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How to Gamble with DEM Contact Models and their Validation

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Abstract

The granular matter is abundant in nature and is one of the starting materials for most industries. To improve industrial processes and equipment for handling bulk solids, the behavior of materials must be understood, modeled, and predicted. The Discrete Element Method (DEM) is a suitable numerical tool for this purpose and has been used by researchers and engineers to analyse various industrial applications and processes. However, before performing mass modeling, the input parameters should be carefully tuned for accurate results. However, the calibration of parameter values requires further research. This work provides a consistent notation for the most widely used contact models used to model materials. Additionally, key differences, characteristics between the models are highlighted to provide a reference for engineers and researchers to select the best model for their particular application. On the other hand, it gives how to gamble the validation process to make a successful simulation. These techniques will help the novice simulator to remove or minimize the impact of some critical parameters.

Keywords: Contact Models, Discrete Element Method, Validation, Gambling

1. Introduction

The handling of granular bulk materials can be found in many industries such as mining, agriculture, pharmaceutical, and food industries. Particulate solids account for many of the materials in the extraction industry. The behavior of particulate matter is complex and exhibits properties of solids, liquids, and gases feature. Our understanding and ability to accurately model and predict the behavior of these materials is restricted, especially when the materials are cohesive. Most of the powders handled in the industry are cohesive, causing significant flow problems during various processes such as mixing, transporting, feeding, storing, packaging, and compacting. The problems associated with agglomerated particles are complex, and the success of numerical and experimental approaches depends on accurate characterization and modeling of their physical behaviour. Although several particle level and bulk-level experiments have been used to characterize the aggregation behavior of powders, many problems remain in the numerical modeling of cohesive powders. The Discrete Element Method (DEM) is a numerical tool for modeling particulate matter and predictingits behavior. In a DEM, single or discrete finite number particles are modeled, contact model and particle shape and size distribution determine bulk behavior. Several discrete particle methods are available, but the most popular is the soft contact (DEM) discrete element method developed by Cundall and Strack [1]. DEMs can continuously track the motion of individual particles over various lengths and time scales, providing comprehensive information about the behavior of bulk solids. In contrast to FEM, DEM allows the modeling of dynamic, quasi-static, and static zones within bulk material systems, successfully investigating phenomena such as strain localization, separation, and mixing. Discrete element method numerical calculations use two main equations in the calculation cycle.

The first cycle starts from the forces and torques calculated based on Newton's equations for the translational and rotational motion of each particle and the second cycle applies the Constitutive laws of contact Non-stick material contact models consist of linear or nonlinear springs, damping, and friction sliders. However, when the material is moist (wet), capillary forces lead to bulk cohesive behaviour due to liquid bridging at the contacts [2]. Therefore, coupling elements should be included in the contact model to account for this behaviour. Several such models have been developed, the most common of which are presented clearly in this white paper.Moreover, this paper will give the outline for the appropriate assumption and techniques, when the properties are missing. It will give the understanding for the simulators on how to select the model and how to validating the parameters. Finally, it will give the right perspective on how to make the best use of your simulator and avoid unnecessary mistakes.

2. Characteristics of Contact Models

The entire forces between particles can arise from both non-adhesive forces (like e.g. (also known as body forces or gravitational forces) and adhesive forces. The van der Waals force, the solid bridge force, the electrostatic force, the magnetic force, the liquid bridge force, and other forces are just a few examples of possible sources of adhesive forces. In DEM, contact models are used to simulate the force interaction between the particles. The early development (1970-1980) of DEM primarily focused on simple contact models such as linear springs or Hertzian contactfor spherical particles [3,4]. These models assumed idealized behaviours and were limited in their ability to capture realistic particle interactions. In 1990s,researchers started to incorporate more sophisticated contact models into DEM simulations. Additionally, researchers began to explore more complex geometries and materials beyond spherical particles. The 2000s saw a proliferation of DEM studies across various fields, leading to the development of specialized contact models tailored to specific applications. Models accounting for particle shape, surface roughness, and material properties became more prevalent. The introduction of parallel computing also allowed for more complex simulations with larger numbers of particles. With advancements in computational power and numerical techniques, DEM contact models became increasingly sophisticated and realistic. Hybrid models that combine DEM with other computational methods, such as Computational Fluid Dynamics (CFD) or Finite Element Analysis (FEA), emerged to simulate coupled phenomena.The behavior of particles that are elastic, elastic-adhesive, perfectly plastic, elastoplastic, and elasto-plastic-adhesive has been modeled using a variety of contact models. Some of the contact models and their reference are listed below in the Table 1

