  
445 single sphere particle models. Results indicated that the mechanical response of a granular  
446 assembly subjected to uniaxial compression is significantly affected by the moisture content of  
447 kernels. Both the simulations and experiments revealed differences in the elasticity and the stress  
448 transmission within rapeseed assemblies at various grain moisture contents.

449 The behavior of rapeseed during a direct shear test was modeled by Molenda et al. (2011)  
450 using 2-D circular discs. They used circular elements with size uniformly distributed between 1.8  
451 and 2.2 mm. Numerical simulations were performed using a non-commercial DEM code  
452 (Wassgren 1997) to determine the influence of three different levels of standard deviations in the  
453 coefficient of interparticle friction to the bulk behavior in a direct shear test. Particle interaction  
454 in the normal direction was simulated using a linear viscoelastic model, whereas the tangential  
455 direction was expanded to include a frictional element. Variability in the interparticle friction  
456 was found to influence markedly the stress-strain characteristic during the initiation of motion,  
457 whereas the strength of the assembly (or steady state value of stress) remained constant.

#### 458 ***Grain Coproducts***

459 Grain undergoes different processing methods during conversion into products and  
460 coproducts. The particle characteristics of products derived from grain are generally controlled;  
461 but particle characteristics are not uniform because the bulk contains particles with different  
462 sizes, shapes, and chemical compositions. The challenge in modeling coproduct is in shape  
463 representation using spheres. For example, distillers dried grains with solubles (DDGS), a  
464 coproduct from corn-to-ethanol processing, contains a mixture of fiber, starch, and protein  
465 components that vary in size and shape. Clementson (2010) modeled the flow and segregation of  
466 DDGS using single sphere particle model in EDEM with the Hertz-Mindlin (no-slip) contact  
467 model. The geometric mean diameter of actual DDGS ranged from 0.87 to 1.01 mm, but the  
468 researchers used bigger particles because small particles required longer simulation time in  
469 DEM; the log-normal bimodal distribution of these particles was kept similar to the actual  
470 particle size distribution. The author found that the magnitude of changes in discharge rates in  
471 the experiments were not the same as in the simulation, and the numerical simulation predicted

472 the same flow patterns as observed during funnel flow but not mass flow experiments. DEM has  
473 not been widely used to predict the bulk behavior of coproducts from the grain-based food and  
474 feed industry, partially because of the computational load from the higher number of spheres  
475 required to obtain accurate shape representation.

## 476 **Modeling Grain Handling Operations**

477 Bulk behavior of cereal grains, oilseeds, and their products vary based on the quantity,  
478 environmental factors, method of processing, and handling equipment used. The grain handling  
479 and processing operations that have been modeled using DEM were subdivided into processes  
480 dealing with free-flowing grain, such as filling and emptying of silos, and confined grain, such as  
481 storage and compression.

### 482 ***GRAN POSTHARVEST OPERATIONS MODELED OR STUDIED USING DEM***

- 483 • Free-flowing grain
  - 484 ○ Filling and discharge of silo
  - 485 ○ Bulk behavior during grain conveying
  - 486 ○ Grain cleaning and separation
  - 487 ○ Impacting grain kernels
- 488 • Confined grain
  - 489 ○ Silo probing
  - 490 ○ Compression
  - 491 ○ Shear testing
- 492 • Grain drying

493 Table 2 summarizes the model and references associated with these postharvest processing.

494 **MODELING FREE-FLOWING GRAIN**

495 ***Filling and Discharge of Silo***

496 Due to the complexity of physical and chemical parameters, hopper flow of grain and grain  
497 products usually encounters challenges such as ratholing, arching, caking, etc. Use of discharge  
498 aids in grain-based food and feed industries is a common practice to achieve uniform flow of  
499 material from hoppers and silos. DEM is increasingly applied to simulate bulk flow  
500 characteristics of grain and products for better bin design and process optimization.

501 Different grain filling approaches have been used to simulate grain storage systems.  
502 Progressive filling is the more common method used in DEM simulation where particles are  
503 generated continuously, whereas in *en masse* filling, all particles are generated simultaneously,  
504 thus reducing computation time. In *en masse* filling, particles are allowed to fall under gravity  
505 until a static equilibrium is reached. Gonzalez-Montellano et al. (2012a) used the *en masse* filling  
506 approach for glass beads and corn kernels filling in a silo. Particles were deposited rapidly on top  
507 of each other, leading to many particles being trapped by the others without having dissipated  
508 their initial energy. During emptying, the movement of the material diluted these effects, and the  
509 observed pressures were similar to the expected pattern (Gonzalez-Montellano et al. 2012a). If  
510 the *en masse* method is used in simulations, prediction errors should be taken into account when  
511 studying pressures during filling of silos.

512 Gonzalez-Montellano et al. (2012b) improved their simulations by using a modified particle  
513 model for corn (Gonzalez-Montellano et al. 2011) and the progressive method of filling a silo  
514 (Gonzalez-Montellano et al. 2012a) from their previous work. Results highlighted a difference in  
515 the vertical distributions of pressure between corn and glass beads. During both filling and  
516 discharge, the peak pressure at the silo-hopper transition was much higher for corn than for glass  
517 beads. Pressure values also fluctuated less for corn. For horizontal pressure distribution during



518 filling and at any time during the discharge of corn, maximum horizontal pressure was in the  
519 central region of the silo walls then slowly decreased toward the corners. This result was the  
520 same for glass beads, except that the distributions were less stable over time. In both models, the  
521 velocity profile at the center was greater than at the walls. For corn, the distribution of the bulk  
522 density in the vertical section was not as random as with glass beads. These researchers  
523 demonstrated DEM's usefulness in studying the behavior of granular materials in silos and  
524 hoppers and the degree of detailed information that could be obtained from simulations.

525 Chung and Ooi (2008b) simulated silo discharge by emptying corn through a circular orifice  
526 of a flat-bottom silo unloading onto a flat surface. Although the purpose of the study was to  
527 examine the influence of gravity on a granular solid, the terrestrial aspects of experiments closely  
528 simulated earth-bound processes using DEM. DEM simulation showed that the mass flow rate  
529 decreases as gravity decreases, with a corresponding increase in discharge time. The simulation  
530 also correlated with Beverloo's relationship that the mass flow rate is proportional to the square  
531 root of the gravitational force. In addition to corn discharge parameters, DEM also predicted  
532 reasonably the angle of repose of corn discharged from the silo (Chung and Ooi 2008b).

533 Mass flow rate and size of hopper outlet opening influence discharge of granular materials.  
534 Coetzee and Els (2009a) studied the discharge of corn kernels from a glass rectangular silo in  
535 two dimensions using PFC2D. Two silo openings were used in this study. The authors found that  
536 the corn particles modeled as clumps composed of two discs could reasonably predict the flow  
537 patterns observed during experiments. The results indicated that a 2-D clump particle model had  
538 higher accuracy in predicting the flow of corn through a larger silo opening where the flow was  
539 less restricted. Accuracy of DEM simulations depend on the particle models and the particle

540 parameter values used in the simulations. In this study, the two disc particle model could have  
541 influenced the prediction accuracy.

542 Monitoring the density of material that flows from hoppers or bins is one method used to  
543 evaluate segregation. Clementson (2010) used DEM to predict the bulk density of DDGS  
544 particles during funnel flow and mass flow from hoppers. The hopper half angles used were 33  
545 degrees for the mass flow and 65 degrees for funnel flow. DEM predicted a funnel flow for  
546 DDGS that was observed during experiments. The results reported by Clementson (2010)  
547 supported the hypothesis that the heterogeneity of DDGS does not facilitate true mass flow,  
548 irrespective of the hopper design.

