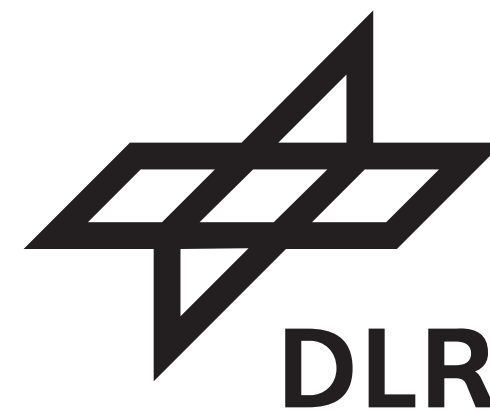


Benjamin Kellers, Martin P. Lautenschläger, Julius Weinmiller, Timo Danner

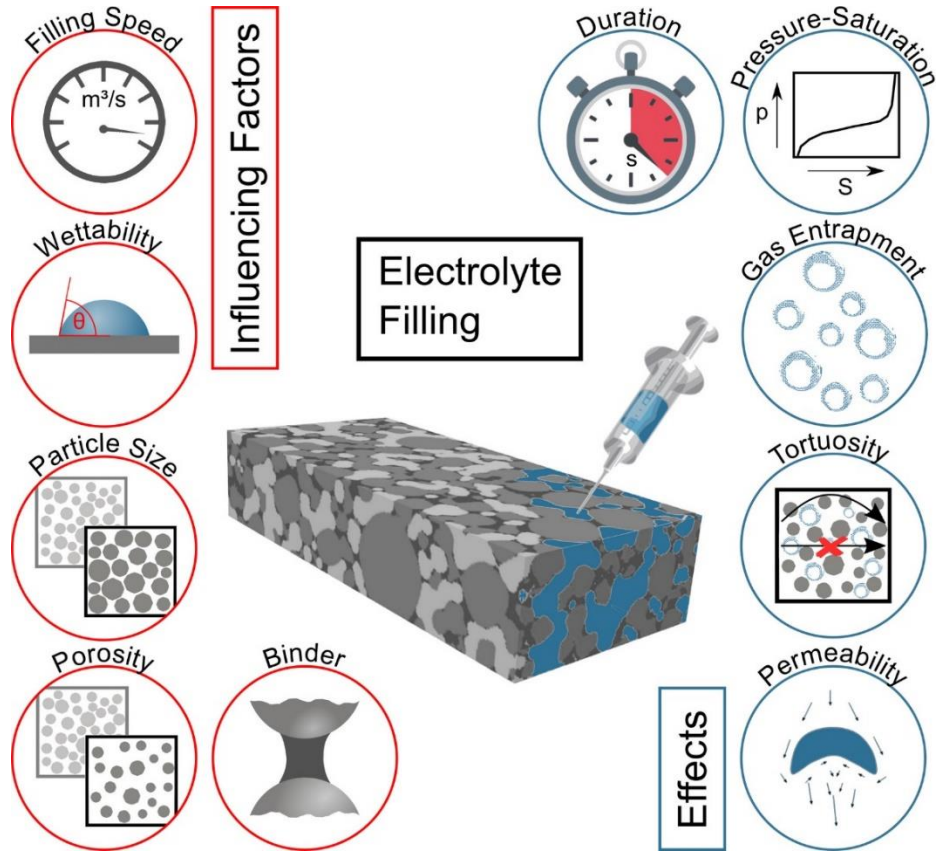
# A Geometry-based Throat Shape Correction of Pore Network Models