Table1: List of Dem Contact Models

Authors (References)	DEM Contact Models
Hertz [5] Brilliantov, Nikolai V [6] Bommireddy [7] JKR [8]	Elastic contact model
C.Thornton and Ning [9] S.Luding [10-12] M.Pasha [13]	Elastoplastic contact model
G.Kuwabara [14] Y.Tsuji [15] H.Kruggel-Emden [16] L.Vu-Quoc [17]	Plastic Contact Model
C.Thornton and Ning [18] J.Tomas [19,20]	Cohesive contact model
R.D,Mindlin [21]	Tangent model
J.Ai [22]	Rolling friction model
J.P Morrissey [23] S.C.Thakur [24]	Elastoplastic Adhesion Model (EEPA)
Feiyang Chen [25]	Hysteretic nonlinear contact models (type I & II) with numerical correction.
N.J.Brown [26] N.Estrada [27] M.J.Jiang [28] S.Utili [29] Yuan Guo [30]	Bonded Contact Model
M.Mascara [31]	Viscoelastic Bonded Model

To witness the continuous development in DEM contact model, the Figure 1will give the overview of the contact model developed over the years and the usage level of contact model. The average usage of contact model was evaluated based on the number of citation on the specific articles.

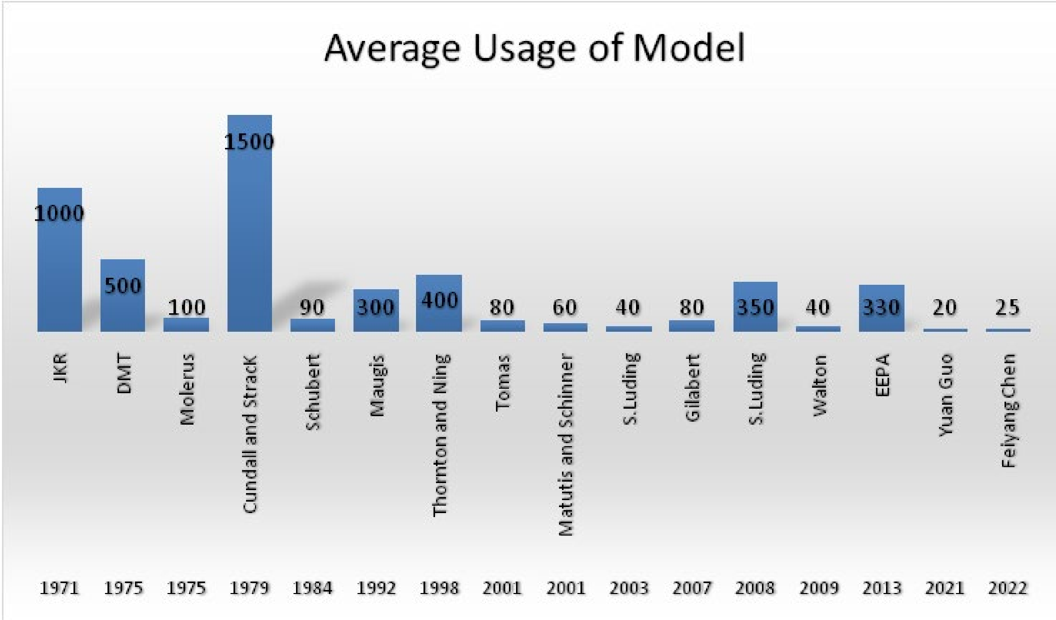

Figure 1: Average Usage of Different Contact Model Over the Years (Web of Science)

The main characteristics feature of a DEM contact model; particle contact detection, contact force calculation, force-displacement relationships, friction, cohesion, damping, viscoelastic, contact stiffness, shape and interaction. Some of the characteristics of discussed contact models are seen inTable 2below.

