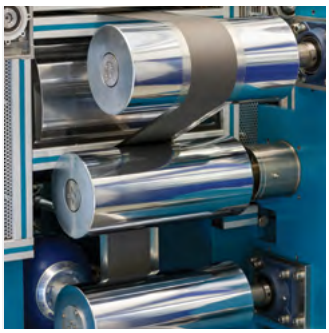
TECHNICAL UNIVERSITY OF MUNICH OPTIMIZES BATTERY PRODUCTION

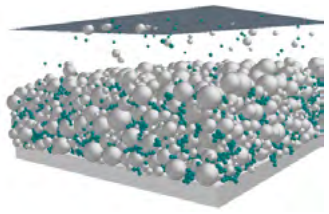
The Battery Production Group at the Institute for Machine Tools and Industrial Management at the Technical University of Munich (TUM) researches the production of innovative battery cells. The core of the work is process development and the optimization of processes within battery production — from mixing, coating, and calendering of the electrode materials to the formation of the final battery cells. All battery production steps are carried out in-house using the TUM's electrode and battery production line.

Challenge

The performance of battery cells depends not only on the materials used, but also on the composition and the microstructure of the electrodes. Each electrode material requires a new design of the manufacturing processes, which is why a deeper understanding of these processes is necessary. The TUM research group considers all aspects of electrode production from the handling of powdered active material to the finishing of electrodes, and includes research into processes such as mixing and dispersing, coating and drying, and calendering of the electrodes.

Calendering, as the final step in electrode production, is a critical process that significantly influences the mechanical and electrochemical properties of the electrode. To date, knowledge of the calendering process has been gathered at TUM through experiments. However, since the parameters of the calendering process have a significant influence on it, a profound understanding of the calendering process and its effects on the electrode is necessary. This includes process parameters such as roll temperature and speed, structural parameters (e.g., layer thickness and adhesive strength), and material and composition, as well as parameters of machine behavior (displacement and bending line).





The Technical University of Munich uses Altair EDEM to simulate the calendering process for lithium-ion batteries

Solution

With Altair EDEM™ simulation, an enhancement of the process design for calendering can be established where potential calendering parameters can be identified and assessed through simulation. The concept for calendering process design encompasses three main modules: modeling of the electrode, parametrization of the electrode, and identification of potential process parameters.

First, the input and output product of the calendering process, the electrode, is defined and then modeled. Therefore, based on the particle size distribution, density, and thickness of the electrode, the control volume is defined and filled with particles. This is done by a combination of two contact models, EEPA and Bonding. A verification of the electrode density and the particle distribution within the electrode concludes the model of the electrode. Since the composition of the electrode is variable, the sensitive simulation parameters of the modeled electrode are parameterized. In order to reduce the time and effort required for calendering settings, a tool for determining the calendering parameters is developed.

Results

Comparing scanning electron microscope (SEM) images with EDEM simulation images show very good agreement with the EDEM-modeled electrodes. In addition, SEM close-up images of NMC particles show that the NMC is embedded in the binder and carbon black matrix, confirming that the assumption of spherical particles is qualitatively verified.

The electrode to be simulated is composed of NMC622 active materials, conductive carbon black and binder. For this purpose, a constant particle size was assumed for the binder and the conductive carbon black, whereas for NMC a logarithmic normal distribution of the particle size was selected based on experimental measurements. In the simulation the electrode was generated by a dynamic

factor into a representative control volume. The parameterization of the model is performed by pressure-displacement curves resulting from nanoindentation experiments.

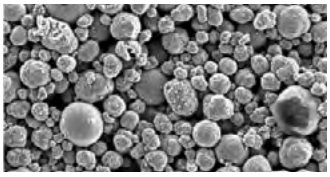
The method was tested and verified against experiments that compared pressure-displacement response. Furthermore, sensitivity analyses of different parameters of the selected contact models — Edinburgh Elasto-Plastic Adhesion Model (EEPA) and Bonded Particle Model — were performed.

In summary, the combination of EEPA and Bonded Particle Model enables a good description of the behavior of the electrode microstructure during calendering. Finally, the modeled and parameterized electrode is used to determine suitable calendering parameters and to predict the effects of individual parameters.

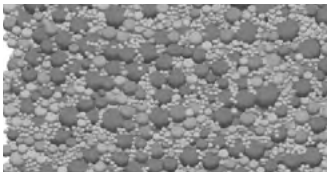
Testimonial

"TU Munich has extensive expertise in calendering and the effects on lithium-ion-battery electrodes," says David Schreiner, research associate at TUM. "So far, however, for each new material system a large number of experiments are necessary to determine suitable process parameters. Even with the same material system but changed thickness and density, the identification of suitable process parameters results in high experimental effort and therefore high expense."

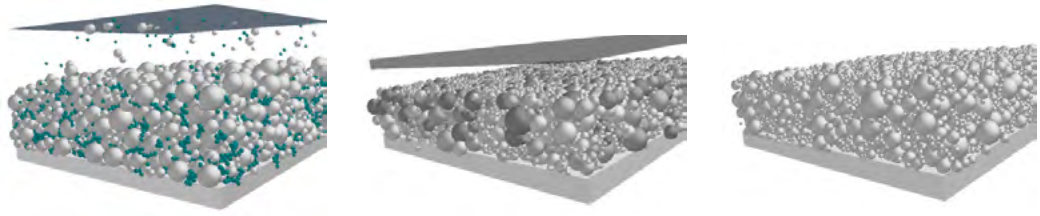
"By coupling the EDEM contact models, EEPA and Bonded Particle Model, as well as their calibration on battery electrode materials," says Schreiner, "we are able to identify possible process parameters during calendering. This provides additional value in the determination of parameters and helps us to gain an even better understanding of the calendering process, especially the possibility to track individual areas and particles during the compaction process."



Scanning electron microscope (SEM) image: NMC cathode from TU Munich, iwb, David Schreiner



Modeled particle bed: an EDEM-modeled NMC electrode from TU Munich, iwb, David Schreiner



LEFT TO RIGHT: Generation of NMC-particles and binder-conductive-matrix; electrode section before compaction; electrode section after compaction