549 DEM can be used to predict bulk density after filling a silo in addition to flow pattern and  
550 discharge rate. González-Montellano et al. (2011) used corn kernels and glass beads in EDEM  
551 simulations to model silo filling and discharge. For corn, three successive DEM models were  
552 tested to identify the coefficients of interparticle and particle-wall friction. High interparticle  
553 friction led to low bulk densities after the silo filling, which agreed with Boac et al.'s (2010)  
554 results in simulated bulk density tests. High interparticle friction also increased the discharge  
555 time. For glass beads, the velocity profile was qualitatively similar to corn but showed a more  
556 fluctuating velocity profile. This result may be explained by the development of crystalline  
557 packing configurations when single sphere particles were used (Chung and Ooi 2008a;  
558 Gonzalez-Montellano et al. 2011). For discharge rates, results for the glass beads showed wider  
559 fluctuation than those for corn kernels, which was a consequence of the relatively larger ratio  
560 between particle size and silo opening used for glass beads (0.24) than for corn (0.17).

561 An axi-symmetric multi-sphere approach is a recent development that could be used to  
562 develop particle models for irregularly shaped cereal grains. Markauskas and Kačianauskas

563 (2011) used this approach to simulate the filling and discharge of rice from a small-plane wedge-  
564 shaped hopper with a rectangular orifice. The authors simulated the angle of repose of the pile of  
565 rice after its discharge from the hopper and modeled friction effects on the flow of rice through  
566 an orifice. To model the friction effects, two rice particle models, with and without rolling  
567 friction, were used. The researchers found that rolling friction must be taken into account to  
568 avoid artificial local rotation of particles when using axi-symmetric multi-sphere particle models  
569 to represent elongated, irregularly shaped particles. Numerical results provided quantitative  
570 evidence of increased rolling friction owing to geometric deviations of the particle shape from  
571 the axi-symmetric geometry. Simulations with zero rolling friction in the model resulted in a  
572 lower angle of repose and discharge time compared with experimental values. The authors also  
573 investigated the rotational energy of particles inside the hopper using both models (Markauskas  
574 and Kačianauskas 2011). The rolling friction practically suppressed local spin, whereas the  
575 perpendicular rotation occurred because of the collective particle arrangement. The authors  
576 showed the effects of rolling friction to rotational behavior of the particles and that neglecting  
577 the rolling friction led to increased capability of particles to rotate by falling on the pile.

578 The effect of moisture content on the mass flow rate of rapeseed from a silo was modeled by  
579 Parafiniuk et al. (2013), who verified the applicability of the elastoplastic model for dry seeds  
580 and the viscoelastic model for wet seeds adapted from Wojtkowski et al. (2010) in DEM  
581 simulations. Simulation results revealed that the proposed contact models reproduced the  
582 experimental results for slower rate of particle flow. At higher flow rates (or larger openings),  
583 however, the dissipation of energy led to higher noise in the force simulated on the silo bottom  
584 than indicated by experimental results. This discrepancy was higher in simulations where the  
585 elastoplastic contact model (for dry seeds) was used. In DEM simulations, mass flow rates of dry

586 and wet seeds did not differ if the mass flow rates were calculated as a sum of masses of particles  
587 falling into the receiving container per time unit, but differences in the mass flow rates of dry and  
588 wet rapeseeds were observed if calculated using the sum of vertical forces exerted by particles on  
589 walls and floor of receiving container. The authors did not include cohesion parameters in  
590 particle models, which resulted in the differences between predictions and experimental results.

591 The major concern when using DEM to study bin pressures is that it assumes rigid silo walls  
592 in the simulations (Gonzalez-Montellano et al. 2012b). This results in overprediction of the  
593 horizontal distribution of normal pressure at the central positions on the walls. Gonzalez-  
594 Montellano et al. (2012b), after continued efforts to simulate grain bins using DEM,  
595 recommended that hybrid models combine DEM and the finite element method (FEM) to  
596 compensate for DEM's limitations. DEM allows a more accurate simulation of the dynamic  
597 behavior of the granular material itself, and FEM will allow flexible walls to be included, thus  
598 yielding a complete model.

### 599 ***Bulk Behavior During Grain Conveying***

600 Shear zone theory was applied by Coetzee and Els (2009a) to simulate bucket filling using  
601 DEM. The authors used a rig geometry that resembled a dragline bucket, which was pulled in the  
602 drag direction by a set of ropes but with freedom of motion in all other directions, based on the  
603 Shear Zone Theory developed by Rowlands (1991). DEM can accurately predict the filling  
604 process of a bucket or scoop, the force acting on the bucket, and the fill rate. During the  
605 experiments, the flow regimes as predicted by the Shear Zone Theory (Rowlands, 1991) were  
606 also observed. DEM predicted these different flow zones (Coetzee 2009a, 2009c), and the  
607 authors recommended that knowledge of the flow zones can be used to optimize buckets in terms  
608 of fill rate, bucket force, and bucket wear.

609 Grain commingling is an unintentional introduction of a different grain type during typical  
610 handling operations that directly reduces the level of purity in grain that enters an elevator  
611 facility. Three approaches address commingling during grain handling: (1) ignore it, (2) identity-  
612 preserve (IP) the grain in dedicated containers, and (3) segregate or handle the IP grain in non-  
613 dedicated facilities. Due to limited scientific data on grain commingling in normal handling  
614 operations, it is not possible to predict the level of purity that could be achieved with the third,  
615 less expensive approach (Boac 2010). Boac et al. (2012) simulated grain commingling in a pilot-  
616 scale grain elevator boot using DEM models and evaluated the tradeoffs of computational speed  
617 versus accuracy for 3D and quasi-2D boot models. Experimental data from the pilot-scale bucket  
618 elevator showed that the average cumulative commingling was comparable to the values for full-  
619 size bucket elevator legs. To avoid overprediction, the 3D model was refined to account for the  
620 sudden surge of particles during entry and corrected for the effective dynamic gap between the  
621 bucket cups and the boot wall. Comparison of predicted average commingling of five quasi-2D  
622 boot models with reduced control volumes showed that the quasi-2D (5.6 times the particle  
623 diameter) model provided the best option in terms of computation time; it reduced computation  
624 time by 72% to 74% compared with the 3-D model. Results of this study are being applied to  
625 study the commingling of infested and sound kernels (wheat and corn) in bucket elevator boot  
626 systems.

### 627 ***Grain Cleaning and Separation***

628 The macroscopic behavior of paddy and brown rice during shaking separation was modeled  
629 by Sakaguchi et al. (2001) on an oscillating inclined separation plate using a 2-D DEM model.  
630 The grain kernels were represented as circular elements using the model developed by Sakaguchi  
631 et al. (1994). In the DEM simulation, the indents on the separation plate were modeled using

632 virtual walls. Particle exit from an indent was modeled as removal of a virtual wall when the  
633 particle-wall contact exceeded a threshold value. There was good agreement between the results  
634 of the simulation and the experiment in terms of the macroscopic separation behavior of the rice.  
635 The experimental observations such as segregation caused by upward movement of paddy rice  
636 relative to brown rice and the shearing of the grain bed to accumulate paddy rice near the lower  
637 end of the shaker box were also predicted by the DEM simulation. The time required to achieve  
638 maximum separation of brown and paddy rice was the same in both experiment and simulation.  
639 In the simulation, the circular particles moved closer to the lower end of the shaker than in the  
640 experiment, which was due to the ease of rotation of the circular elements. However, the  
641 simulation showed the same wave-like behavior of the grain assembly as in the experiment. The  
642 authors concluded that a simple DEM model using 2-D circular particles and virtual walls was  
643 effective and can be done with reasonable computation times. The model will allow further  
644 investigation of the separation mechanism and exploration of the effects of different physical and  
645 process parameters on the efficiency of grain separation in shaking separators.