Table 2: Characteristics of Normal- Force Contact Models

Authors (References)	Attributes
JKR [32]	Elastic –nonlinear, constant adhesion force, does not consider long-range Van der Waals, suitable for large and soft spheres
DMT [33]	Elastic –nonlinear, constant adhesion force, does not consider long-range Van der Waals, suitable for small and stiff spheres
Molerus [34]	Perfectly plastic, adhesion force is proportional to plastic deformation
Cundall and Strack [1]	Elastic- linear, applied to any material with adhesion force
Schubert [35]	Nonlinear elastic – purely plastic, adhesion force proportional to plastic deformation
Maugis [36]	Elastic –nonlinear, constant adhesion force, can be applied to any materials with low or high adhesion force
Thornton and Ning [9]	Hertzian elastic, linear plastic consider for the plastic flattening of the contact
Matutis and Schinner [37]	Elastic–linear, adhesion force proportional to contact area
Tomas [38]	Hertzian elastic, linear plastic, non-linear elastic unloading, load, time, rate dependent viscoelastic, plastic, viscoplastic adhesion
Luding [39]	Linear elastic, linear plastic, load-dependent unloading stiffness, load-dependent adhesion
Gilabert [40]	Linear elastic, approximately for the long-range Vander Waals, the constant adhesion force
Luding [11]	Linear elastic, linear plastic, load-dependent unloading stiffness, and load-dependent adhesion does not account for the permanent plastic deformation
Walton and Braun [41]	Linear elastic, linear plastic, and load-dependent adhesion, account for the permanent plastic deformation, separating the rate of increase of adhesion force from tensile force-displacement
Edinburgh Elasto-Plastic Adhesion Model (EEPA) [23,42-44]	Linear elastic, linear plastic, both linear and non-linear options (by setting the exponents) load-dependent unloading stiffness, load-dependent adhesion, and high loads (consolidation)

Feiyang Chen [25]	Linear elastic, linear plastic, both linear and non-linear options (by setting the exponents) load-dependent unloading stiffness – numerical correction
Yuan Guo [30]	Linear elastic, linear plastic, load-dependent unloading stiffness and bond interaction are linear plastics.

2.1 Selection of Models and its Parameter

One of the key objectives in doing a successful simulation is how to select the contact models and its parameters used in the equations. This selection will depend upon the right estimation methods. This section will give some tips and tricks to describe the parameters and models needed in the simulation. As an engineer or researcher, you always have to make some assumption in to terms of properties used in the contact models. Selection process of model and its parameters can be done in following ways. First by selecting the appropriate the DEM contact models, second by validating the physical parameters used in the simulation.

2.2 Model Selection

The important step is the selecting the appropriate DEM model, the inappropriate selection will affect any subsequent task in the simulation. Lots of factors need to considered, in previous section you can find the different contact models and their characteristics available for the simulation. Apart from that, some factors you need to consider for the selection. The nature of models, its properties interest, and the availability of parameters. To ease the selection of model process, we suggested using the tree decision diagrams show in *Figure 1*. This tress diagram (contact models) has been drawn based on the linear and non-linear behaviour of the model [45]. In addition to that selection also depend on the nature of the material used (For e.g.: Cohesive, non-cohesive suspension etc.). In this case, we framed the tree diagram based on the two areas one with elasticity and other one with plasticity. The reference mentioned in the tree diagram are already explained in the Table 1.