# AGENDA

- Motivation
- Goals
- Model development & results
- Summary & outlook

# THE FILLING PROCESS OF A LI-ION BATTERY



doi:10.1002/batt.202200090



## DEFACTO

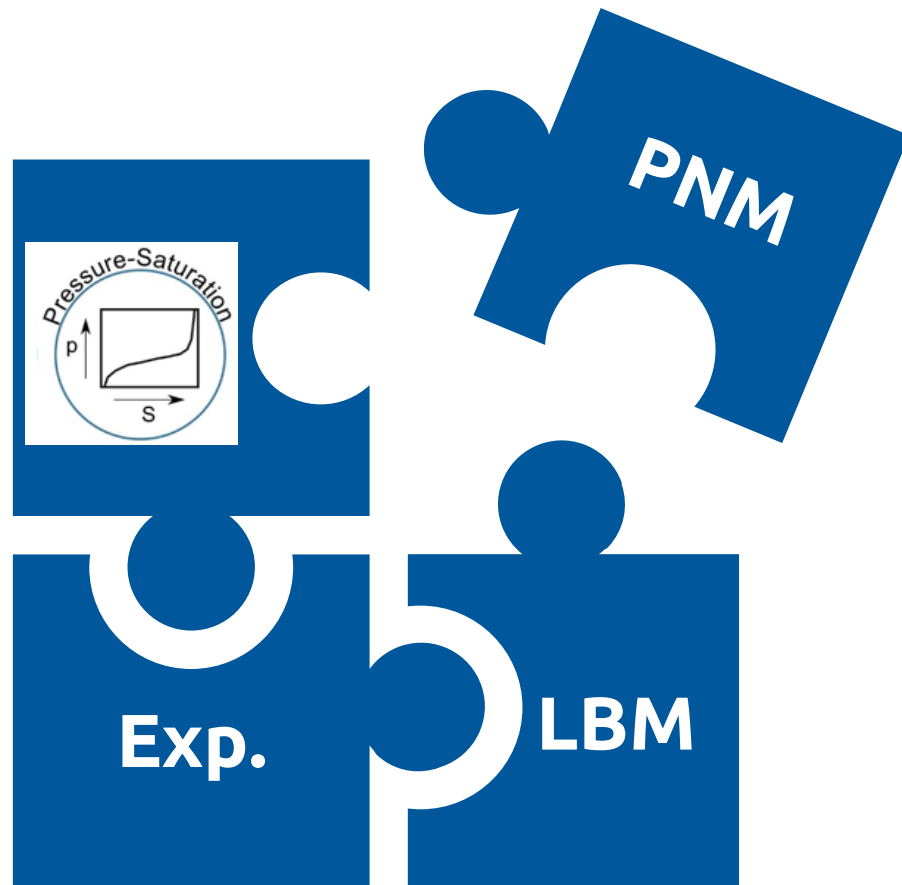
### Software Tool

for the modelling of the  
filling process

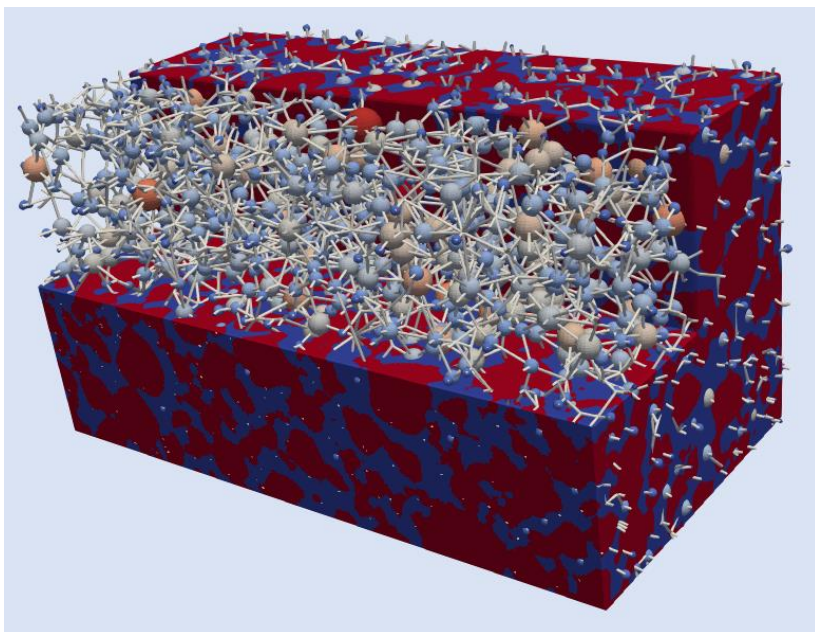
Goals:

1. reduction of computational resources needed
2. reduction of the filling time in the manufacturing

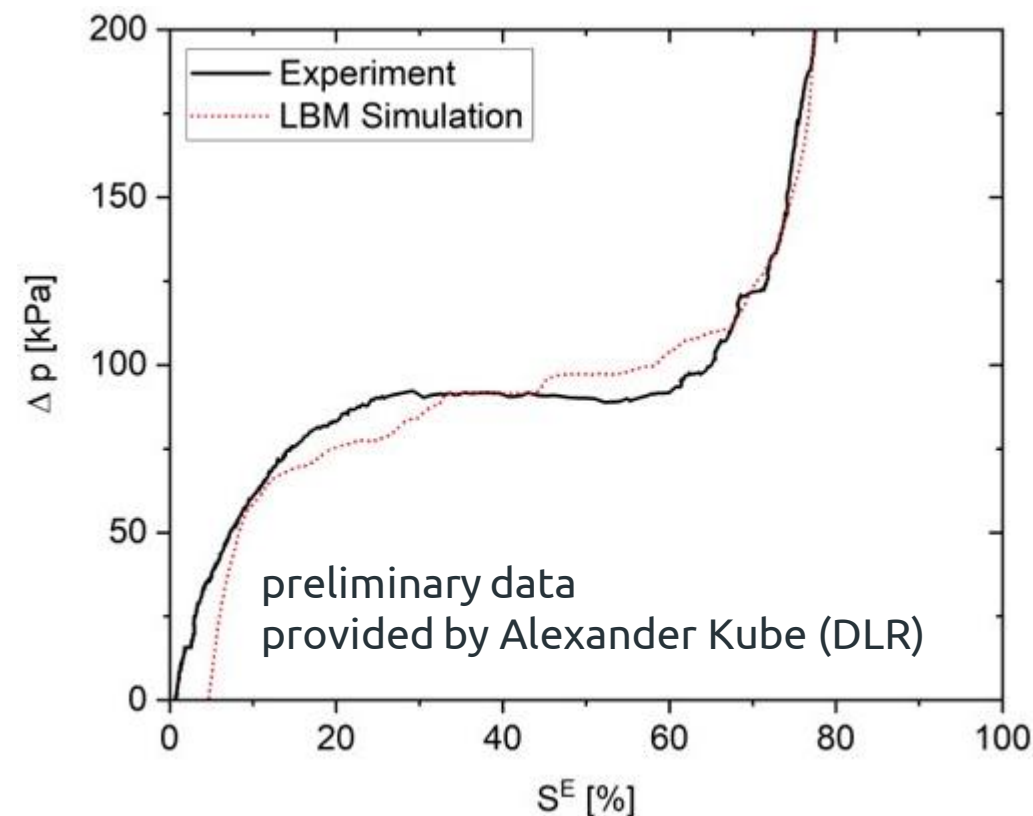
# AGREEMENT OF PNM AND LBM WITH EXPERIMENTAL RESULTS