646 Separation mechanism of grain kernels on sieves is a dynamic process that requires  
647 consideration of various particle parameters such as size, shape, density, loading rate, and other  
648 factors. Li et al. (2002) used a 2-D transient model to calculate the motion of discrete soybean  
649 and mustard seed particles on sieves using DEM. The authors studied the influence of particle  
650 bed depth on undersize particle segregation in an inclined vibrating screen. In the DEM  
651 simulation, the sieving screen was modeled to be made of vibrating circular particles (smaller  
652 than the kernels) with properties of the sieving wires. The numerical simulation indicated that at  
653 a particle bed depth of about 5 times the size of the large particles and 12 times the size of the  
654 screen apertures, most undersize particles segregated to the screen surface. The undersize

655 particles also passed through the apertures within about 40% of the sieve length at the front  
656 section of the screen. For this particle bed depth, the screen length was long enough to ensure the  
657 highest screening efficiency, 100% separation, which means no undersize particle passed over  
658 and joined the overflow of large particles at the end of the screen. The authors concluded that for  
659 a screening system involving granular materials, the critical feeding rate needed to achieve the  
660 most efficient screening process can be determined using DEM simulation. Li et al. (2003)  
661 extended this study to mathematically investigate the particulate motion of polyethylene pellets  
662 on an inclined screening chute using DEM.

663 The coupled DEM-CFD approach has been used recently to predict the solid interaction with  
664 fluids. Li et al. (2012) used a 3-D coupled DEM-CFD model to study the effects of inlet airflow  
665 velocity on the kernels and short straw's longitudinal velocity and vertical height and the  
666 cleaning loss in an air-and-screen cleaning device. The rice grain represented by a spheroid and  
667 the short straw by a cylinder were generated in EDEM and allowed to fall on an inclined  
668 vibrating screen. The CFD portion of the coupling model used the Eulerian-Eulerian model in  
669 FLUENT (ANSYS Inc., Canonsburg, PA). The authors used Hertz-Mindlin contact model to  
670 simulate particle-particle and particle-screen (wall) collisions. Through the coupled DEM-CFD  
671 approach, the authors found that the length of the screen can be shortened if impurity content is  
672 lower. The coupled DEM-CFD modeling approach also could be used to improve the design of  
673 combine harvesters because the model accurately predicts the particle movement in air.

#### 674 ***Impacting of Grain***

675 The impact of grain as it falls on a flat surface influences breakage characteristics, friction,  
676 and coefficient of restitution. Wojtkowski et al. (2010) proposed that different models have to be  
677 used to predict the impact of grain kernels depending on moisture content. The researchers also

678 indicated that to determine a correct contact model, the ratio of the fall time to the rise time (TR)  
679 for the contact force-time characteristics should be considered. For  $TR > 1$ , the authors  
680 recommended the viscoelastic model, whereas the elastoplastic model should be applied for  
681  $TR < 1$ .

682 Another application of DEM in investigating the impact of grain kernel on a surface was  
683 reported by Jiang and Qiu (2011). The authors studied the effects of particle mass and the normal  
684 contact force between a rice particle and the impact board of an inclined elevator during flow of  
685 rice. Rice kernels were represented as ellipsoids composed of seven spheres in EDEM, and  
686 celluloid was used as the material for the impact board to study the effect of elevator belt speeds  
687 of 0.5 m/s to 1.0 m/s on bulk flow. The authors found that the normal contact force between the  
688 flowing rice particles and the impact board increased as the belt speed increased, but belt speed  
689 had no effect on tangential contact force. There was a good linear relationship between the rice  
690 particle mass and the normal contact force when the rice particle mass was from 0.18 to 0.54 kg.  
691 The authors also concluded that the retention stage (i.e., from the time when the normal contact  
692 force is less than 30% of the maximum normal force to when it became zero) during impact was  
693 not beneficial to grain mass flow measurement. Qiu et al. (2012) extended this study to include  
694 the elevator belt speed of 1.5 m/s and the effect of sliding during impact.

## 695 ***MODELING CONFINED GRAIN***

### 696 ***Silo Probing***

697 Managing grain quality in a grain handling facility involves sampling the grain from the  
698 incoming truck and testing it for quality. To assess quality, incoming bulk grain in trucks or rail  
699 cars are probed using mechanical (vacuum) probes. Chung and Ooi (2006), using DEM,  
700 simulated the penetration of probes in a dense granular medium to evaluate the resistance of



701 granular bulk to penetration of a moving object and the dynamic force transmission to a contact  
702 surface. The setup the authors used was comparable to a confined compression arrangement with  
703 a probe to penetrate the bulk granular materials. Glass beads and corn kernels were used in the  
704 simulations for comparison purposes. The authors found that the measured and predicted forces  
705 fluctuated during penetration into each material. The average trend was repeatable, with corn  
706 kernels giving a larger resistance to penetration than glass beads.

### 707 ***Compression***

708 Oil expression by compression is a major processing operation used by grain-based oil  
709 industries. Compression of cereal grains is a complicated process to model because it involves  
710 changes in density, inner porosity/voids due to oil removal, size, and shape. By incorporating the  
711 actual physical changes in the DEM model, Raji and Favier (2004a) developed a numerical  
712 model to predict compression behavior of rapeseeds. The model was based on the actual physical  
713 changes during loading of a low-modulus viscoelastic spherical particles and the resulting  
714 change in shape that are often neglected during DEM model development. The authors avoided  
715 errors in estimating the porosity by compressing beds of rapeseeds before the seedbeds reached  
716 the oil point so the void spaces were not filled with oil. The oil point is the state at which the  
717 bulk density of the seedbed approaches the seed kernel density. When the threshold pressure is  
718 reached, the oil emerges from a seed kernel during mechanical seed-oil expression. DEM  
719 predicted the mechanical compression of oilseeds within a standard error of estimate of 0.20, and  
720 the predicted stress-strain values were not significantly different from the experimental values.  
721 Extending the same modeling approach to canola, soybean, and palm-kernel, Raji and Favier  
722 (2004b) validated their approach of using low-modulus viscoelastic spherical particles for DEM  
723 simulations. Raji and Favier (2004a, b) concluded that DEM is a useful tool to study the behavior

724 of deformable soft particulates and the outputs from modeling could be used to design and  
725 modify oil expression process machinery.

726 The effects of materials' different shapes during compression were investigated by Chung and  
727 Ooi (2006, 2008a), who simulated the confined compression of spherical (glass beads) and non-  
728 spherical (corn kernels) particles. The confined compression test simulation was designed to  
729 investigate the mechanical response of a granular material under confined compression and the  
730 load transfer to the containing walls. The applied vertical load, vertical displacement, vertical  
731 force transmitted to the bottom platen, and force transmitted to the walls were measured, and the  
732 material properties for silo design, the lateral pressure ratio, and the bulk wall friction were also  
733 evaluated. The findings from these studies indicated that accurate representation of particle shape  
734 may not be necessary for prediction of kernels under compression because capturing the key  
735 linear dimensions of a particle may be adequate. DEM results indicated that glass spheres, with  
736 their tendency to spin more than non-spherical particles, were more sensitive to initial packing  
737 arrangement as influenced by the particle generation method. Irregular particles such as corn  
738 kernels were not sensitive to particle spacing as affected by the particle generation method.  
739 Interparticle friction affected the loading for the containing walls for corn kernels but not for  
740 glass beads; this result was attributed to the significant difference in particle stiffness between  
741 two particles. Reducing the contact friction allowed more contacts to reach limiting friction for  
742 corn, thus resulting in a larger lateral pressure ratio and a smaller load on the bottom platen than  
743 for glass beads.

744 Moisture content is a principal factor that influences the compression, size reduction, and  
745 handling behavior of bulk cereal grains. Understanding the effects of moisture on compression  
746 through modeling was initiated by Wiącek and Molenda (2011). The authors used EDEM

747 software with rapeseeds represented as single spheres with 1.9 mm diameter and used the  
748 physical properties obtained from the literature (Wiącek, 2008). The load responses of rapeseed  
749 subjected to uniaxial confined compression quantified at moisture contents of 7.5%, 9%, and  
750 12% and were compared with experimental data. The authors observed that the DEM predicted a  
751 softer response for the spherical assembly of rapeseeds compared with the experimental  
752 observations. Although the model responses deviated from the actual values, this study  
753 illustrated the possibility of using DEM to predict the mechanical behavior of granular materials  
754 of biological origin.