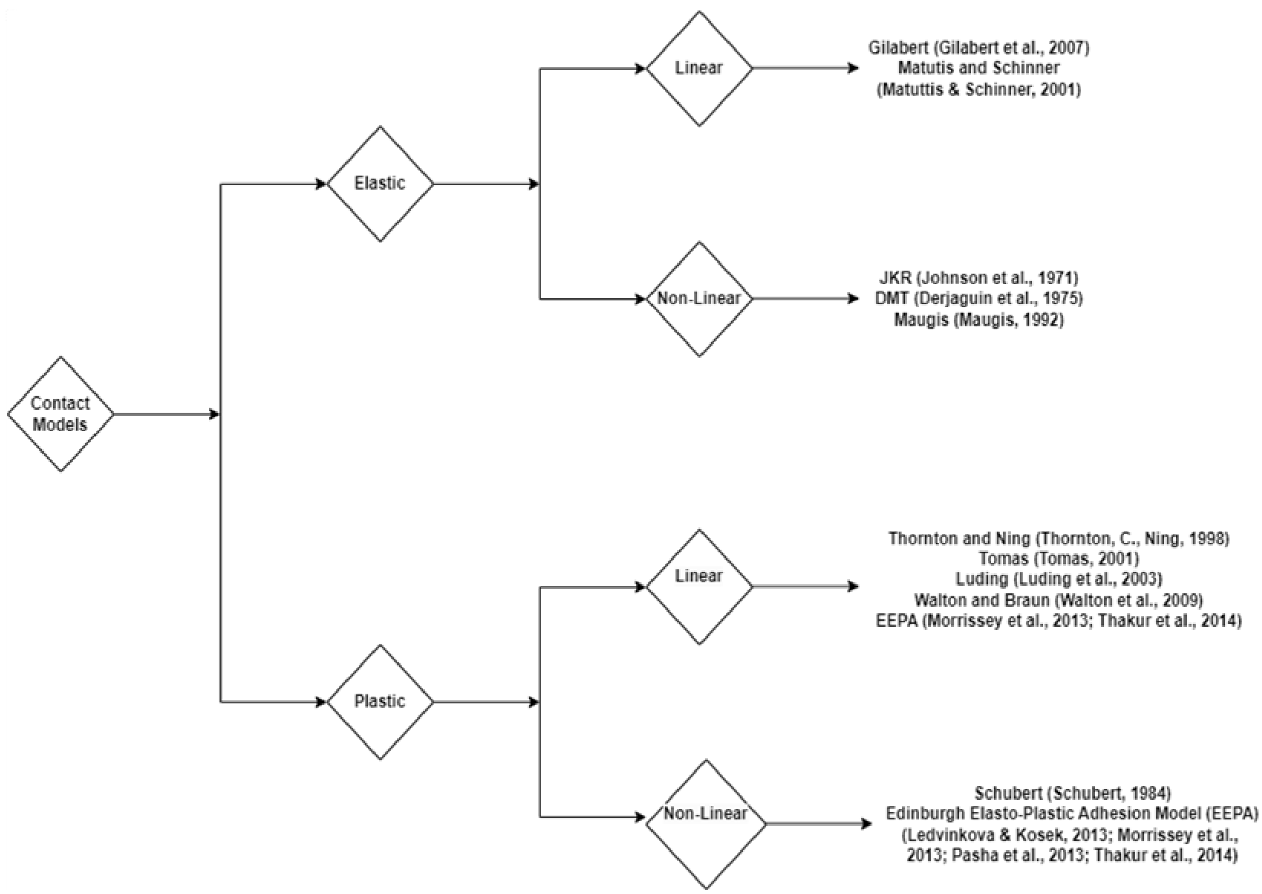

Figure 2: First Step for Selecting Contact Models

Does the choice of model selection matter?Yes, it will affect and that's the main reason for making this method. This way of collecting different models will help to predict the accuracy of the model, its parameter or results that interest to you. Without sufficient parameters (contact area, adhesion force, surface energy etc.), you will not able to calculate the properties of the powders/ particles. You should choose among obtaining and using experimental or literature data and choosing the less rigorous method.

2.3 Validation of Parameter

The much-needed step in any simulation is the validation of the parameters. Generally, this can be done by creating a report, tabulating or plotting for a known parameter values and comparing the results to known data or expected behaviour. By using a tabulation and plotting tools to determine the cause of discrepancies in properties. If particle property is incorrect, investigate if a model and its mathematical formulation is the cause. In some cases, the parameters is not available in the literature or experimental data, regression, estimation etc. then you have to revaluate the choice of parameters and its nature of interest. There are some certain property parameter is always requiring for the simulation such size of the particle, density, young's modulus. Passion ratio, restitution coefficients. Apart from that, it is based on the need for the simulation. Finally, regression of data is important tool to analyse the proper fit to the contact models and its properties.

