Microstructure Simulations of Flow Batteries

Amadeus Wolf
Karlsruhe Institute of Technology

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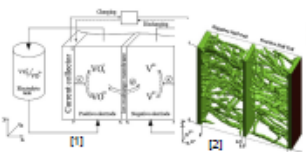
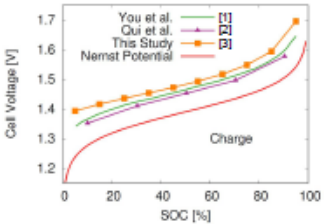
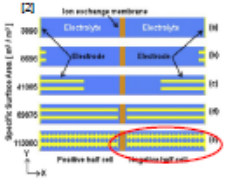
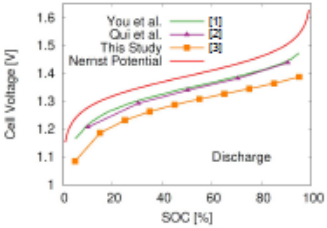
Validation of the model

Vanadium system – full cell – model comparison



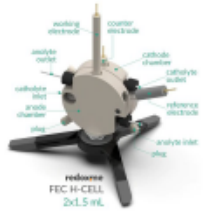


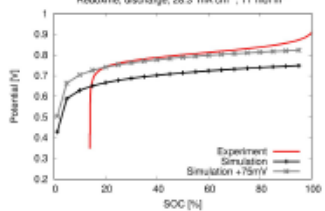


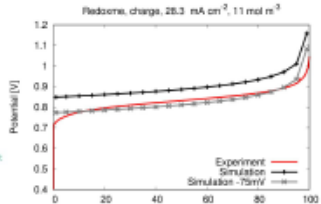


[1] G. Qiu et al., Electrochimica Acta, Volume 64, 2012, Pages 46-64,
[2] D. You et al. Electrochimica Acta, Volume 54, 2009, Pages 6827 - 6836
[3] Wolf, A., Kespe, S. and Nirschl, H. (2023). „Pore-scale Modeling of Flow Batteries." In Flow Batteries. John Wiley & Sons. https://doi.org/10.1002/9783527833757.ch18

TEMPO system – half cell – experiment[4]

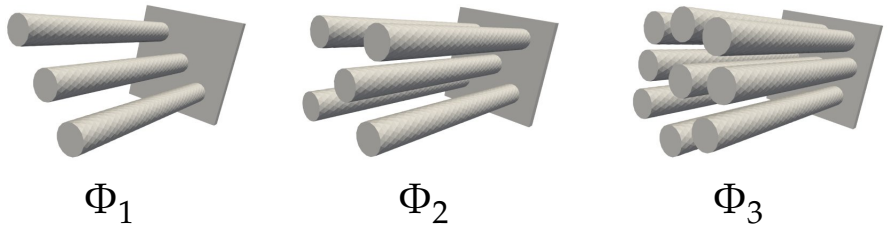






[4] Wolf, A., Baudrin, E., Nirschl, H., (2023) „A Multiscale Flow Battery Modeling Approach Using Mass Transfer Coefficients." Energy Technology. https://doi.org/10.1002/ente.202300175

Numerical investigations on structured electrodes



Φ_1 Φ_2 Φ_3

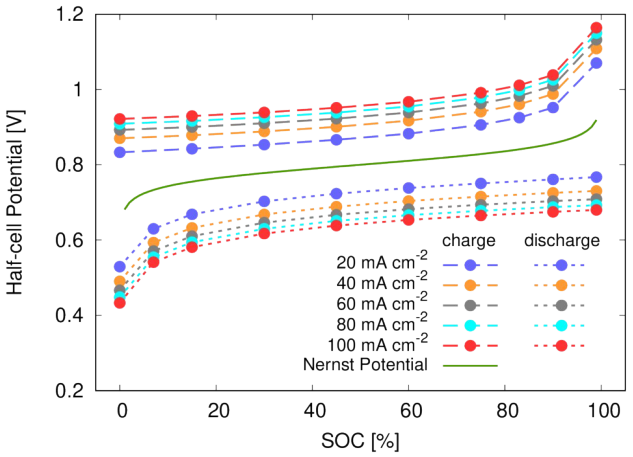
	Φ_1	Φ_2	Φ_3
Domain size	100 µm x 50 µm x 50 µm		
Fiber diameter	10 µm		
Porosity	0.92	0.86	0.75
Specific active surface area	43 761 $m^2\ m^{-3}$	66 269 $m^2\ m^{-3}$	111 283 $m^2\ m^{-3}$
Number of cells	114 077	138 898	168 889