755 Interparticle friction and particle stiffness also influenced the bulk response of grain kernels in  
756 DEM simulations under confined compression. Chung and Ooi (2008b) found that reduction of  
757 particle stiffness by a few orders can provide a huge computational advantage, with secondary  
758 effects on the load transmission in a quasi-static assembly. The researchers also found that  
759 interparticle friction has an effect on the loading of containing walls in simulating confined  
760 compression of corn kernels but not of glass beads. For corn kernels, reduced contact friction  
761 allowed more contacts to reach limiting friction, resulting in a larger lateral pressure ratio and a  
762 smaller load on the bottom of the confined structure.

763 Modeling the compression of grain has been used to calibrate material properties for DEM  
764 simulations (Coetzee and Els 2009a, 2009b) and to determine parameter values of cohesionless  
765 corn kernels. Coetzee and Els (2009a) calibrated particle stiffness using confined compression  
766 tests (also called oedometer tests) by applying stress to corn kernels along the vertical axis at low  
767 compression rates ( $\pm 2 \text{ mm min}^{-1}$ ). Numerical simulation of 2-D corn kernels indicated that the  
768 internal friction angle depended on particle stiffness and the particle friction coefficient. Results  
769 of the confined compression test showed that the simulated macro or bulk stiffness is a linear

770 function of the particle stiffness; thus, particle stiffness can be determined through the confined  
771 compression test. This study showed that DEM simulation could enable determination of particle  
772 properties to enhance understanding of the bulk behavior of cereal grains.

### 773 ***Shear Testing***

774 DEM was used to examine the influence of the friction coefficient between two sliding  
775 particles on the shear behavior of an assembly of rapeseeds in 2-D systems (Molenda et al.  
776 2011). The authors first measured the interparticle friction coefficients for metal plates, pea,  
777 wheat, and rapeseeds. Then they simulated the direct shear test using 2-D DEM models. The  
778 authors found that the degree of variation of the coefficient of interparticle friction did not  
779 influence the final value of shear strength at steady state flow; however, the level of standard  
780 deviation of the coefficient of interparticle friction markedly influenced the shear path (or shear-  
781 strain characteristics) at the initiation of motion.

782 The effects of moisture content on shear testing were simulated by Sarnavi et al. (2013). They  
783 modeled the strength properties of stored wheat kernels at different moisture contents using the  
784 Jenike method of direct shear tests (ASTM 2006). The research group implemented linear and  
785 nonlinear models. Three types of particle models were used to create kernels by a multi-sphere  
786 approach: (1) spherical, (2) 4-spheres, and (3) 8-spheres. The simulation of bulk behavior was  
787 strongly affected by the interparticle interactions and particle shape representation in modeling.  
788 Linear models are more capable of representing the variation in strength properties with moisture  
789 content than nonlinear models. In general, both linear and nonlinear models have an equal  
790 chance of correctly predicting strength properties of the wheat assembly. Spherical grain models  
791 best simulated wheat kernels in bulk properties tests. Both the values of internal angle of friction  
792 and apparent cohesion have about a 70% chance of prediction by the DEM model.

793 **GRAIN DRYING**

794 Although grain is considered free-flowing during grain drying, the dense arrangement of the  
795 particles inside the grain dryer make them behave like confined particles. Iroba et al. (2011a, b)  
796 examined the physical phenomena that control particle flow in mixed-flow dryers (MFDs). They  
797 investigated the residence time distribution (RTD), particle vertical velocity profiles, and particle  
798 trajectories using PFC2D. Simulation results were validated with experiments using a semi-  
799 technical dryer test station with a transparent Plexiglas front wall. Experiments were conducted  
800 with moist wheat as a bed material, with an average moisture content of 18% wet basis (w.b.)  
801 and a bulk density of  $783 \text{ kg m}^{-3}$ . Colored tracer particles were employed in the residence time  
802 analysis in the mixed-flow dryer (MFD) to detect particle flow inhomogeneity and design deficit.  
803 Simulation results showed that the DEM model adequately predicted particle flow during drying.  
804 Through DEM simulation, it was understood that two flow regimes exist in MFDs, the near-wall  
805 region and the central region. Particles at the near-wall region had lower particle velocity,  
806 whereas the central region had high particle velocity. Wall friction dominated the particle flow  
807 near-wall region and had a large effect on the bulk particle movement, whereas particle-particle  
808 forces were dominant in the central region. Kernels passing through the MFD have different  
809 vertical velocities, thus resulting in different residence times. The presence of two different flow  
810 regimes will affect overall dryer capacity and drying efficiency. Kernels flowing at lower  
811 velocities may be over-dried, while those moving at high velocities may be under-dried. The  
812 authors concluded that the present design of MFDs did not provide adequate cross-mixing, with  
813 the effect of the half air ducts dominant on the sidewalls. Consequently, the current design may  
814 lead to broad moisture content distribution at the outlet (inhomogeneous drying) with the risk of  
815 product quality deterioration during subsequent storage. This study underlined the importance of

816 updated MFD design, such as the need to adjust the size and positions of the half air ducts.  
817 Although the 2-D DEM model predicted the residence time distributions and the flow patterns,  
818 improvements in the approach are needed to map velocity profiles. To depict the grain drying  
819 process accurately, numerical simulation should also account for the shrinkage of kernels during  
820 drying because this shrinkage alters the particle properties.

821 To improve the prediction of drying process using DEM, Mellman et al. (2011) modeled the  
822 effects of design elements and air duct arrangements on MFDs. The authors articulated the same  
823 findings as Iroba et al. (2011a, b) regarding the RTD in mixed-flow grain dryers. Simulation and  
824 experimental results showed that the DEM can adequately predict the main features of particle  
825 flow. The half air ducts at the sidewalls obstructed the free flow of grain, resulting in the long  
826 tail of the RTD. The studies indicated that the diagonal duct arrangement showed a more even  
827 grain moisture and temperature distribution than the horizontal duct arrangement. The airflow  
828 distribution in the grain bed in the diagonal arrangement was considered degraded, however,  
829 because of the dead zones, which were not flushed by the drying air, in the MFD. The authors  
830 concluded that grain bulk and particle moisture content as well as grain temperature distributions  
831 fluctuate strongly over the cross-section of the dryer, resulting in inhomogeneous drying. The  
832 analysis displayed deficits in the present design of MFDs, namely the arrangement and allocation  
833 of the air ducts.

834 Due to variations in grain properties, dryer design, and drying parameters, optimizing dryer  
835 design and understanding particle movement inside the dryer is of continued interest researchers  
836 as well as industry. The influence of dryer walls and air ducts on particle velocity distribution in  
837 an MFD was investigated by Keppler et al. (2012), who modeled the effects of particle-wall  
838 friction, air duct apex angle, and wall angle on the vertical direction of particle velocity

839 distribution. The effects of different construction modifications for more even vertical grain  
840 particle velocity distribution were analyzed using DEM. The authors found from experiments  
841 and simulations that the sidewalls have a strong impact on grain flow, causing segregation; these  
842 were similar to the findings by Iroba et al. (2011a). Both studies indicated that segregation  
843 caused big differences in the residence time of single grain portions and caused uneven drying.