# CATHODES, EXTRACTED NETWORKS & LBM VALIDATION



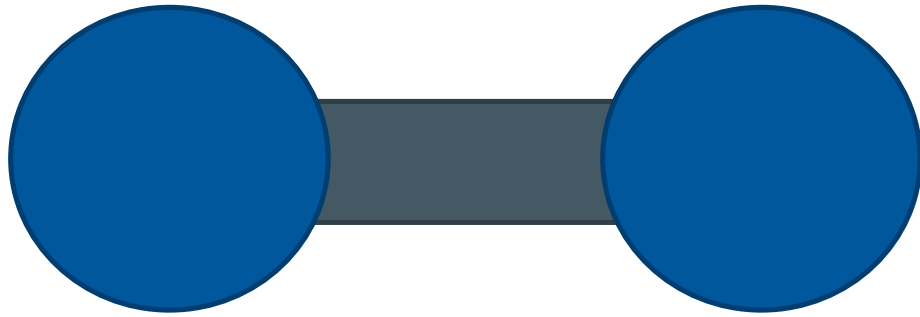
- stochastically generated cathode material
- porosity 40% (also 50% and 30%)
- medium particle size (relative to other cathodes)
- the number of pores and throats in the extracted network range from the order of  $10^4$  to  $10^5$ , otherwise the structures will be too large for LBM simulations



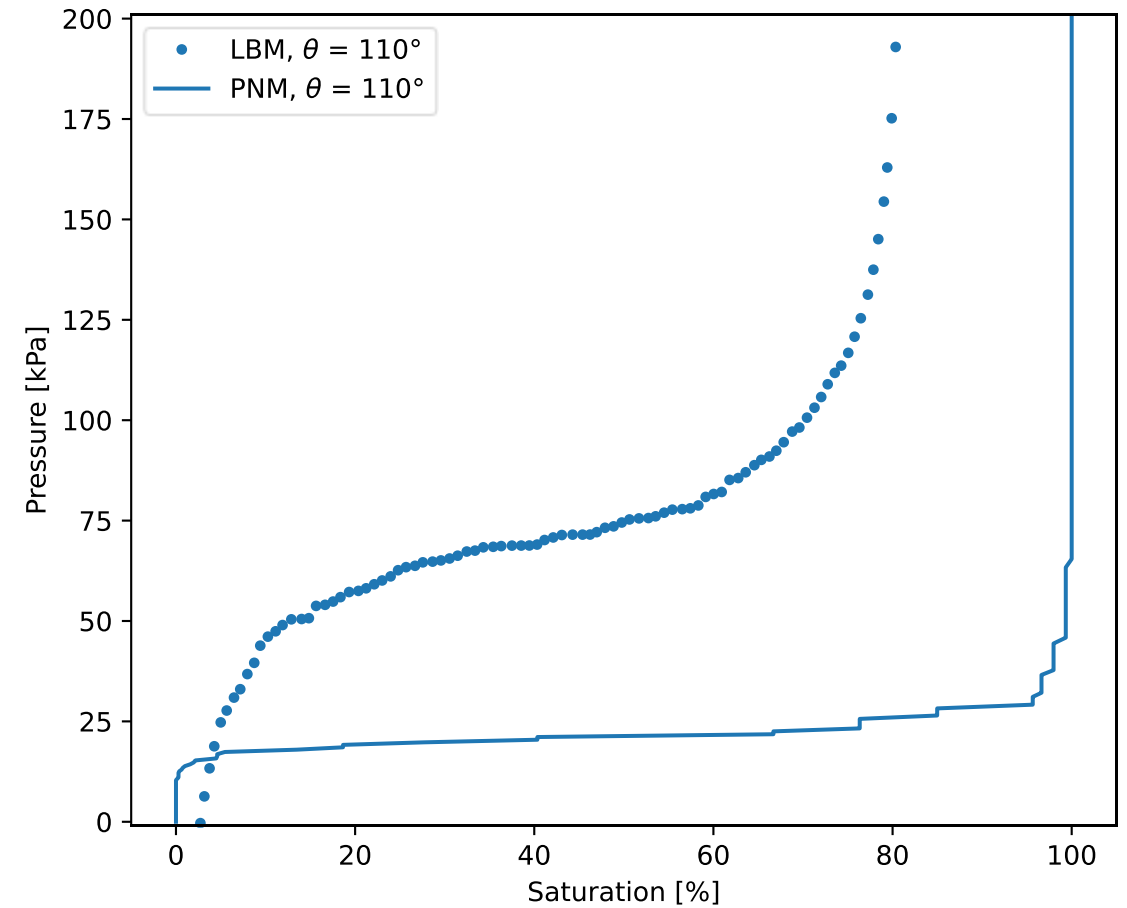
setup analogous to  
<https://doi.org/10.1016/j.jpowsour.2022.231381>