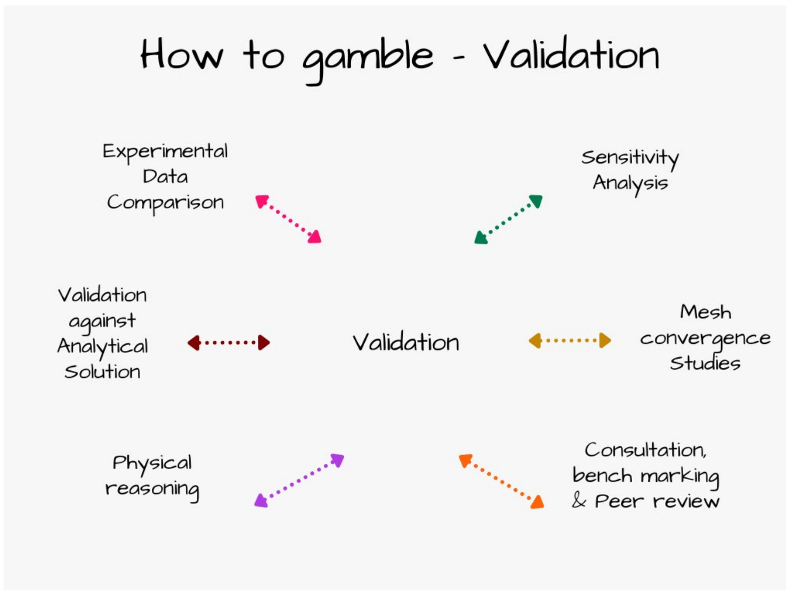

Figure 3: How to Gamble – Validation

Normally property estimation will be done after a data search is performed, to supply missing property parameters. Here we suggest using built in estimation methods to fill the gaps of your property parameter requirements. However, technically this validation can be done with the following ways such as: experimental data comparison, sensitivity analysis, validation against analytical solution, mesh convergence studies, benchmarking, physical reasoning, consultation and peer review.Gambling this validation is crucial for ensuring accurate and reliable simulation. This is the vital step in the any simulation and it can be performed for existing parameters or derived parameters. Compare your simulation results with experimental data. This could include data on material behaviour, such as stress-strain relationships, particle velocities, or any other relevant properties. Quantitatively compare key parameters like bulk density, porosity, flow characteristics, and angle of repose with experimental data. Performing sensitivity analysis on key parameters such as particle size, particle shape, friction coefficients, and particle-particle interaction parameters. Observe how variations in these parameters affect the overall simulation results. This can help in identifying which parameters have significant impacts on the simulation outcomes. For simpler scenarios, there might be analytical solutions (repeatability and reproducibility) available. Validate your simulation results against these analytical solutions to ensure correctness. In case of using a mesh-based approach in your DEM simulation, perform mesh convergence studies. Gradually refine the mesh and observe changes in the simulation results. Ensure that the results converge to a stable solution, as the mesh is refined. Physical reasoning aids in interpreting simulation results in the context of fundamental principles of granular mechanics, enhancing the understanding of material behavior. Additionally, peer review and consultation with experts provide valuable feedback and validation of the simulation approach.

In order to understand in a better way, we came up with one validation example. In this case how physical experiments was calibrated, validated against simulation. For this approach, we use framework of V-model for verification and validation [46, 47]. It is a software development and testing methodology that emphasizes the importance of early testing and verification activities to ensure the quality of a system.

