6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11-15 June 2018, Glasgow, UK

DISCRETE ELEMENT METHOD FOR THE MODELING OF LITHIUM ION BATTERY CATHODES AND AN APPROACH FOR MORE GENERAL PARTICLE SHAPES

Verena Becker[1], Oleg Birkholz[1], Yixiang Gan[2] and Marc Kamlah[1]

[1] KIT (IAM-WBM), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, verena.becker@kit.edu, oleg.birkholz@kit.edu, marc.kamlah@kit.edu and *https://www.iam.kit.edu/wbm/*

[2] The University of Sydney, Darlington NSW 2006, yixiang.gan@sydney.edu.au and *https://sydney.edu.au/engineering/people/yixiang.gan.php*

Keywords: *Lithium Ion Batteries, Random Close Packing, Discrete Element Method, Superquadric, Non-spherical particles*

In a multitude of engineering processes particles and their movements play a significant role. Lithium Ion Batteries (LIB) are composed of two electrodes consisting mainly of granular material. The static and dynamic behavior of such particulate structures is still not completely understood. However, for suitable designs, e.g. cathodes with determined mechanical or electrical properties, the knowledge of this behavior is of major importance.

For Discrete Element simulations (DEM) [1] randomly distributed and overlap-free particle assemblies are generated with the so-called Random Close Packing (RCP) [2] algorithm. Further, these inital structures are densified and arising percolated pathways are identified. Thus the electrical resistance of the cathode can be calculated with the Resistor Network (RN) [3] approach.

Spherical particles are preferably utilized in simulations due to the well known contact force models and simple implementation. Though in reality particles mostly show non-spherical shapes. An approach for more common particle forms [4] is finally presented.

REFERENCES

[1] P. Cundall and O. Strack, A discrete numerical model for granular assemblies. *Geotechnique*, Vol. **29**, pp. 47–65, 1979.

[2] W. Jodrey, E. Tory, Computer simulation of close random packing of equal spheres. *Physical Review A*, Vol. **34**, pp. 2347–2351, 1986. *Journal of Power Sources*, Vol. **301**, pp. 151–159, 2016.

[3] J. Ott, et al., A micromechanical model for effective conductivity in granular electrode structures. *Acta Mechanica Sinica*, Vol. **29**, pp. 682–698, 2013.

[4] A. Podlozhnyuk, et al., Efficient implementation of superquadric particles in Discrete Element Method within an open-source framework. *Computational Particle Mechanics*, Vol. **4**, pp. 101–118, 2017.