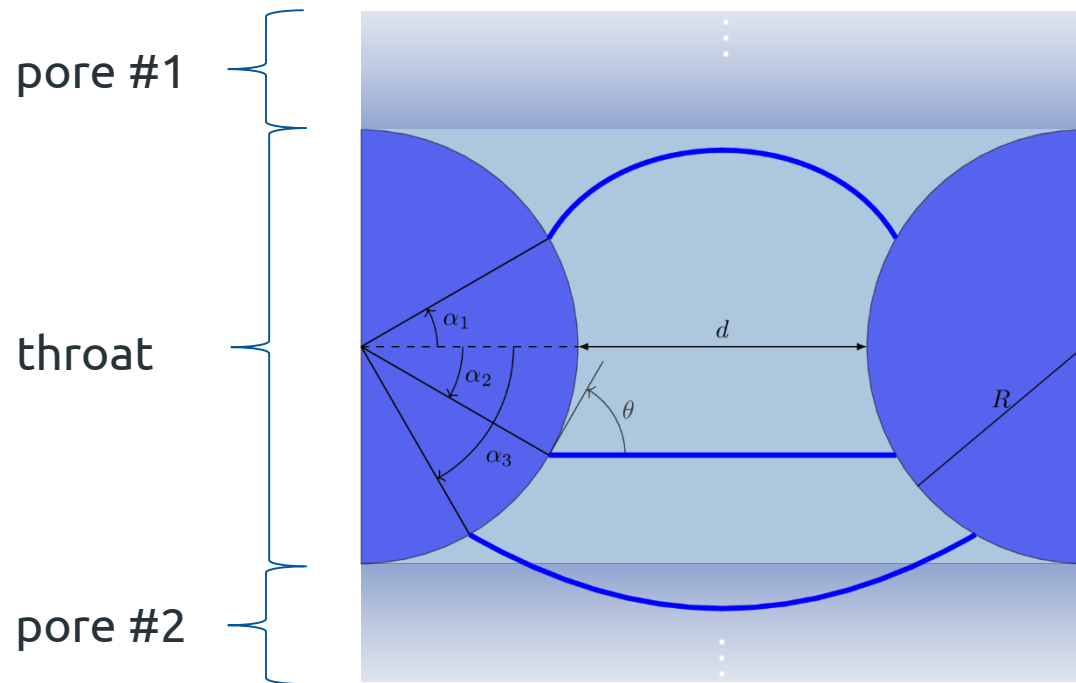
# WASHBURN PHYSICS



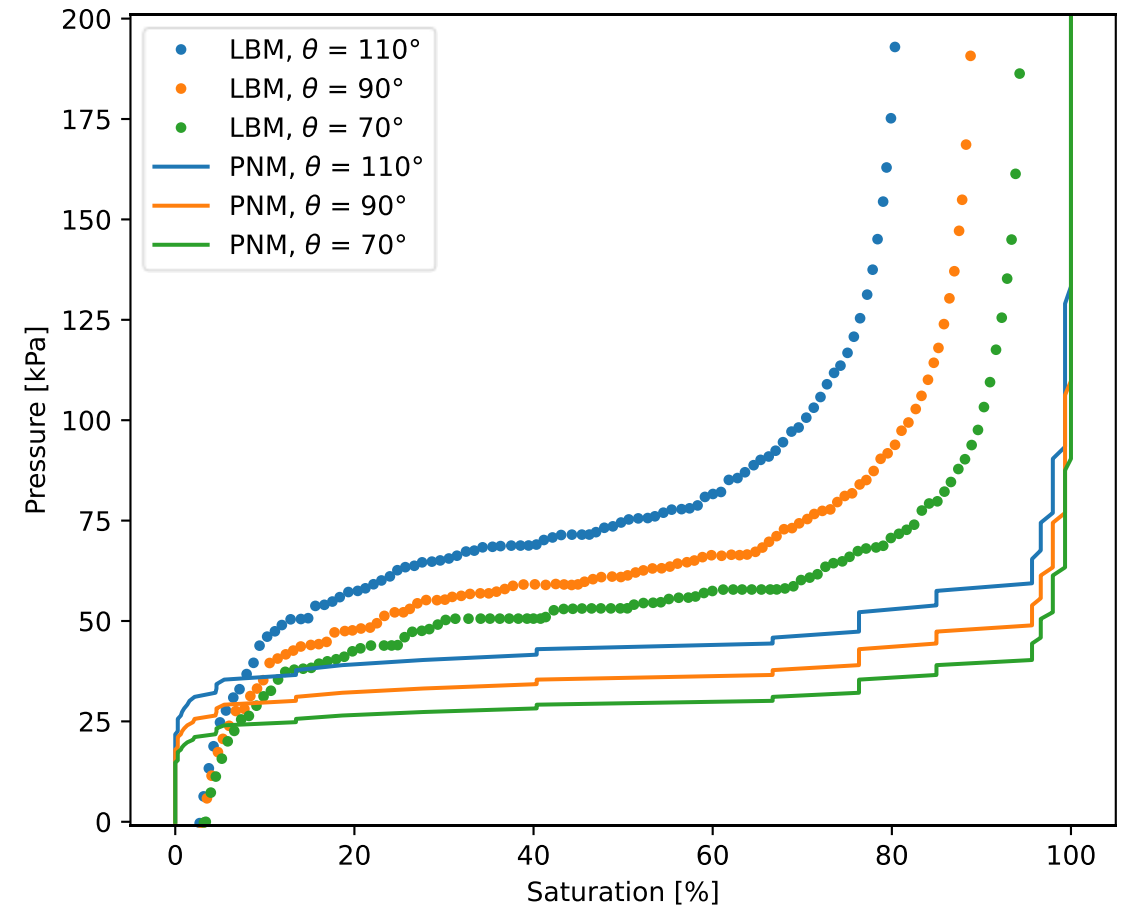
$$|p_c| = \frac{2\sigma \cos(\theta)}{r}$$



