Abstract for oral presentation

Analysis of local heterogeneities and their effect on DMFC performance with a physical 2D cell model

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In order to develop direct methanol fuel cells (DMFCs) with enhanced lifetime and performance, it is important to understand the physical phenomena inside the cell. During operation, the local conditions inside a DMFC can be very heterogeneous, leading to non-homogeneous performance and degradation. Together with experimental validation, physical modelling can help to understand the processes that are causing those heterogeneities.
DMFC exhibit a pronounced performance loss during operation, which can partially be recovered by adjusting the operating strategy, as Bresciani et al. have shown [1]. This temporary performance degradation is to a great extent dependent on conditions like the local potential and the species distribution. Those parameters are not easy to measure experimentally but can be studied in detail in numerical simulations.

We present a two-dimensional DMFC cell model, which allows transient simulation of a single cell, including the possibility to simulate impedance spectra. The model is implemented in *NEOPARD-FC*, a code developed at DLR based on the open source CFD-framework DuMu^x [2]. It accounts for two-phase flow and multicomponent transport in channels and electrodes, as well as for electrochemical phenomena in the catalyst layers. All layers are spatially resolved. We use a multiphase Darcy approach to describe the behavior of gas and liquid in the porous media. Furthermore, the crossover of methanol and water through the membrane and the resulting mixed potential on the cathode are included. The model is validated using experimental data from segmented cells. The occurrence of local heterogeneities and their effect on cell performance is discussed.

References:
[1] F. Bresciani, C. Rabissi, A. Casalegno, M. Zago and R. Marchesi, International Journal of Hydrogen Energy **39**, 21647–21656 (2014).
[2] B. Flemisch, M. Darcis, K. Erbertseder, B. Faigle, A. Lauser, K. Mosthaf, et al., Advances in Water Resources **34,** 1102–1112 (2011).