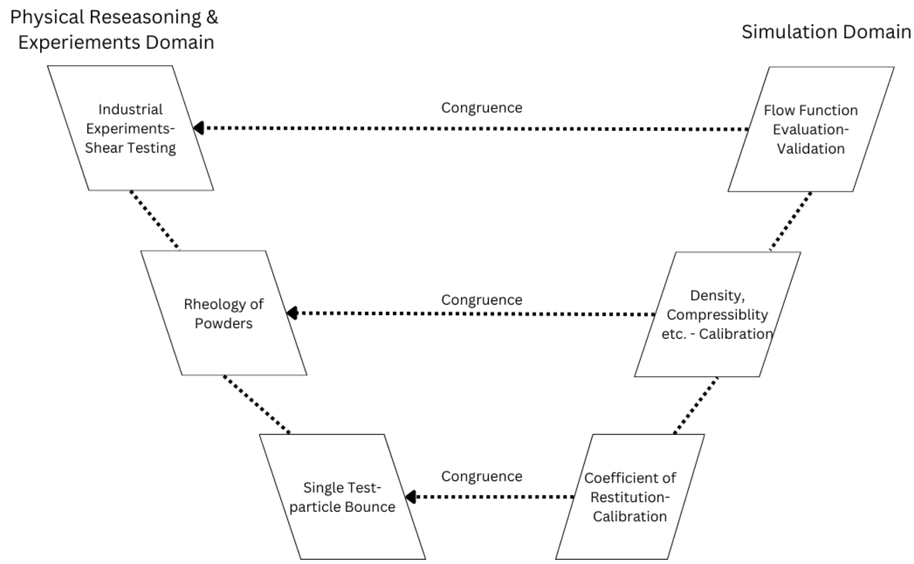

Figure 4: V-Model for Calibration and Validation (For e.g. Powders)

The above *Figure 4* explains the calibration of DEM model parameters by conduction to single test to industrial experiments. On the other hand, validation part explains the overall output that we get it from the simulation domain. Ensuring that individual particle properties are accurately represented through a single particle bounce test alone does not guarantee that the overall behavior of the particle population aligns with real-world material characteristics. Therefore, a secondary calibration process, focusing on the rheology of powders through experiments, becomes necessary. This additional calibration aims to ensure that the collective behaviour resulting from all model parameters corresponds well within a specified range of accuracy. Finally, validation at the highest level is conducted through shear testing applications, where simulation results are compared against real-scale experimental data[48]. This above V model example explains how we can gamble the validation part.By following these steps, you can systematically validate the Particle DEM parameters and ensure that your simulations accurately represent the behaviour of the granular materials being studied.

3. Conclusion

A summary and formulation of the most prominent DEM contact models used for the modeling of cohesive granular materials are presented. The adhesive contact models in DEM, forces causing adhesion, the relationship between adhesion and bulk cohesion, and measurement of cohesion are reviewed. There is a need for a model that can capture the key elements of the contact mechanics and reproduce the stress history of the powder. Many studies have been done on the measurement of contact model parameters using a variety of techniques, but they tend to be on either highly idealized particles or specially manufactured perfect spheres and suffer from enormous scatter and uncertainty concerning the accuracy. On the other hand, it gives the way in order to select the appropriate DEM model and how its parameters are validating, estimating etc. This help to develop a set of results and relationships that can execute complex concepts gently. The validation of DEM parameters is a comprehensive gambling process involving multiple steps and considerations. By following these steps diligently, researchers can ensure that their simulations accurately represent the behavior of granular materials or particulate systems, enabling informed decision-making and advancing understanding in various fields. Using a consistent notation, this paper should help future users and researchers to easily compare the different models and to select the most appropriate model for a specific application.

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References

1. Cundall, P. A., & Strack, O. D. (1979). A discrete numerical model for granular assemblies. *geotechnique, 29*(1), 47-65.
2. Farmani, Z., & Dijksman, J. A. (2024). Rate dependence in adhesive particle–particle contacts affect ceramic suspension bulk flow behavior. *Powder Technology, 434,* 119353.
3. Maw, N., Barber, J. R., & Fawcett, J. N. (1976). The oblique impact of elastic spheres. *Wear, 38*(1), 101-114.
4. Mindlin, R. D. (1949). Compliance of elastic bodies in contact.
5. Hertz, H. R. (1882). Über die Berührung fester elastischer Körper und über die Härte. *Verhandlungen des Vereins zur Beförderung des Gewerbfleißes, Berlin: Verein zur Beförderung des Gewerbefleisses, 1882,* 449-463.
6. Brilliantov, N. V., Spahn, F., Hertzsch, J. M., & Pöschel, T. (1996). Model for collisions in granular gases. *Physical review E, 53*(5), 5382.
7. Bommireddy, Y., Agarwal, A., Yettella, V., Tomar, V., & Gonzalez, M. (2019). Loading-unloading contact