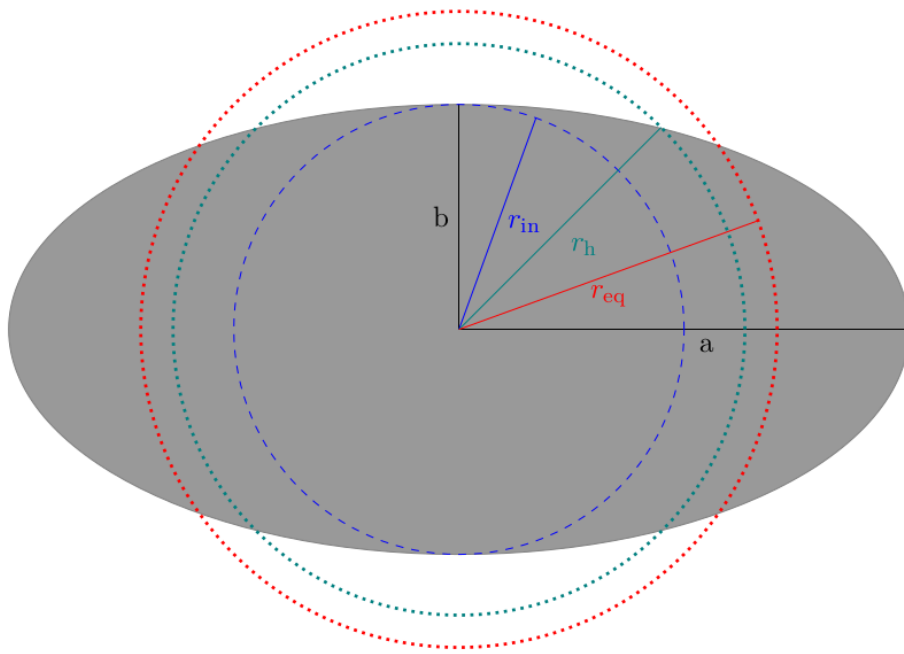
# PURCELL PHYSICS



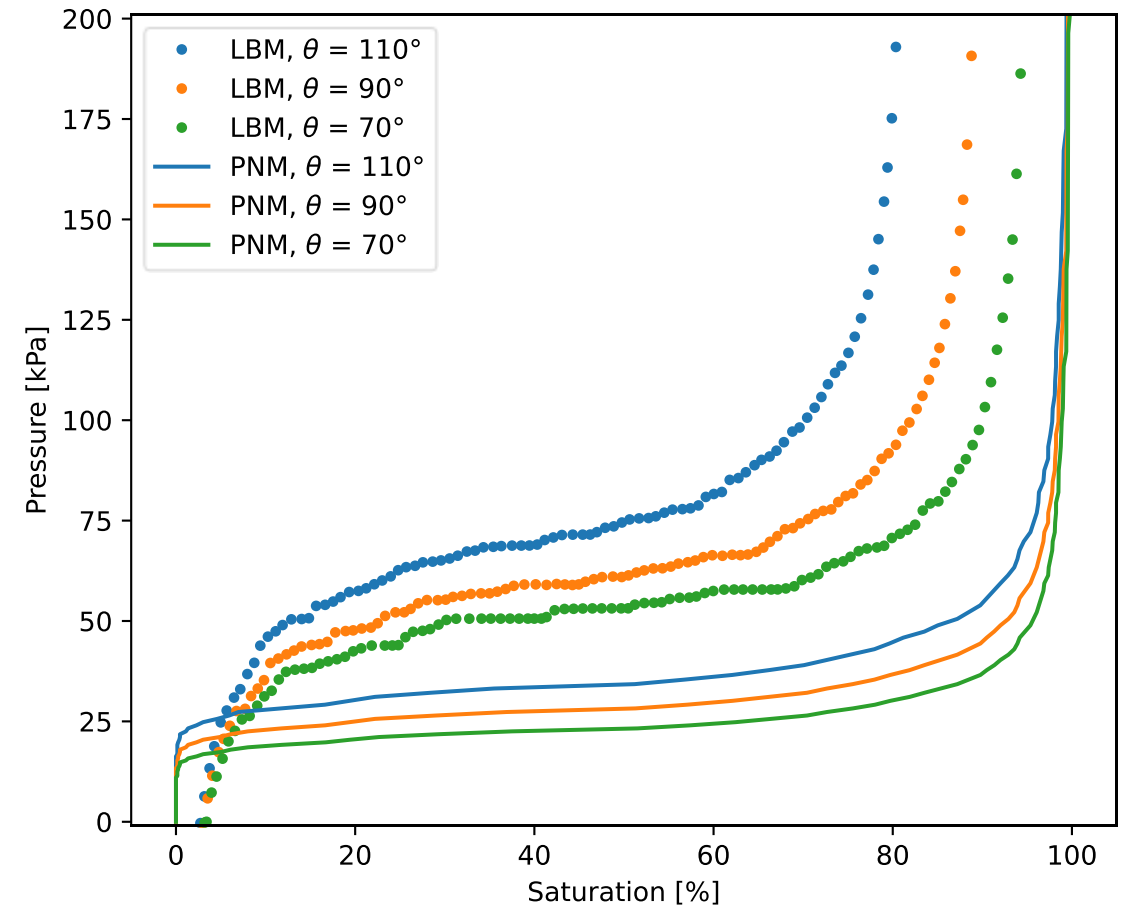
$$|p_c| = \frac{2\sigma}{r} \frac{\cos(\theta - \alpha)}{1 + \frac{R}{r}(1 - \cos \alpha)}$$



