Contribution ID: **398** Type: **Oral Presentation**

Lattice Boltzmann simulation in the context of battery systems

Tuesday, 1 June 2021 11:45 (15 minutes)

Simulations based on the Lattice Boltzmann method are a powerful and efficient tool for the investigation of mesoscopic processes that are hard to study experimentally. Such simulations have been used successfully to study redox flow batteries [1]. But they have rarely been used to study transport mechanisms in other battery systems [2,3]. In the present work, the wetting process during the electrolyte filling in the battery production is investigated by means of the flow of electrolyte through realistic three-dimensional porous battery electrodes. The electrode microstructures are generated using a sophisticated stochastic model [4] for the active material which is complemented by an additional binder phase. The focus of the study is on determining the capillary pressure-saturation relation during electrolyte intrusion and drainage. The main influencing factors investigated in the present work, are the porosity of the electrodes, the proportion of the binder phase as well as the wetting behavior of both the active material and the binder. Besides, also the effect of spatially non-resolved nanopores in the binder is studied using a homogenization approach. Lattice Boltzmann simulations with different multiphase flow methods, i.e. the Shan-Chen pseudopotential method [5] and the color gradient method [6], are conducted. Results from both methods are compared with each other. For validation purposes, they are also compared against results determined using the pore morphology method. The results from the present study are shown to agree well with results from the literature. They are especially useful for optimizing the electrolyte filling process which is a time-determining step in the battery production.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

[1] D. Zhang et al.; J. Power Sources, 447 (2020), pp. 227249
[2] T. Danner et al.; J. Power Sources, 324 (2016), pp. 646–656
[3] Z. Jiang et al.; J. Power Sources, 324 (2018), pp. 500–513
[4] J. Feinauer et al.; Comput. Mater. Sci., 109 (2015), pp. 137–146
[5] X. Shan et H. Chen; Phys. Rev. E, 47 (3) (1993), pp. 1815–1819
[6] J. Leclaire et al.; Phys. Rev. E, 95 (3) (2017), pp. 033306

Acceptance of Terms and Conditions

Click here to agree

Newsletter

Student Poster Award

Primary author: Dr LAUTENSCHLÄGER, Martin (Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU), Ulm, Germany; German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Stuttgart, Germany)

Co-authors: Mr WEINMILLER, Julius (Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU), Ulm, Germany; German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Stuttgart, Germany); DANNER, Timo (German Aerospace Center (DLR)); Prof. LATZ, Arnulf (Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU), Ulm, Germany; German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Stuttgart, Germany; Ulm University, Institute of Electrochemistry, Ulm, Germany)

Presenter: Dr LAUTENSCHLÄGER, Martin (Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU), Ulm, Germany; German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Stuttgart, Germany)

Session Classification: MS19

Track Classification: (MS19) Electrochemical processes in porous media