law for micro-crystalline cellulose particles under large deformations. *Mechanics Research Communications, 99,* 22-31.
8. A. D. Johnson, K.L., Kendall, K., Roberts, "Surface energy and the contact of elastic solids," *R. Soc. London,* vol. 324, no. 1558, 1971.
9. Thornton, C., & Ning, Z. (1998). A theoretical model for the stick/bounce behaviour of adhesive, elastic-plastic spheres. *Powder technology, 99*(2), 154-162.
10. S. Luding, "Anisotropy in cohesive, frictional granular media," *J. Phys. Condens. Matter*, vol. 17, no. 24, 2005,
11. Luding, S. (2008). Cohesive, frictional powders: contact models for tension. *Granular matter, 10*(4), 235-246.
12. Luding, S. (2004). Micro–macro transition for anisotropic, frictional granular packings. *International Journal of Solids and Structures, 41*(21), 5821-5836.
13. Pasha, M., Dogbe, S., Hare, C., Hassanpour, A., & Ghadiri, M. (2014). A linear model of elasto-plastic and adhesive contact deformation. *Granular Matter, 16,* 151-162.
14. Kuwabara, G., & Kono, K. (1987). Restitution coefficient in a collision between two spheres. *Japanese journal of applied physics, 26*(8R), 1230.
15. Tsuji, Y., Tanaka, T., & Ishida, T. (1992). Lagrangian numerical simulation of plug flow of cohesionless particles in a horizontal pipe. *Powder technology, 71*(3), 239-250.
16. Kruggel-Emden, H., Simsek, E., Rickelt, S., Wirtz, S., & Scherer, V. (2007). Review and extension of normal force models for the discrete element method. *Powder Technology, 171*(3), 157-173.
17. Vu-Quoc, L., & Zhang, X. (1999). An elastoplastic contact force–displacement model in the normal direction: displacement–driven version. *Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences, 455*(1991), 4013-4044.
18. Thornton, C., & Ning, Z. (1998). A theoretical model for the stick/bounce behaviour of adhesive, elastic-plastic spheres. *Powder technology, 99*(2), 154-162.
19. Tomas, J. (2007). Adhesion of ultrafine particles—a micromechanical approach. *Chemical Engineering Science, 62*(7), 1997-2010.
20. Tomas, J. (2003). Mechanics of nanoparticle adhesion–a continuum approach. *Particles on surfaces, 8*, 183-229.
21. Mindlin, R. D., & Deresiewicz, H. E. R. B. E. R. T. (1953). Elastic spheres in contact under varying oblique forces.
22. Ai, J., Chen, J. F., Rotter, J. M., & Ooi, J. Y. (2011). Assessment of rolling resistance models in discrete element simulations. *Powder Technology, 206*(3), 269-282.
23. P. J. Morrissey, J. Ooi, and J.-F. Chen, "Discrete Element Modelling of Iron Ore Pellets to Include the Effects of Moisture and Fines," University of Edinburgh, Edinburgh, 2013.
24. Thakur, S. C., Morrissey, J. P., Sun, J., Chen, J. F., & Ooi, J. Y. (2014). Micromechanical analysis of cohesive granular materials using the discrete element method with an adhesive elasto-plastic contact model. *Granular Matter, 16,* 383-400.
25. Chen, F., Xia, Y., Klinger, J. L., & Chen, Q. (2022). A set of hysteretic nonlinear contact models for DEM: Theory, formulation, and application for lignocellulosic biomass. *Powder Technology, 399*, 117100.
26. Brown, N. J., Chen, J. F., & Ooi, J. Y. (2014). A bond model for DEM simulation of cementitious materials and deformable structures. *Granular Matter, 16*, 299-311.
27. Estrada, N., & Taboada, A. (2013). Yield surfaces and plastic potentials of cemented granular materials from discrete element simulations. *Computers and Geotechnics, 49,* 62-69.
28. Jiang, M., Zhang, F., & Sun, Y. (2014). An evaluation on the degradation evolutions in three constitutive models for bonded geomaterials by DEM analyses. *Computers and Geotechnics, 57*, 1-16.
29. Utili, S., & Nova, R. O. B. E. R. T. O. (2008). DEM analysis of bonded granular geomaterials. *International Journal for Numerical and Analytical Methods in Geomechanics, 32*(17), 1997-2031.
30. Guo, Y., Chen, Q., Xia, Y., Klinger, J., & Thompson, V. (2021). A nonlinear elasto-plastic bond model for the discrete element modeling of woody biomass particles. *Powder Technology, 385*, 557-571.
31. M. Mascara, A. Mayrhofer, S. Radl, and C. Kloss, "A Viscoelastic Bonded Particle Model to Predict the Rheology of Hydrogels," *Granul. Matter* 26, no. February, 2023,
32. Johnson, K. L., Kendall, K., & Roberts, A. A. D. (1971). Surface energy and the contact of elastic solids. *Proceedings of the royal society of London. A. mathematical and physical sciences, 324*(1558), 301-313.
33. Derjaguin, B. V., Muller, V. M., & Toporov, Y. P. (1975). Effect of contact deformations on the adhesion of particles. *Journal of Colloid and interface science, 53*(2), 314-326.
34. Molerus, O. (1975). Theory of yield of cohesive powders. *Powder Technology, 12*(3), 259-275.
35. Schubert, H. (1984). Capillary forces-modeling and application in particulate technology. *Powder Technology, 37*(1), 105-116.
36. Maugis, D. (1992). Adhesion of spheres: the JKR-DMT transition using a Dugdale model. *Journal of colloid and interface science, 150*(1), 243-269.
37. Matuttis, H. G., & Schinner, A. (2001). Particle simulation of cohesive granular materials. *International Journal of Modern Physics C, 12*(07), 1011-1021.
38. Tomas, J. (2001). Assessment of mechanical properties of cohesive particulate solids. Part 1: Particle contact constitutive model. *Particulate science and technology, 19*(2), 95-110..
39. Luding, S., Tykhoniuk, R., & Tomas, J. (2003). Anisotropic Material Behavior in Dense, Cohesive-Frictional Powders. *Chemical Engineering & Technology: Industrial Chemistry-Plant Equipment-Process Engineering-Biotechnology, 26*(12), 1229-1232.
40. Gilabert, F. A., Roux, J. N., & Castellanos, A. (2007). Computer simulation of model cohesive powders: Influence of assembling procedure and contact laws on low consolidation states. *Physical review E, 75*(1), 011303.
41. Walton, O. R., & Johnson, S. M. (2009, June). Simulating the effects of interparticle cohesion in micron-scale powders. In *AIP conference proceedings* (Vol. 1145, No. 1, pp. 897-

