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A mixed-wet pore network model for electrolyte imbibition in gas diffusion electrodes

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Knowledge of electrolyte distribution inside Gas Diffusion Electrodes (GDE) is a key feature to improve the electrochemical behaviour of these electrodes. In processes like the chlor-alkali-electrolysis, a porous silver electrocatalyst is brought in contact with the liquid electrolyte and the gaseous reactants at the so-called three-phase boundary. To prevent flooding and to alter the wettability of the electrodes, non-wetting polytetrafluoroethylene is added in the manufacturing process. As shown by experimental work [1], the PTFE content has a high impact of the PTFE content on the electrode performance.

Based on FIB/SEM images of the silver electrodes, Direct Numerical Simulations (DNS) inside the pore system have been carried out using Smoothed Particle Hydrodynamics (SPH). This allows us to track the interface movement in a mixed-wettable porous electrode. Fig. 1 shows snapshots of the simulated filling process of a pore system. Hydrophobicity of the electrode significantly changes with consideration of the contact angle due to the electrowetting-effect [2], which had also been seen in experimentally for this GDE [3].

The DNS is computationally too expensive to model larger parts of the electrode while pore network models are computationally far less demanding. Therefore we combined pore network modelling and rigorous hydrodynamic simulations. First, a skeleton from pore space was extracted from the FIB/SEM-images. Then the skeleton is segmented into different parts of the pore systems. Second, characteristic properties like pore diameter and PTFE-Fraction that covers the pore wall are extracted along the connecting paths.

In a mixed-wet system, the entry pressure does not only depend on geometry and **averaged** wettability, but as well on the **locally resolved** wettability degree. In contrast to conventional pore network models, the highest entry pressure can be not determined by the narrowest nor the widest part of the pore system, but on the **most hydrophobic one**. This can be found by DNS or by more simplified models. Using this data as input, the electrolyte imbibition can be modelled by pore network models on representative electrode volumes.

Participation

In-Person

References

References:

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- [2] F. Mugele and J.-C. Baret, "Electrowetting: from basics to applications," *J. Phys. Condens. Matter*, vol. 17, no. 28, pp. R705–R774, Jul. 2005.
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