844 Weigler et al. (2012) extended the work of Iroba et al. (2011a, b) and Mellman et al. (2011) by  
845 investigating the particle and airflows in MFDs using DEM and CFD. The particle flow behavior  
846 of wheat in the traditional MFD was simulated using PFC2D. Two different particle  
847 representations of wheat, spherical and ellipsoidal, were studied and compared when simulating  
848 particle flow. A diagonal air duct arrangement led to dead zones in airflow. Airflow through the  
849 grain bed was simulated using CFD, applying the commercial software ANSYS CFX (Release  
850 14.0, ANSYS, Inc., Canonsburg, Penn.). The airflow domain in the dryer apparatus was  
851 discretized by generating a finite volume grid employing the software ANSYS ICEM (ANSYS,  
852 Inc., Canonsburg, Penn.). The authors found that over- and under-drying occurred in traditionally  
853 designed mixed-flow dryers because of unfavorable air duct arrangements; core flow of particles  
854 due to the wall friction effect and the half air ducts fixed at the sidewalls, characterized by  
855 retarded flow at the dryer walls and a fast flow region in the center; and dead zones in airflow,  
856 resulting in uneven airflow, grain flow, and drying conditions over the cross-section. They  
857 recommended a new dryer design with the airflow distribution adjusted to the particle flow  
858 distribution. In regions with higher particle velocities, higher air velocities should be provided.  
859 The sidewalls of the dryer should be inclined, and the half air ducts should be removed.  
860 Researchers also added that future design development would require a tool that couples the

861 airflow characteristics with the particle flow characteristics, including the heat and mass transfer,  
862 such as coupled CFD and DEM simulation.

863 Weigler et al. (2013) used the model they developed for MFDs (Weigler et al. 2012) to study  
864 the flow of grain in the process of designing an efficient MFD using PFC2D. The particle flow  
865 was studied by tracing the differently colored kernels through the transparent sidewall of the  
866 dryer. Based on the observations, the authors developed a new MFD geometry that results in  
867 uniform drying of kernels. The greatest advantage of using DEM modeling techniques in grain  
868 drying is the ability to study the grain velocity distribution within the dryer as affected by  
869 constructional modifications. This will be of great interest to industry because understanding  
870 grain behavior within the dryer allows analysis of drying without requiring an expensive  
871 prototype.

## 872 **A Case Study**

873 In this case study, the commingling of two types of grain in a bucket-type grain elevator boot  
874 system is considered based on Boac et al. (2012). Previous research in commercial elevator  
875 equipment (Ingles, et al., 2003; 2006; Ingles, 2005) showed large variations between and within  
876 facilities for commingling of grain lots, which can greatly increase the number of experiments  
877 necessary to make widely-applicable inferences. However, DEM was used in this case study to  
878 model the commingling in a grain elevator boot system and avoid the time and expense of many  
879 more experiments.

880 A 3-D computer-aided design (CAD) drawing (DS SolidWorks Corp., Concord, Mass.) of the  
881 pilot-scale bucket elevator leg and boot geometry (model B3, Universal Industries, Inc., Cedar  
882 Falls, Iowa) was imported in EDEM 2.3. Grain commingling in the pilot-scale boot was  
883 simulated using 3-D and quasi-2-D DEM models. Simulations were performed at 20% Rayleigh



884 time step. The Hertz-Mindlin no-slip model (DEM Solutions, 2013) was implemented as the  
885 contact model for all simulations.

886 Two types of soybeans with different intrinsic properties were colored red and yellow in the  
887 simulation to illustrate their difference. The particle model developed by Boac et al. (2010) for  
888 soybeans was used. Red soybeans were allowed to flow inside the grain elevator boot geometry.  
889 The grain elevator leg (composed of bucket cups) was allowed to run for 15 s of simulation time,  
890 until the red soybeans stabilized as the residual grain at the bottom of the boot. With red  
891 soybeans as the residual grain, yellow soybeans were generated in the simulation and allowed to  
892 accumulate in the left-hand side (LHS) hopper for 15 s before opening the slide gate. Yellow  
893 soybeans were then continuously run in the boot for approximately 8 min in simulation time  
894 (Figure 3a).

895 The same simulation procedure was followed for a quasi-2-D DEM model using a periodic  
896 boundary and domain width equivalent to 5.6 times the particle diameter (Figure 3b). The total  
897 particle mass of red and yellow soybeans was determined from each bucket cup in all  
898 simulations. Predicted average commingling data were computed, plotted at each time interval,  
899 and compared with experimental data. Figure 4 shows that the predicted average commingling  
900 from 3-D and quasi-2-D DEM models of the boot closely matched the experimental data,  
901 especially after the flow has stabilized after 100 s. The quasi-2-D (5.6d) model reduced  
902 simulation run time by 72% to 74% compared to the 3-D model, with both models being run on  
903 the same workstation (Table 4). This case study showed that grain commingling in a bucket  
904 elevator boot system can be simulated with both 3-D and quasi-2-D DEM models, giving results  
905 that agreed with experimental data.

## 906 **Application of DEM in Other Food Engineering Operations**

907 Postharvest operations in any food engineering applications are complex and modeling has  
908 proved to be effective for prediction, process calculation and process design purposes. Ho et al.  
909 (2013) suggested that parallel multiscale modeling, with a complete understanding of the  
910 structural aspect of food material, will be the best approach for analyzing and designing food  
911 processing systems.

912 In specific, fresh horticultural crop produce are difficult to model due to their non-uniformity  
913 in size and shape and for their higher vulnerability to changes in surface and textural  
914 characteristics during handling and transport (Ambaw et al. 2013). Delele et al. (2010) developed  
915 a combined DEM and computational fluid dynamics (CFD) model to analyze the airflow during  
916 cooling through stacks of boxes with horticultural produce. DEM was used to generate random  
917 stacking of spheres in the box. Cooling was simulated at different heights of the stack with  
918 different diameter spheres. The results indicate that DEM helped identify that random filling has  
919 less influence on the air flow resistance than other factors such as confinement ratio, size,  
920 porosity, and box vent hole ratio. Through this coupled DEM-CFD approach, the flow profile in  
921 individual pores could be analyzed that could not be done through porous media approaches.

922 Van Zeebroeck et al. (2006 ab) applied DEM to study impact damage in apples during  
923 transport and handling. The authors used the nonlinear Kuwbara and Kono contact force model  
924 and the parameters were derived experimentally. The model findings were validated using a  
925 shaking box approach of vibrating apples in an electro-hydraulic shaker. Though the authors  
926 predicted the bruising damage with reasonable accuracy, multi-impact bruise surfaces and the  
927 bruise volume could not be predicted. For vibration damage, the Kuwabara and Kona contact  
928 model predicted the condition of apple as influenced by fruit properties and mechanical

929 parameters such as vibration frequency and stack height. Further, the model accurately predicted  
930 the existence of damage chains within the apple stack.

## 931 **Summary and Conclusions**

932 Existing literature that used DEM to simulate postharvest handling and processing, limited to  
933 grain and its coproducts, was reviewed. The soft-sphere approach of DEM was commonly used  
934 to develop these grain and food processing industry process simulations. The advantage of soft-  
935 sphere models was their capability of handling multiple particle contacts, which are of  
936 importance when modeling bulk grain systems. The deformations that a grain kernel undergoes  
937 during handling and processing were used to calculate elastic, plastic, and frictional forces  
938 between particles, and the motion of particles was described by Newton's laws of motion.

939 Particle models varied with the type of grain. For near-spherical kernels such as soybean and  
940 rapeseed, single sphere particle models predicted particle behavior with greater accuracy. For  
941 non-spherical kernels such as rice, wheat, and corn, particle representation using a multi-sphere  
942 approach reduced specific simulation errors, but increased simulation time and computational  
943 load because of the higher number of contact points requiring force and deformation calculation  
944 at each contact point. To avoid this excess computation time problem, most researchers have  
945 used single sphere models and had reasonable success in predictions. Rotation of the single-  
946 sphere particles must be properly described, however, because these particles rotate more easily  
947 in the simulation than observed in experiments. Thus, the rolling friction coefficient is an  
948 important component when using spherical particle models to simulate non-spherical kernels.  
949 Depending on the software used, both linear and non-linear (Hertz-Mindlin) contact models have  
950 been used effectively to study grain handling and processing operations.