900). American Institute of Physics.

42. Thakur, S. C., Ahmadian, H., Sun, J., & Ooi, J. Y. (2014). An experimental and numerical study of packing, compression, and caking behaviour of detergent powders. *Particuology, 12*, 2-12.
43. Pasha, M., Dogbe, S., Hare, C., Hassanpour, A., & Ghadiri, M. (2013, June). A new contact model for modelling of elastic-plastic-adhesive spheres in distinct element method. In *AIP Conference Proceedings* (Vol. 1542, No. 1, pp. 831-834). American Institute of Physics.
44. Ledvinkova, B., & Kosek, J. (2013). The effects of adhesive forces on the collision behavior of polyolefin particles. *Powder technology, 243,* 27-39.
45. I. Carlson, Eric C. (Aspen Technology, "Don't gamble with physical properties for simulations," *Chem. Eng. Prog*., pp. 35–46, 1996.
46. Hofmann, M. (2005). On the complexity of parameter calibration in simulation models. *The Journal of Defense Modeling and Simulation, 2*(4), 217-226.
47. Zeng, H., Xu, W., Zang, M., Yang, P., & Guo, X. (2020). Calibration and validation of DEM-FEM model parameters using upscaled particles based on physical experiments and simulations. *Advanced Powder Technology, 31*(9), 3947-3959.
48. J. Quist and M. Evertsson, "Framework for DEM Model Calibration and Validation," *Proc. 14th Eur. Symp. Comminution Classif*., no. September, pp. 103–108, 2015.