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Abstract

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Quantifying the influence of 3D microstructure on effective conductivity and permeability of composite and porous materials

Joint with Matthias Neumann, Ole Stenzel, François Willot and Lorenz Holzer

Effective conductivity and permeability of a versatile, graph-based model of random structures are investigated numerically. This model, originally introduced in [1] allows one to simulate a wide class of realistic materials. In the present work, an extensive dataset of two-phase microstructures with wide-ranging morphological features is used to assess the relationship between microstructure and effective transport properties, which are computed using Fourier-based methods on digital images. Our main morphological descriptors are phase volume fractions, mean geodesic tortuosity, two "hydraulic radii" for characterizing the length scales of heterogeneities, and a "constrictivity" parameter that describes bottleneck effects. This additional parameter, usually not considered in homogenization theories, is an essential ingredient for predicting transport properties, as observed in [1]. We modify the formula originally developed in [2] for predicting the effective conductivity and propose a formula for permeability. For the latter one, different geometrical definitions of the hydraulic radius are compared. Our predictions are validated using tomographic image data of fuel cells.

References

[1] G. Gaiselmann, M. Neumann, O. M. Pecho, T. Hocker, V. Schmidt, L. Holzer (2014): Quantitative relationships between microstructure and effective transport properties based on virtual materials testing. *AIChE Journal 60*, 1983–1999.

[2] O. Stenzel, O. M. Pecho, L. Holzer, M. Neumann, V. Schmidt (2016): Predicting effective conductivities based on geometric microstructure characteristics. *AIChE Journal 62*, 1834–1843.