951 DEM simulations have been used in different grain processing environments, such as those  
952 dealing with free-flowing grain and with confined grain, for optimizing processes and to improve  
953 equipment design. In general, DEM has adequately simulated postharvest processing of grain  
954 and grain coproducts. In some processes, such as the analysis of discharge from a silo and design  
955 of grain dryers, coupling DEM with computational fluid dynamics is recommended for better  
956 predictions. Although DEM has been increasingly used to study grain kernel processes, it has not  
957 been widely applied. The huge variation in particle characteristics such as size, shape, surface  
958 roughness, density, friction coefficients, composition, and other factors could be hindering the  
959 use of DEM. Computational cost also limits DEM application; specifically, most of the particles  
960 in grain-based food industries are smaller, which leads to higher computation time. Development  
961 of precision particle models could help spur adoption of this numerical modeling concept and  
962 optimize process and equipment design in the grain handling and processing industry.

963 ***ACKNOWLEDGEMENTS***

964 This is contribution no. 14-278-J from the Kansas State University Agricultural Experiment  
965 Station.

966

967 **References**

- 968 Ambaw A, Delele MA, Defraeye T, Ho QT, Opara LU, Nicolai BM, Verboven P (2013) The use  
969 of CFD to characterize and design post-harvest storage facilities: past, present and future.  
970 *Computers and Electronics in Agriculture* 93: 184-194
- 971 ASTM. 2006. Standard test method for shear testing of bulk solids using the Jenike shear cell.  
972 D6128. American Society for Testing and Materials, West Conshohocken, PA
- 973 Boac JM (2010) Quality changes, dust generation, and commingling during grain elevator  
974 handling. Ph.D. Dissertation. Kansas State University, Manhattan, Kansas
- 975 Boac JM, Casada ME, Maghirang RG, Harner JP (2010) Material and interaction properties of  
976 selected grains and oilseeds for modeling discrete particles. *Transactions of the ASABE*  
977 53(4):1201–1216
- 978 Boac JM, Casada ME, Maghirang RG, Harner JP (2012) 3-D and quasi-2-D discrete element  
979 modeling of grain commingling in a bucket elevator boot system. *Transactions of the*  
980 *ASABE* 55(2):659–672
- 981 Boukouvala F, Gao Y, Muzzio F, Ierapetritou MG (2013) Reduced-order discrete element  
982 method modeling. *Chemical Engineering Science* 95: 12-26
- 983 Campbell CS (2006) Granular material flows – an overview. *Powder Technology* 162:208-229
- 984 Chung YC, Ooi JY, Favier JF (2004) Measurement of mechanical properties of agricultural  
985 grains for DE models. In: *17th ASCE Engineering Mechanics Conference*. American  
986 Society of Civil Engineers, Newark, Delaware

987 Chung YC, Ooi JY (2006) Confined compression and rod penetration of a dense granular  
988 medium: discrete element modeling and validation. In: Wu W, Yu HS (eds.) *Modern*  
989 *trends in geomechanics*. pp. 223–239. Springer, Berlin

990 Chung YC, Ooi JY (2008a) Influence of discrete element model parameters on bulk behavior of  
991 a granular solid under confined compression. *Particulate Science and Technology*  
992 26(1):83–96

993 Chung YC, Ooi JY (2008b) A study of influence of gravity on bulk behaviour of particulate  
994 solid. *Particuology* 6(6):467–474

995 Clementson CL (2010) The granulometric heterogeneity of distillers dried grains with solubles  
996 (DDGS) and its effect on the bulk physical and chemical properties. Ph.D. Thesis. Purdue  
997 University, West Lafayette, Indiana

998 Coetzee CJ, Els DNJ (2009a) Calibration of discrete element parameters and the modelling of  
999 silo discharge and bucket filling. *Computers and Electronics in Agriculture* 65(2):198–  
1000 212

1001 Coetzee CJ, Els DNJ (2009b) Calibration of granular material parameters for DEM modelling  
1002 and numerical verification by blade-granular material interaction. *Journal of*  
1003 *Terramechanics* 46(1):15–26

1004 Coetzee CJ, Els DNJ (2009c) The numerical modelling of excavator bucket filling using DEM.  
1005 *Journal of Terramechanics* 46(5):217–227

1006 Coetzee CJ, Els DNJ, Dymond GF (2010) Discrete element parameter calibration and the  
1007 modelling of dragline bucket filling. *Journal of Terramechanics* 47(1):33–44

1008 Cundall PA (1988a) Computer simulations of dense sphere assemblies. In: Satake M, Jenkins JT  
1009 (eds.) *Micromechanics of granular materials*. pp. 113–23. Elsevier, Amsterdam

1010 Cundall PA (1988b) Formulation of a three-dimensional distinct element method. Part I: A  
1011 scheme to detect and represent contacts in a system composed of many polyhedral  
1012 blocks. *International Journal of Rock Mechanics and Mining Sciences and*  
1013 *Geomechanics Abstracts* 25(3):107–116

1014 Cundall PA, Hart RD (1989) Numerical modeling of discontinua. In Mustoe GGW, Henriksen  
1015 M, Huttelmaier HP (eds) *Proceedings of the 1st U.S. Conference on Discrete Element*  
1016 *Methods*. CSM Press, Golden, Colorado

1017 Cundall PA, Strack ODL (1979) A discrete numerical model for granular assemblies.  
1018 *Geotechnique* 29(1):47–65

1019 de Bruyn, JR (2012) When does a granular material behave like a continuum fluid? *Journal of*  
1020 *Fluid Mechanics* 704:1–4

1021 Delaney G, Inagaki S, Aste T (2007) Fine tuning DEM simulations to perform virtual  
1022 experiments with three dimensional granular packings. In: Aste Y, Di Matteo T,  
1023 Tordesillas A (eds) *Granular and Complex Materials*. pp. 141-168. World Scientific

1024 Delele MA, Tijskens E, Atalay YT, Ho QT, Ramon H, Nicolai BM, Verboven, P (2008)  
1025 Combined discrete element and CFD modelling of airflow through random stacking of  
1026 horticultural products in vented boxes. *Journal of Food Engineering* 89(1): 33-41

1027 DEM Solutions (2013) EDEM 2.5 User Guide. DEM Solutions, Ltd., Edinburgh, UK

1028 Dewicki G (2003) Bulk material handling and processing – numerical techniques and simulation  
1029 of granular material. *Bulk Solids Handling: International Journal of Storing and*  
1030 *Handling Bulk Materials* 23(2):110–113

1031 Di Renzo A, Di Maio FP (2004) Comparison of contact-force models for the simulation of  
1032 collisions in DEM-based granular flow codes. *Chemical Engineering Science* 59(3):525–  
1033 541

1034 Di Renzo A, Di Maio FP (2005) An improved integral non-linear model for the contact of  
1035 particles in distinct element simulations. *Chemical Engineering Science* 60(5):1303–1312

1036 FAO (2013) Zae mays L. Food and Agriculture Organization of the United Nations, Rome, Italy

1037 Favier JF, Abbaspour-Fard MH, Kremmer M, Raji AO (1999) Shape representation of axi-  
1038 symmetrical, non-spherical particles in discrete element simulation using multi-element  
1039 model particles. *Engineering Computations* 16(4):467–480

1040 Ferrellec JF, McDowell GR (2010) A method to model realistic particle shape and inertia in  
1041 DEM. *Granular Matter* 12(5):459–467

1042 Fortin J, Millet O, de Saxce G (2004) Numerical simulation of granular materials by an  
1043 improved discrete element method. *International Journal for Numerical Methods in*  
1044 *Engineering* 62:639-663

1045 Ghaboussi J, Barbosa R (1990) Three-dimensional discrete element method for granular  
1046 materials. *International Journal for Numerical and Analytical Methods in Geomechanics*  
1047 14(7):451–472

1048 González-Montellano C, Ramirez A, Gallego E, Ayuga F (2011) Validation and experimental  
1049 calibration of 3D discrete element models for the simulation of the discharge flow in  
1050 silos. *Chemical Engineering Science* 66(21):5116–5126

