

Abstract for oral presentation**Elementary kinetic modeling for the investigation of direct-methanol fuel cell degradation****T. Jahnke^{*1}, Wolfgang G. Bessler²**¹German Aerospace Center (DLR), Institute of Technical Thermodynamics, Stuttgart, Germany²Offenburg University of Applied Sciences, Offenburg, Germany

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In order to become competitive to conventional energy conversion systems, the lifetime of direct-methanol fuel cells (DMFCs) still has to be increased. Therefore it is important to get a deeper understanding of the mechanisms responsible for cell degradation.

We present a detailed one-dimensional model of a direct-methanol fuel cell, based on the in-house modeling framework DENIS^{1,2}, including gas diffusion layers, catalyst layers and membrane. Two-phase transport for the methanol-water mixture within GDL and CL is taken into account. Within the membrane methanol crossover due to diffusion and electro-osmotic drag is considered. The electrochemistry (methanol oxidation and oxygen reduction reactions) is described by means of an elementary kinetic approach including the most relevant surface-adsorbed intermediate species on the anode (Pt-Ru) and cathode (Pt) catalysts. The kinetic coefficients are parameterized using quantum chemical data available from literature. The model allows for steady state, transient as well as impedance simulations.

Based on this cell model, degradation mechanisms which cause changes in catalyst active surface area are studied in detail. A mechanism which is considered to be crucial for lifetime of DMFC is ruthenium dissolution. We demonstrate a model for this degradation mechanism implemented into the cell model and discuss its effect on the cell performance. In the elementary mechanism, ruthenium is responsible for activating water molecules that inhibit poisoning of the Pt surface due to adsorbed CO molecules. The feedback on Ru dissolution on this mechanism is quantified.

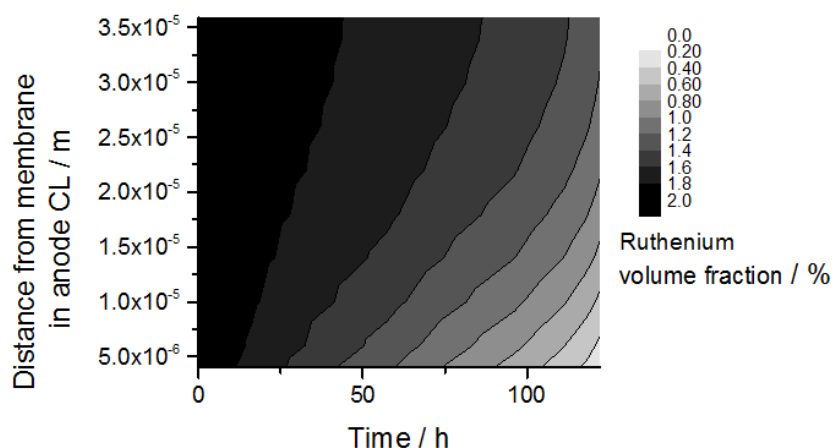


Figure 1. Spatially resolved analysis of ruthenium dissolution in the anode catalyst layer

References:

1. W. G. Bessler, S. Gewies, and M. Vogler, *Electrochimica Acta*, **53**, 1782-1800 (2007)
2. J. P. Neidhardt et al., *Journal of the Electrochemical Society*, **159**, A1528-A1542 (2012)