Contribution ID: **471** Type: **Poster (+) Presentation**

Incompressible Smoothed Particle Hydrodynamics as a tool for modelling electrolyte distribution in Gas Diffusion Electrodes

Wednesday, 2 June 2021 10:00 (1 hour)

In electrochemical synthesis processes like chlor-alkali electrolysis with oxygen-depolarized-cathodes, porous Gas Diffusion Electrodes (GDE) have to ensure the intimate contact between the silver catalyst, the gaseous reactants and the liquid electrolyte. In the manufacturing process of the electrodes non-wetting Polytetrafluoroethylene (PTFE) is added to change the wettability of this electrodes. Electrochemical experiments showed a strong dependence of the PTFE content on the performance of such electrodes [1]. Understanding the electrolyte distribution in GDE enables the possibility for further improvements of the process.

To model the mixed-wet behaviour, the Lagrangian Smoothed Particle Hydrodynamics Method (SPH) can be used to solve flow-problems on the microscale. Recently, Kunz et al. showed the capability of the SPH-code SiPER (Smoothed Particle Hydrodynamics in Process Engineering) to model these structures based on FIB-SEM images [2]. We present simulation results based on dynamic SPH simulations of the electrolyte imbibition process to estimate the pore entry pressure dependent on wettability effects at the fluid-fluid-solid-interfaces resulting from the PTFE-distribution, external pressure gradients and flow configuration. However, modelling of representative volumes is still challenging due to the high computational demand.

As an outlook, we will present several ways to model larger structures of the GDE. Beside the improvement of scalability and the numerical methods for the SPH-method, the separate treatment of single pores, to use the corresponding entry pressure as an input for a Pore Network Model (PNM), can be used to model the electrolyte distribution on larger parts of the porous structure.

References:

[1] Franzen, D., Ellendorff, B., Paulisch, M.C. et al. Influence of binder content in silver-based gas diffusion electrodes on pore system and electrochemical performance. Journal of Applied Electrochemistry 49, 705–713 (2019).

[2] Kunz, P., Paulisch, M., Osenberg, M. et al. Prediction of Electrolyte Distribution in Technical Gas Diffusion Electrodes: From Imaging to SPH Simulations. Transp Porous Med 132, 381–403 (2020).

Time Block Preference

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

References

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