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Harald Kruggel-Emden

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Telefon: 02407 / 95 96 - 0 • Telefax: 02407 / 95 96 - 9
Internet: www.shaker.de • E-Mail: info@shaker.de

Abstract of the Dissertation

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Several processes in nature as well as many industrial applications involve static or dynamic granular materials. Granulates can adopt solid, liquid or gas like states and thereby reveal intriguing physical phenomena not observable in its versatility for any other form of matter. The frequent occurrence of phase transitions and the related characteristics thereby strongly affect their processing quality and economics. This situation demands for prediction methods for the behavior of granulates. In this context simulations provide a feasible alternative to experimental investigations. Advantageous are their better reproducibility, their less expenditure of time and their lower costs. Several different simulation approaches are applicable to granular materials. The time-driven Discrete Element Method turns out to be the most complex but also as the most general method. It is based on tracking each particle's movement and its interactions with the surrounding over time. The method provides detailed information on particle positions, orientations and translational and angular velocities. These properties are obtained by integrating numerically a set of fully deterministic differential equations which are explicitly depending on the contact forces.

The time-driven Discrete Element Method is a simulation approach which has been used in a wide variety of scientific fields for more than thirty years. With the tremendous increase in available computer power, especially in the last years, the method is more and more developing to the state of the art simulation technique for granular materials. Despite of the long time of usage, model advances and theoretical and experimental studies are not harmonized in the different branches of application, providing a large potential for improvements.

Therefore, the scope of this work is a review of methods and models based on theoretical considerations and experimental data from literature. Through model advances it is intended to contribute to a general enhancement of techniques, which are then directly available for simulations.

In detail, force displacement models which are usually separated in normal and tangential direction are reviewed for a broad range of experimental data. Model improvements and new methods for the derivation of simulation parameters are proposed. For a special combination of force models an analytical solution is derived, which is later used as a benchmark case for the evaluation of different integration schemes. With the Discrete Element Method even today being mostly limited to simple spherical bodies a method for the implementation of complex shapes based on multi-sphere particles is reviewed. The applicability of this approach is verified based on a study on collision properties under different impact situations. As a final application outlining the advantages of particle orientated modeling the Discrete Element Method incorporating the derived improvements is used for a comparative study of mixing on grates.