Multiscale models for wetting dynamics in porous materials

Tobias Gebäck, Alexei Heintz and Irina Pettersson

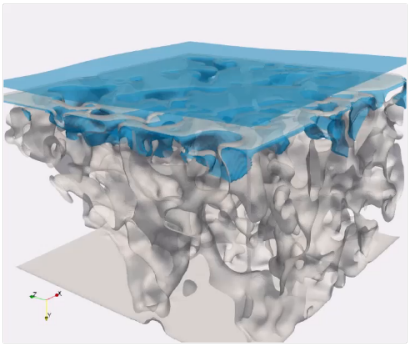

Figure 1: Simulation of water penetration into a paperboard coating layer.

Background

The project is closely related to the ongoing CoSiMa project at the Mathematical Sciences funded by Vinnova. CoSiMa aims at the development of novel, sustainable materials using computational tools to study transport of liquids and molecules in porous materials. It is a collaboration with several major Swedish companies, with applications including the development of paper straws at TetraPak, products for controlled drug release at AstraZeneca, and hygiene product development at Essity.

At the department of Mathematical Sciences, we develop models and methods as well as software which are currently used in industry. This work was awarded the "Chalmers impact award 2020" for most valuable contribution to society. In particular, the transport simulation software *Gesualdo*, that uses the lattice Boltzmann method, and the material structure analysis software *Mist* have contributed to this success. These software are used on real 3D material geometries obtained through microscopy, as shown in Figure 1.

Project description

The current project focuses on modeling and simulations of wetting in porous materials. Such models include several phases (e.g. water and air), and take into account the liquid transport driven by capillary forces and/or pressure gradients. This is achieved by coupling the Navier-Stokes equations for flow with a nonlinear phase-field equation of advection-diffusion-type, describing the distribution of phases. Due to the microstructure, there are several natural scales in such materials, and the multiscale analysis (homogenization technique) may be used for describing the macroscopic behavior and the effective characteristics of such media.

Many challenges arise in these models, giving rise to several research topics, including

- Homogenization methods to rigorously derive effective/macroscopic equations from microscopic ones.
- Development of stable, accurate and efficient computational methods to compute transport properties on the pore scale using the above-mentioned models.
- Investigation of how structural properties such as porosity, surface area, connectivity, etc. influence the liquid transport into the material.

The precise focus of the PhD project can be adapted to the experience and interests of the student.