1051 González-Montellano C, Ramirez A, Fuentes JM, Ayuga F (2012a) Numerical effects derived  
1052 from *en masse* filling of agricultural silos in DEM simulations. *Computers and*  
1053 *Electronics in Agriculture* 81:113–123



1054 González-Montellano C, Gallego E, Ramirez-Gomez A, Ayuga F (2012b) Three dimensional  
1055 discrete element models for simulating the filling and emptying of silos: Analysis of  
1056 numerical results. *Computers and Chemical Engineering* 40:22–32

1057 González-Montellano C, Fuentes JM, Ayuga- Tellez E, Ayuga F (2012c) Determination of the  
1058 mechanical properties of maize grains and olives required for use in DEM simulations.  
1059 *Journal of Food Engineering* 111(4):553–562

1060 Jiang G, Qiu B (2011) Discrete element method simulation of impact-based measurement of  
1061 grain mass flow. In *Proceedings of the 2011 International Conference on Computer  
1062 Distributed Control and Intelligent Environmental Monitoring* 5747847:419–422

1063 Hart R, Cundall PA, Lemos J (1988) Formulation of a three-dimensional, distinct element  
1064 method, Part II: Mechanical calculations for motion and interaction of a system  
1065 composed of many polyhedral blocks. *International Journal of Rock Mechanics and  
1066 Mining Sciences and Geomechanics Abstracts* 25(3):117–125

1067 Ho QT, Carmeliet J, Datta AK, Defraeye T, Delele MA, Herremans E, Opara L, Ramon H,  
1068 Tijskens E, Sman Rvd, Liedekerke PV, Verboven P, Nicolai BM (2013) Multiscale  
1069 modeling in food engineering. *Journal of Food Engineering* 114: 279-291

1070 Hocking G (1992) The discrete element method of analysis of fragmentation of discontinua.  
1071 *Engineering Computation* 9(2):145–155

1072 Hogue C (1998) Shape representation and contact detection for discrete element simulations of  
1073 arbitrary geometries. *Engineering Computations* 15(3):374–390

1074 Hoomans BPB, Kuipers JAM, Briels WJ, Van Swaaij WPM (1996) Discrete particle simulation  
1075 of bubble and slug formation in a two-dimensional gas-fluidized bed: A hard-sphere  
1076 approach. *Chemical Engineering Science* 51(1):99–118

1077 Hustrulid AI (1998) Transfer station analysis. Paper presented at the 1998 SME Annual Meeting,  
1078 Orlando, Florida

1079 Hustrulid AI, Mustoe GGW (1996) Engineering analysis of transfer points using discrete  
1080 element analysis. Paper presented at the 1996 SME Annual Meeting, Phoenix, Arizona

1081 Ingles MEA (2005) Identity preservation of grain in elevators. Unpublished PhD dissertation.  
1082 Kansas State University Department of Biological and Agricultural Engineering,  
1083 Manhattan, Kansas

1084 Ingles MEA, Casada ME, Maghirang RG (2003) Handling effects on commingling and residual  
1085 grain in an elevator. *Transactions of the ASAE* 46(6):1625-1631

1086 Ingles MEA, Casada ME, Maghirang RG, Herrman TJ, Harner JP III (2006) Effects of grain-  
1087 receiving system on commingling in a country elevator. *Applied Engineering in*  
1088 *Agriculture* 22(5):713-721

1089 Iroba KL, Mellman J, Weigler F, Metzger T, Tsotsas E (2011a) Particle velocity profiles and  
1090 residence time distribution in mixed-flow grain dryers. *Granular Matter* 13(2): 159–168

1091 Iroba KL, Weigler F, Mellman J, Metzger T, Tsotsas E (2011b) Residence time distribution in  
1092 mixed-flow grain dryers. *Drying Technology* 29(11):1252–1266

1093 Isik E (2007) Some Engineering Properties of Soybean Grains. *American Journal of Food*  
1094 *Technology* 2:115–125

1095 Itasca (2008) PFC3D Particle flow code in 3 dimensions: Theory and background. Itasca  
1096 Consulting Group, Minneapolis, Minn. 40pp

1097 Jean M, Moreau JJ (1991) Dynamics of elastic or rigid bodies with frictional contact: numerical  
1098 methods. *Publications du L.M.A.* 124:9-29

1099 Kačianauskas R, Maknickas A, Kačeniauskas A, Markauskas D, Balevičius R (2010) Parallel  
1100 discrete element simulation of poly-dispersed granular material. *Advances in Engineering*  
1101 *Software* 41(1):52–63

1102 Keppler I, Kocsis L, Oldal I, Farkas I, Csatar A (2012) Grain velocity distribution in a mixed  
1103 flow dryer. *Advanced Powder Technology* 23(6):824–832

1104 Kuwabara G, Kono K (1987) Restitution coefficient in a collision between two spheres.  
1105 *Japanese Journal of Applied Physics* 26(8):1230–1233

1106 Li H, Li Y, Gao F, Zhao Z, Xu L (2012) CFD-DEM simulation of material motion in air-and-  
1107 screen cleaning device. *Computers and Electronics in Agriculture* 88:111–119

1108 Li J, Webb C, Pandiella SS, Campbell GM (2002) A numerical simulation of separation of crop  
1109 seeds by screening – effect of particle bed depth. *Food and Bioproducts Processing:*  
1110 *Transactions of the Institution of Chemical Engineers, Part C* 80(2):109–117

1111 Li J, Webb C, Pandiella SS, Campbell GM (2003) Discrete particle motion on sieves – a  
1112 numerical study using the DEM simulation. *Powder Technology* 133(1–3):190–202

1113 Li Y, Xu Y, Thornton C (2005) A comparison of discrete element simulations and experiments  
1114 for ‘sandpiles’ composed of spherical particles. *Powder Technology* 160(3):219–228

1115 Lin X, Ng TT (1997) A three-dimensional discrete element model using arrays of ellipsoids.  
1116 *Geotechnique* 47(2):319–329

1117 LoCurto GJ, Zhang X, Zarikov V, Bucklin RA, Vu-Quoc L, Hanes DM, Walton OR (1997)  
1118 Soybean impacts: experiments and dynamic simulations. *Transactions of the ASAE*  
1119 40(3):789–794

1120 Lu M, McDowell GR (2007) The importance of modelling ballast particle shape in the discrete  
1121 element method. *Granular Matter* 9(1–2):69–80

1122 Markauskas D, Kačianauskas R (2011) Investigation of rice grain flow by multi-sphere particle  
1123 model with rolling resistance. *Granular Matter* 13(2):143–148

1124 Markauskas D, Kačianauskas R, Džiugys A, Navakas R (2010) Investigation of adequacy of  
1125 multi-sphere approximation of elliptical particles for DEM simulations. *Granular Matter*  
1126 12(1):107–123

1127 Mellman J, Iroba KL, Metzger T, Tsotsas E, Mészáros C, Farkas I (2011) Moisture content and  
1128 residence time distributions in mixed-flow grain dryers. *Biosystems Engineering* 109(4):  
1129 297–307

1130 Metzger MJ, Glasser BJ (2013). Simulation of the breakage of bonded agglomerates in a ball  
1131 mill. *Powder Technology* 237: 286-302

1132 Miller GF, Pursey H (1955) On the partition of energy between elastic waves in a semi-infinite  
1133 solid. *Proceedings of the Royal Society of London Series A: Mathematical and Physical*  
1134 *Sciences* 233(1192):55–69

1135 Mindlin RD (1949) Compliance of elastic bodies in contact. *Journal of Applied Mechanics*  
1136 16:259–268

1137 Mindlin RD, Deresiewicz H (1953) Elastic spheres in contact under varying oblique forces.  
1138 *Transactions of ASME, Series E. Journal of Applied Mechanics* 20:327–344

