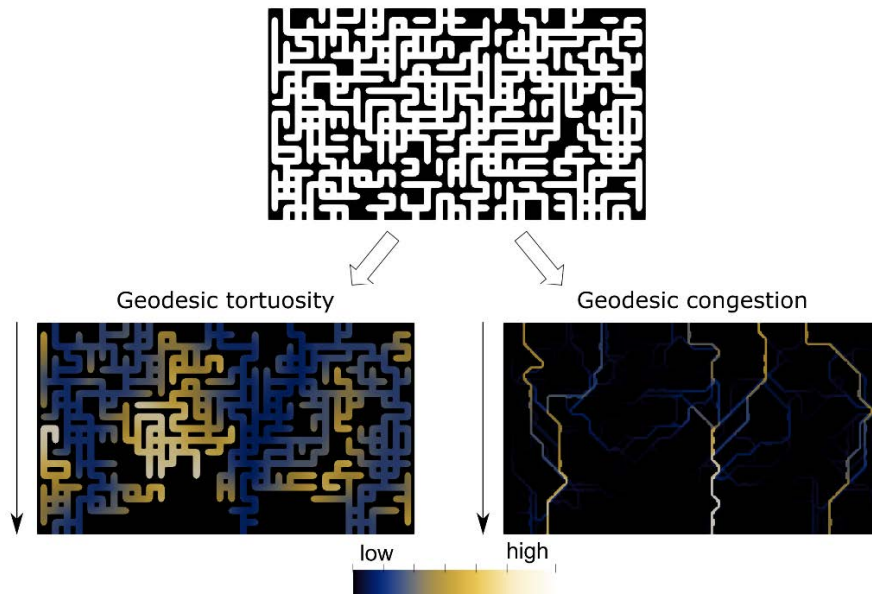


Sandra Barman (Chalmers University of Technology)

Characterization of pore connectivity using geodesic paths

To understand macroscopic properties of a porous material – such as diffusive transport, heat transfer, electrical conductivity, fluid permeability and mechanical strength – it is important to be able to quantify aspects of the pore geometry that influence the macroscopic property of interest. One such aspect is the connectivity of the pore network, which can be quantified using so called geodesic paths through the pore system. A geodesic path in this context is a shortest path that connects a point in the pore system to both the inlet and the outlet. The length of a geodesic path is called the geodesic tortuosity. This path-length measure has been shown to be a very good predictor of diffusive transport [1, 2] (and thus also of heat transfer and electrical conductivity since the governing equations are equivalent), especially if the geodesic tortuosity is computed for the whole pore network [2] as in the 2-D example shown in the figure below. We develop new methods for characterizing and visualizing the connectivity of the pore geometry based on geodesic paths. For characterization, we develop a measure that captures large scale bottleneck effects in the pore network. Our new measure, called geodesic congestion [3] (see the figure below), counts how many geodesic paths pass through each point in the pore space and thus captures bottlenecks caused by path congestion. Bottlenecks are an important factor influencing diffusive transport, and bottlenecks caused by variations in pore size have previously been shown to perform well as a predictor of diffusive transport [1]. For visualization, we compute geodesic paths starting at a specific pore and divide the paths into categories by length. The categories are visualized separately, giving an idea of how the pore network is connected which can be difficult to find from just visual inspection of a 3-D pore network [4].



References

- [1] O. Stenzel, O. Pecho, L. Holzer, M. Neumann, and V. Schmidt. Predicting effective conductivities based on geometric microstructure characteristics. *AIChE Journal*, 62:1834–1843, 2016.
- [2] S. Barman, H. Rootzén, and D. Bolin. Prediction of diffusive transport through polymer films from characteristics of the pore geometry. *AIChE Journal*, 65(1):446–457, 2018.
- [3] S. Barman, C. Fager, M. Röding, A. Olsson, N. Lorén, C. von Corswant, E. Olsson, A. Särkkä, D. Bolin and H. Rootzén. Characterization of Pore Shape and Connectivity of Coatings used for Controlled Drug Release. Manuscript.
- [4] C. Fager, S. Barman, M. Röding, A. Olsson, N. Lorén, C. von Corswant, E. Olsson, A. Särkkä, D. Bolin and H. Rootzén. 3D Visualisation of Transport Paths in Coatings for Controlled Drug Release using FIB-SEM. Manuscript.