# THROAT SHAPE CORRECTION

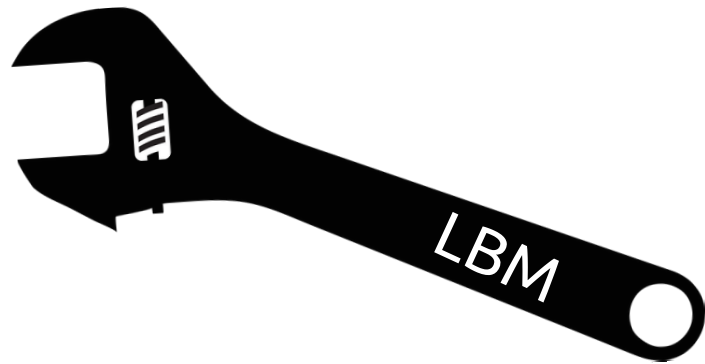


$$|p_c| = \frac{2\sigma \cos(\theta - \alpha)}{r_h + R(1 - \cos \alpha)}$$

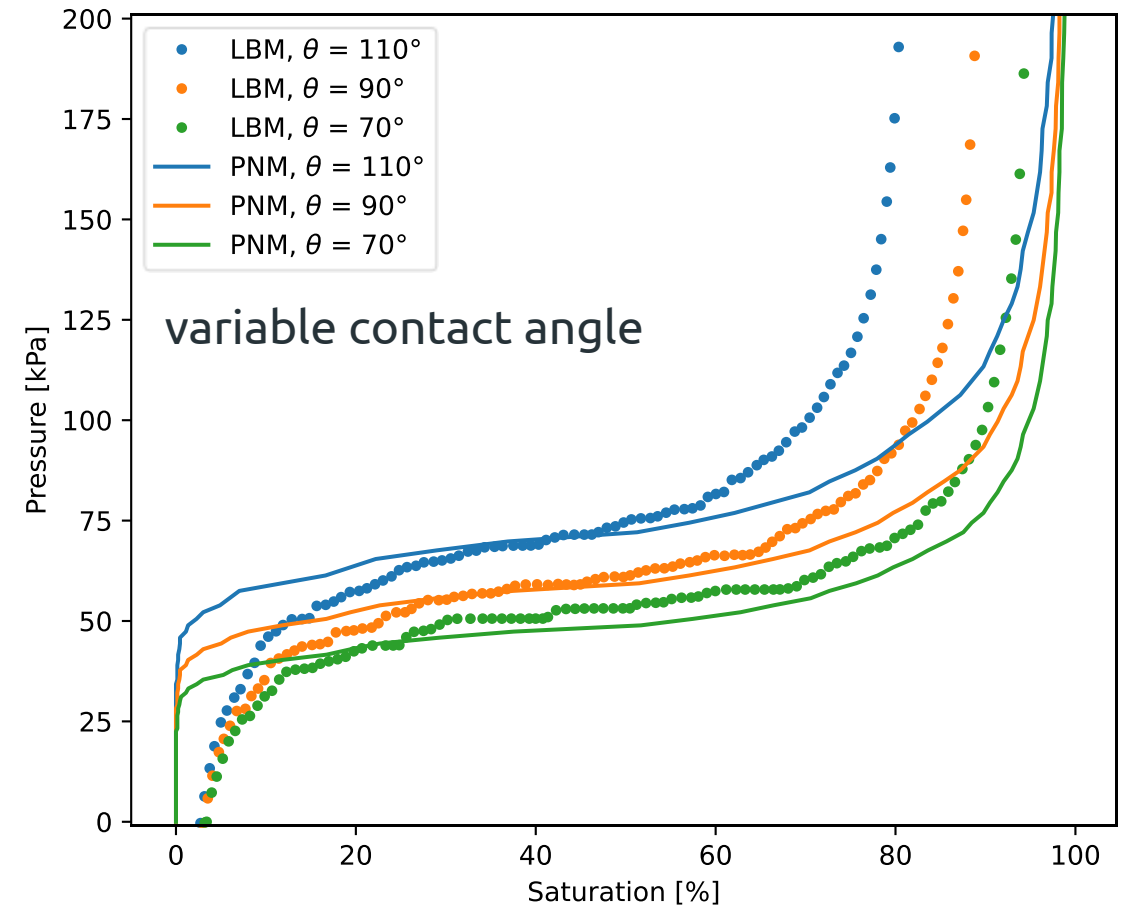