1139 Mishra BK (2003) A review of computer simulation of tumbling mills by the discrete element  
1140 method: Part I – contact mechanics. *International Journal of Mineral Processing* 71(1–  
1141 4):73–93

1142 Molenda M, Horabik J, Lukaszuk J, Wiącek J (2011) Variability of intergranular friction and its  
1143 role in DEM simulation of direct shear of an assembly of rapeseeds. *International*  
1144 *Agrophysics* 25(4): 361–368

- 1145 O’Sullivan C (2011a) Particle-based discrete element modeling: Geomechanics perspective.  
1146 *International Journal of Geomechanics* 11(6):449–464
- 1147 O’Sullivan C (2011b) Particulate discrete element modelling: A geomechanics perspective. Spon  
1148 Press, New York, NY
- 1149 Parafiniuk P, Molenda M, Horabik J (2013) Discharge of rapeseeds from a model silo: physical  
1150 testing and discrete element method simulations. *Computers and Electronics in*  
1151 *Agriculture* 97: 40–46
- 1152 Potyondy DO, Cundall PA (2004) A bonded-particle model for rock. *International Journal of*  
1153 *Rock Mechanics and Mining Sciences* 41(8):1329–1364
- 1154 Qiu B, Jiang G, Yang N, Guan X, Xie J, Li Y (2012) Discrete element method analysis of impact  
1155 action between rice particles and impact-board. *Transactions of the Chinese Society of*  
1156 *Agricultural Engineering* 28(3):44–49 (Chinese)
- 1157 Raji AO, Favier JF (2004a) Model for the deformation in agricultural and food particulate  
1158 materials under bulk compressive loading using discrete element method. Part I: Theory,  
1159 model development and validation. *Journal of Food Engineering* 64(3):359–371
- 1160 Raji AO, Favier JF (2004b) Model for the deformation in agricultural and food particulate  
1161 materials under bulk compressive loading using discrete element method. Part II:  
1162 Compression of oilseeds. *Journal of Food Engineering* 64(3):373–380
- 1163 Remy B, Khinast JG, Glasser BJ (2009) Discrete element simulation of free-flowing grains in a  
1164 four-bladed mixer. *AIChE Journal* 55(8):2035–2048
- 1165 Rowlands, JC (1991) Dragline bucket filling. Ph.D. Thesis. University of Queensland,  
1166 Queensland, Australia

1167 Sakaguchi E, Kawakami S, Tobita F (1994) Simulation on flowing phenomena of grains by  
1168 distinct element method. Eur. Ag. Eng. Paper No. 94-G-025. Ag. Eng. '94, Milano

1169 Sakaguchi E, Suzuki M, Favier JF, Kawakami S (2001) Numerical simulation of the shaking  
1170 separation of paddy and brown rice using the discrete element method. *Journal of*  
1171 *Agricultural Engineering Research* 79(3):307–315

1172 Sarnavi HJ, Mohammadi AN, Motlagh AM, Didar AR (2013) DEM model of wheat grains in  
1173 storage considering the effect of moisture content in direct shear test. *Research Journal of*  
1174 *Applied Sciences, Engineering and Technology* 5(3):829–841

1175 Theuerkauf J, Dhodapkar S, Jacob K (2007) Modeling granular flow using discrete element  
1176 method – from theory to practice. *Chemical Engineering* 114(4):39–46

1177 Thornton C, Ning Z (1998) A theoretical model for the stick/bounce behaviour of adhesive,  
1178 elastic-plastic spheres. *Powder Technology* 99(2):154–162

1179 Ting JM, Khwaja M, Meachum L, Rowell JD (1993) An ellipse based discrete element model for  
1180 granular materials. *International Journal for Numerical and Analytical Methods in*  
1181 *Geomechanics* 17(9):603–623

1182 Tsuji Y, Tanaka T, and Ishida T (1992) Lagrangian numerical simulation of plug flow of  
1183 cohesionless particles in a horizontal pipe. *Powder Technology* 71(3):239–250

1184 USDA ERS (2013) Oil Crops Yearbook. U.S. Department of Agriculture Economic Research  
1185 Service, Washington, D.C. [http://www.ers.usda.gov/data-products/oil-crops-](http://www.ers.usda.gov/data-products/oil-crops-yearbook.aspx#.UupiItJdUS4)  
1186 [yearbook.aspx#.UupiItJdUS4](http://www.ers.usda.gov/data-products/oil-crops-yearbook.aspx#.UupiItJdUS4)

1187 Van Zeebroeck M, Tijskens E, Dintwa E, Kafashan J, Loodts J, De Baerdemaeker J, Ramon H  
1188 (2006 a) The discrete element method (DEM) to simulate fruit impact damage during

1189 transport and handling: Model building and validation of DEM to predict bruise damage  
1190 of apples. *Postharvest Biology and Technology* 41: 85-91

1191 Van Zeebroeck M, Tijskens E, Dintwa E, Kafashan J, Loodts J, De Baerdemaeker J, Ramon H  
1192 (2006 b) The discrete element method (DEM) to simulate fruit impact damage during  
1193 transport and handling: Case study of vibration damage during apple bulk transport.  
1194 *Postharvest Biology and Technology* 41: 92-100

1195 Vu-Quoc L, Zhang X, Walton OR (2000) A 3-D discrete-element method for dry granular flows  
1196 of ellipsoidal particles. *Computer Methods in Applied Mechanics and Engineering*  
1197 187(3–4):483–528

1198 Walton OR (1983) Particle – dynamics calculations of shear flow. In: Jenkins JT and Satake M  
1199 (eds) *Micromechanics of granular materials: new models and constitutive relations*. pp.  
1200 327–338. Elsevier, Amsterdam

1201 Wassgren CR (1997) Vibration of granular materials. Ph.D. Thesis. California Institute of  
1202 Technology, Pasadena, California

1203 Weigler F, Scaar H, Mellmann J (2012) Investigation of particle and air flows in a mixed-flow  
1204 dryer. *Drying Technology* 30(15):1730–1741

1205 Weigler F, Mellmann J, Franke G, Scaar H (2013) Experimental studies on a newly developed  
1206 mixed-flow dryer. *Drying Technology* 31: 1736-1743

1207 Wiącek J (2008) Discrete element modeling of quasi-static effects in grain assemblies. PhD  
1208 Thesis, Institute of Agrophysics, PAS, Lublin, Poland

1209 Wiącek J, Molenda M (2011) Moisture-dependent physical properties of rapeseed – experimental  
1210 and DEM modeling. *International Agrophysics* 25(1):59–65

1211 Wightman C, Moakher M, Muzzio FJ, Walton OR (1998) Simulation of flow and mixing of  
1212 particles in a rotating and rocking cylinder. *Journal of American Institute of Chemical*  
1213 *Engineers* 44(6):1266-1276

1214 Williams JR, Hocking G, Mustoe GGW (1985) The theoretical basis of the discrete element  
1215 method. *NUMETA '85 Numerical Methods in Engineering, Theory and Applications*.  
1216 Balkema, Rotterdam, The Netherlands

1217 Williams JR, Pentland AP (1989) Superquadrics and modal dynamics for discrete elements in  
1218 concurrent design. In: *1<sup>st</sup> U.S. Conference on the Discrete Element Method*, Golden,  
1219 Colorado

1220 Wojtkowski M, Pecen J, Horabik J, Molenda M (2010) Rapeseed impact against a flat surface:  
1221 physical testing and DEM simulation with two contact models. *Powder Technology*  
1222 198(1):61–68

1223 Zhou YC, Xu BH, Yu AB, Zulli P (2001) Numerical investigation of the angle of repose of  
1224 monosized spheres. *Physical Review E: Statistical, Nonlinear, and Soft Matter Physics*  
1225 64(2):213011–213018

1226 Zhu HP, Zhou ZY, Yang RY, Yu AB (2007) Discrete particle simulation of particulate systems:  
1227 theoretical developments. *Chemical Engineering Science* 62(13):3378–3396  
1228