Contribution ID: **637**   Type: **Oral Presentation**

Stochastic 3D microstructure modeling for three-phase electrode materials with an emphasis on transport relevant characteristics

Wednesday, 2 June 2021 15:15 (15 minutes)

We use parametric stochastic 3D microstructure modeling to generate digital twins representing the complex microstructure of three-phase electrode materials observed by tomographic imaging. For this purpose, we consider two models based on methods of stochastic geometry. The first model is based on random networks, while the second one is based on excursion sets of two independent Gaussian random fields [1]. Both models, for which we have derived new relationships between model parameters and morphological characteristics, are fitted to 3D image data representing anodes in solid oxide fuel cells consisting of nickel, a ceramic phase (Yttrium-stabilized zirconia) and pores. Model validation is performed with respect to the transport relevant microstructure characteristics mean geodesic tortuosity and constrictivity, *i.e.*, a geometrically defined radius of the characteristics bottleneck normalized by the median value of the continuous phase size distribution. Moreover, permeability of the pore space and effective conductivities of the solid phases are numerically simulated using Fourier methods [2]. This allows us to investigate quantitative relationships between morphological characteristics and effective properties, which is an essential question in the field of heterogeneous materials [3], for the considered anode materials. Additionally, we show that excursion sets of two correlated Gaussian random fields can be used to model the microstructure of gas-diffusion electrodes consisting of silver, polytetrafluorethylen and pores [4]. We present a method for parameter estimation by means of two-point cross-coverage probability functions. After having fitted the model to 3D image data, model validation shows that mean geodesic tortuosity and the geometrically defined radius of the characteristic bottleneck are nicely reproduced.

Time Block Preference

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

References

[1] M. Neumann, B. Abdallah, L. Holzer, F. Willot, and V. Schmidt. Stochastic 3D modeling of three-phase microstructures for the prediction of transport properties in solid oxide fuel cells. Transport in Porous Media, 128:179-200, 2019.

[2] F. Willot, B. Abdallah, and Y.-P. Pellegrini. Fourier-based schemes with modified green operator for computing the electrical response of heterogeneous media with accurate local fields. International Journal for Numerical Methods in Engineering, 98:518-533, 2014.

[3] S. Torquato. Random Heterogeneous Materials: Microstructure and Macroscopic Properties. Springer, New York, 2002.

[4] M. Neumann, M. Osenberg, A. Hilger, D. Franzen, T. Turek, I. Manke, and V. Schmidt. On a pluri-gaussian model for three-phase microstructures, with applications to 3D image data of gas-diffusion electrodes. Computational Materials Science, 156:325-331, 2019.

Acceptance of Terms and Conditions

Click here to agree

Newsletter

Student Poster Award

Primary authors: Dr NEUMANN, Matthias (Ulm University, Institute of Stochastics, D-89069 Ulm, Germany); Prof. SCHMIDT, Volker (Ulm University, Institute of Stochastics, D-89069 Ulm, Germany)

Presenter: Dr NEUMANN, Matthias (Ulm University, Institute of Stochastics, D-89069 Ulm, Germany)

Session Classification: MS14

Track Classification: (MS14) Uncertainty Quantification in Porous Media