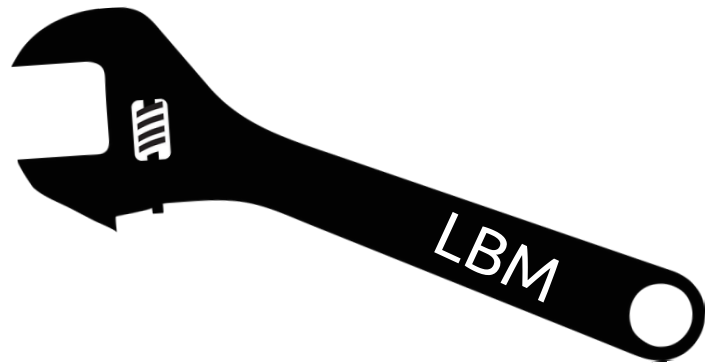
# LBM-CALIBRATION



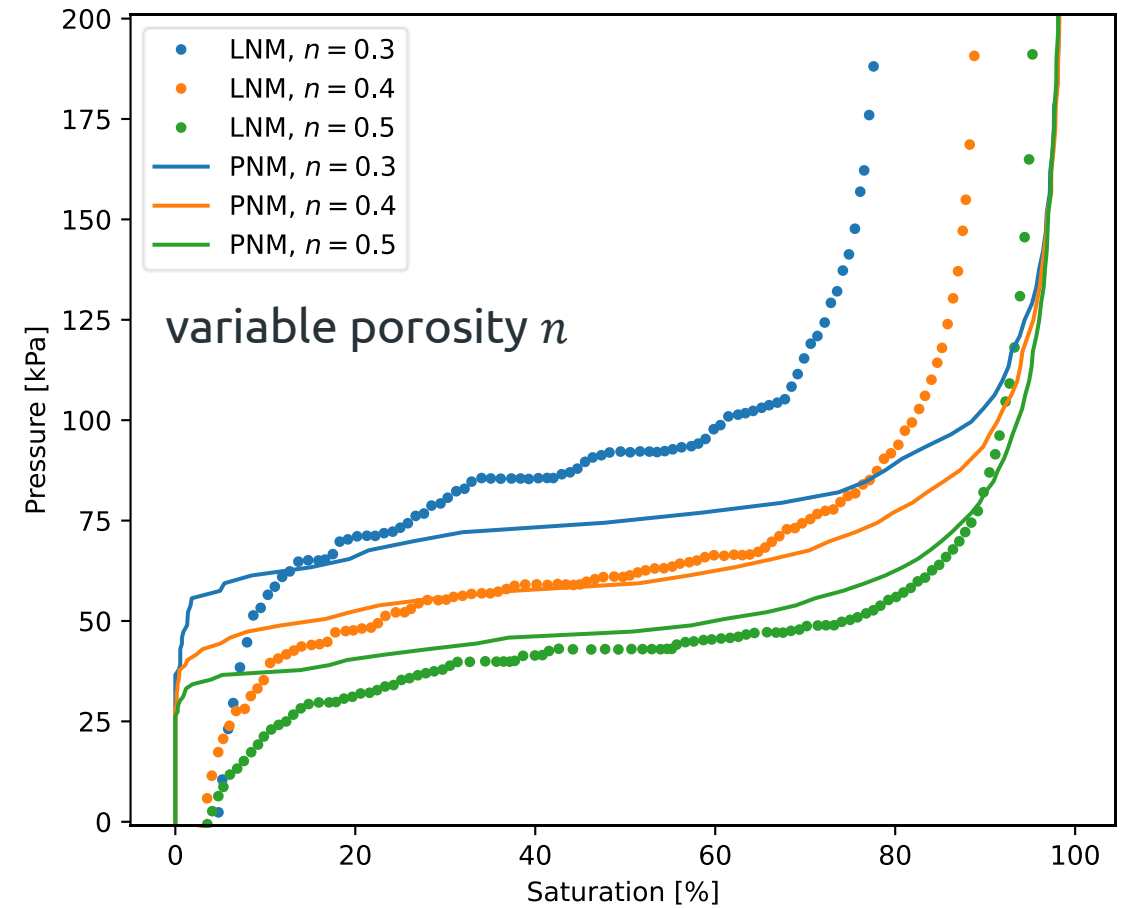
$$|p_c| = c_{\text{geo}} \frac{2\sigma \cos(\theta - \alpha)}{r_h + R(1 - \cos \alpha)}$$