Concentration ↑ → Voltage efficiency ↑

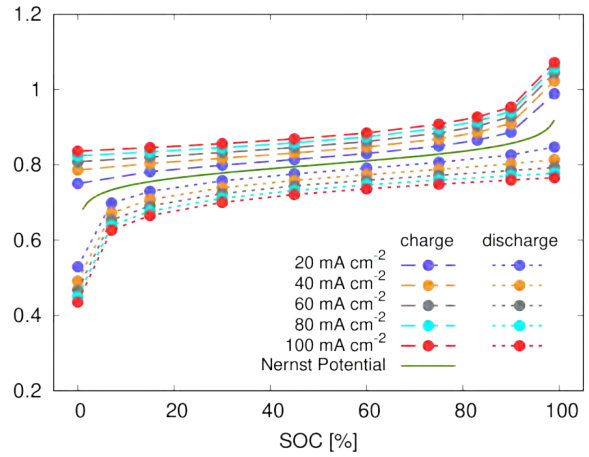
Active surface ↑ → Voltage Efficiency ↑

Active surface ↑ → Pressure drop ↑

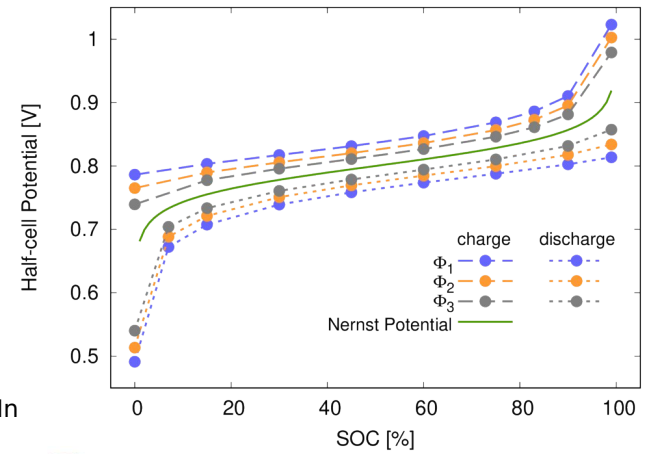
0.1M TEMPO in 1.0M NaCl



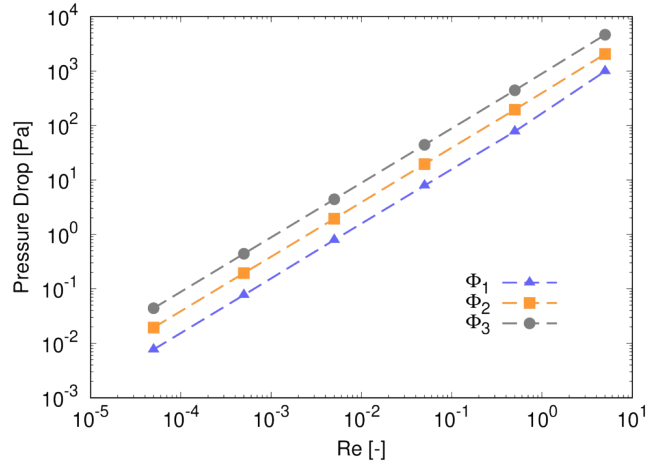
0.5M TEMPO in 1.5M NaCl



Active Surface

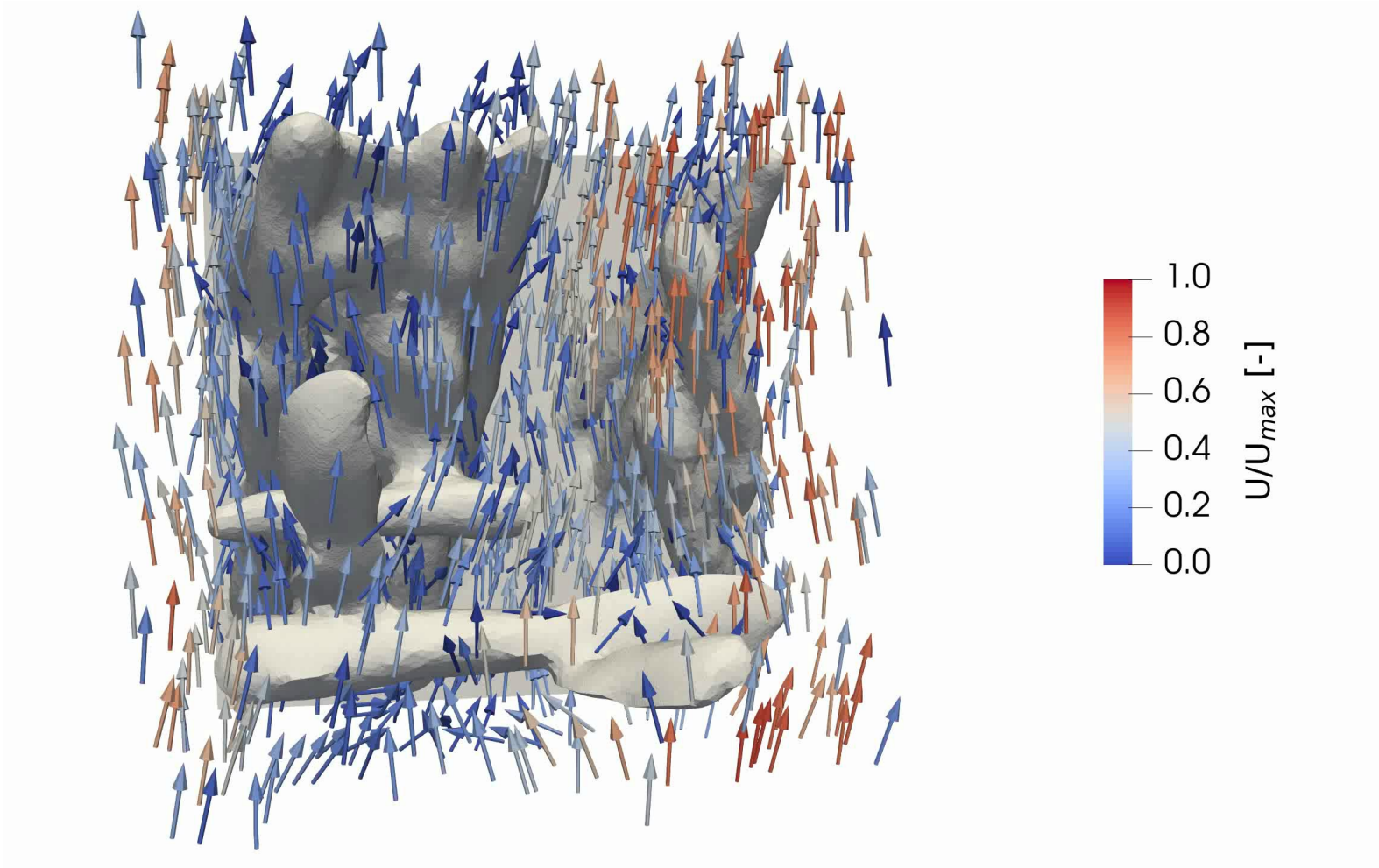


Pressure drop



[1] Wolf, A., Kespe, S. and Nirschl, H. (2023). „Pore-scale Modeling of Flow Batteries." In Flow Batteries, John Wiley & Sons (eds C. Roth, J. Noack and M. Skyllas-Kazacos). https://doi.org/10.1002/9783527832767.ch18

Numerical investigations on reconstructed microstructure



Volume-weighted mean of normalized concentration