Porous materials: spatial models of 3D geometries with specific global connectivity structures & new methods for capturing the connectivity

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Porous materials are widely used in industry, e.g., as packaging materials; in hygiene products; for pharmaceutical applications such as controlled drug release; and as electrodes controlling electrochemical processes in fuel cells and re-chargeable batteries. The properties of these materials (flow, diffusion and/or electrical conductivity) are determined by the 3D geometry of the pores. It is becoming more and more common to use 3D microscopy data of the material and models informed by that data when developing new materials. With this data, there is a need for new spatial statistical models that capture the features of the 3D geometry that are most relevant for the materials properties.

In this talk I will show new methods for capturing the global connectivity of a porous material which are based on computing shortest (geodesic) paths through the 3D geometry. This type of global connectivity is highly correlated with the materials properties. An example is poor connectivity in battery electrodes, caused by pore heterogeneity, which can lead to quick degradation and even battery failure. Methods for capturing global connectivity, geodesic tortuosity and geodesic channels, have been implemented in a freely available software Mist which will soon be available to download from https://mist.math.chalmers.se

I will also show a new method of constructing spatial statistical models with specific global connectivity properties. The method is based on constructing a pore network representation of the 3D geometry and thinning the network by removing links based on a resistance network simulation of diffusion/electrical conductivity. Links in the network are removed iteratively based on how much of the simulated mass transport (diffusion) that goes through the link.

References

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