RANDOM SET MODELS FOR THREE-PHASE ELECTRODE MATERIALS WITH AN EMPHASIS ON TRANSPORT RELEVANT CHARACTERISTICS

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Abstract. We use parametric random closed set models to describe the complex microstructure of three-phase electrode materials observed by tomographic imaging. For this purpose, we consider a model based on β-skeletons of Poisson point processes [1] as well as a model based on excursion sets of two independent Gaussian random fields [2]. 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 certain ceramic phase and pores [3]. 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. These morphological characteristics have been recently defined for stationary random closed sets in [4], where properties of the corresponding estimators are discussed. Moreover, permeability of the pore space and effective conductivities of the solid phases are numerically simulated using Fourier methods [5]. This allows us to investigate quantitative relationships between morphological characteristics and effective properties—an essential question in the field of heterogeneous materials [6]—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 [7]. 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.

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