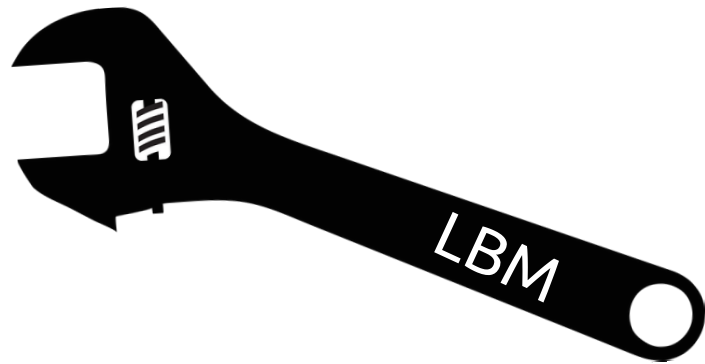
# LBM-CALIBRATION



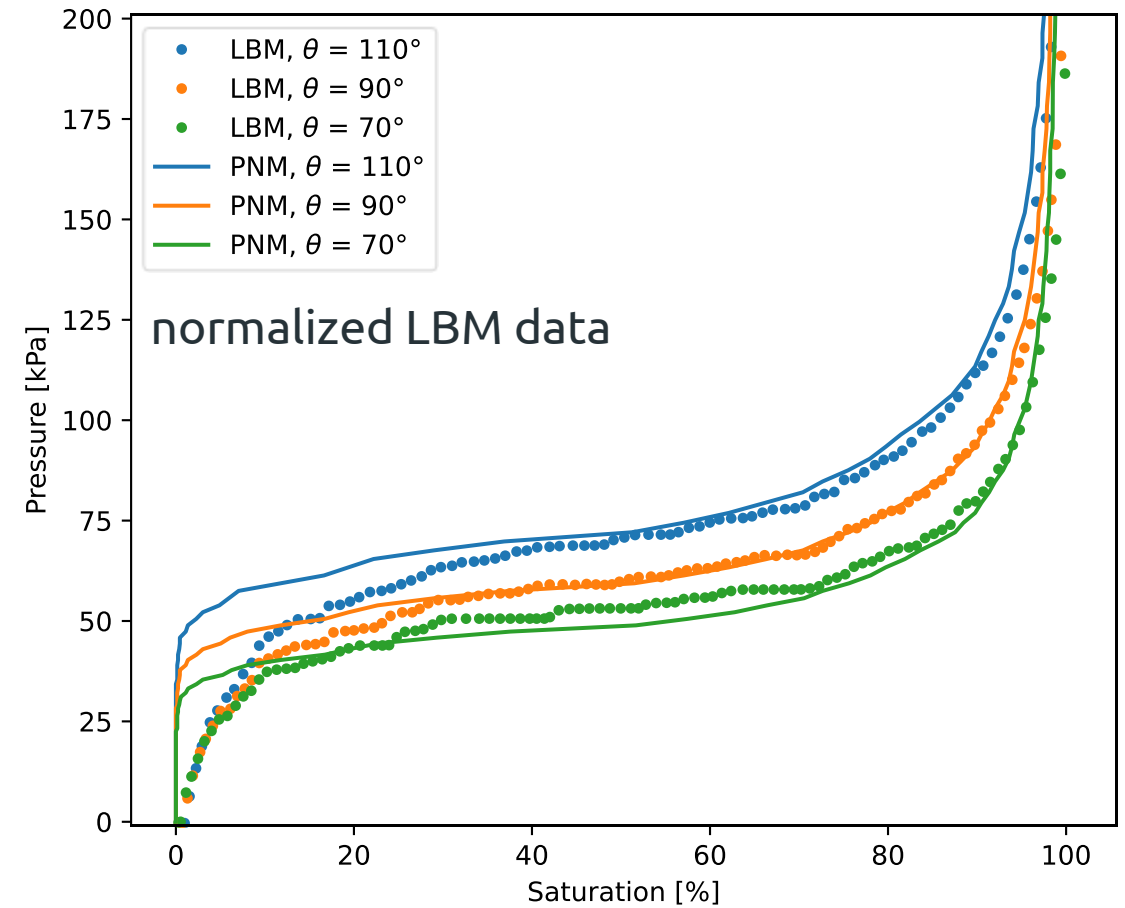
$$|p_c| = c_{\text{geo}} \frac{2\sigma \cos(\theta - \alpha)}{r_h + R(1 - \cos \alpha)}$$



# LBM-CALIBRATION



$$|p_c| = c_{\text{geo}} \frac{2\sigma \cos(\theta - \alpha)}{r_h + R(1 - \cos \alpha)}$$



# SUMMARY

- throat shape correction leads to much smoother pS-curves that agree well with LBM
- variation of contact angle (and also surface tension) requires only one LBM calibration
- the calibration might be sufficient for different volume fraction (depending on the required accuracy), as long as overall structural properties are similar

## FUTURE STEPS

- incorporation of a binder phase and modelling of gas entrapment
- fully geometrical correction without calibration
  - this works for some structures already, but most battery materials are still problematic; the problem is still being investigated
- study of saturation dependend permeability (again compared to LBM)

# ACKNOWLEDGEMENT

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- This work contributes to the research performed at CELEST (Center for Electrochemical Energy Storage Ulm-Karlsruhe).
- All our LBM results are published in  
M. P. Lautenschlaeger, B. Prifling, B. Kellers, J. Weinmiller, T. Danner, V. Schmidt, A. Latz:  
Batteries & Supercaps 2022, e202200090, doi:10.1002/batt.202200090

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