

Abstract of the poster for the Summer School on Topics in Space-Time Modeling and Inference, Aalborg 2013

by Henrike Häbel, Ph.D. student at Chalmers University of Technology

Title: Spatial modeling of micro-structures of materials

In several industrial areas mass transport of liquids in a material is crucial for its properties and function. The aim of this project is to construct and fit spatial models to given data on biomaterial in order to understand and control mass transport properties such as diffusion through these complex geometrical micro-structures. Such micro-structures can be polymer blended films, cellulose fibers, foams or gels, for instance. Images of these structures are obtained using Confocal Laser-Scanning Microscopy, Scanning Electron Microscopy or similar methods. After having converted these images using statistical image analysis techniques, 2D or 3D models are constructed and fitted to the given data applying methods from stochastic geometry and spatial statistics. In this poster I will present some ideas how porous Ethyl cellulose (EC) / Hydroxypropyl cellulose (HPC) blended films used for controlled drug release can be studied. Their micro-structure is mainly determined by the percentage of HPC which acts as a pore former. The pores can be modeled as unions of overlapping spheres. In particular, they will be modeled by marked point processes, where the centers of the pores are the points and the radii of the spheres the corresponding marks. In order to account for heterogeneity and correlation, the chain like structure of the HPC pores can be constructed based on continuum percolation or by involving Markov chains. The fitted models can be evaluated as input to lattice-Boltzmann computations numerically simulating multicomponent fluids. Consequently, the models can be validated by comparing mass transport characteristics of simulated structures to the same characteristics of real micro-structures with the lattice-Boltzmann method.