Karlsruhe Institute of Technology

Institute for Chemical Technology and Polymer Chemistry
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Announcement of student theses

At the Institute for Chemical technology and Polymer Chemistry at the Karlsruhe Institute of Technology

Master Thesis

with the Topic

Morphological and topological analysis of disordered porous media

is open and the position is to be assigned at the earliest possible date

Description:

Obtaining three-dimensional (3D) structural information from porous materials is a critical component of materials science, catalysis and porous media research. Pore characteristics such as size, volume, shape, connectivity and tortuosity greatly affects the performance of materials. In heterogeneous catalysis, designing catalysts with a suitable pore size and connectivity allows reactant molecules of the desired size to enter and products of the reaction to leave the catalyst without diffusion limitations, enabling precise control of concentration profiles around the catalytic site. Porosity and pore accessibility can also be compromised by catalyst deactivation processes, which can negatively impact catalytic performance. Quantitative information about the morphology of pore systems therefore leads to better understanding of their microstructure and correlation between the structure itself, the manufacturing procedures, the physical properties and the engineering performance. Moreover, extracting the required 3D information is necessary for further modelling and simulation.

In the “X-ray Microscopy in Catalysis” (XRM) research group, hard X-ray computed tomography is used as an optimal and novel characterisation tool for 3D catalyst characterization. In the field of catalysis, until now little research has been devoted to investigate how pores are coordinated and connected, as well as how tortuous are the pathways through the pore. Therefore, the main focus of characterization in this research aims in this direction. Different methods and algorithms are available for pore structure characterization. We want to apply and compare these different approaches on our 3D tomography images to quantify the pore connectivity, the pore and pore throat coordination, and the geometric tortuosity. Most of the algorithms and codes are open source and can be improved based on the project requirements.

Tasks:

- Apply and compare various image analysis methods for pore structure characterization:
  - ✓ Skeleton analysis combined with maximum inscribed sphere: Pore 3D package in IDL environment can be used
  - ✓ Snow algorithm method (Improved version of watershed segmentation): available as python scripts
  - ✓ Watershed segmentation with Avizo software
- Explore accurate definitions for 3D tortuosity and apply these in tomographic image analysis

Requirement:

- Interest in the field of porous media characterization (e.g. catalyst characterization)
- Master student in the field of chemistry or chemical engineering
- Programming experience (e.g. preferably in Matlab, Python)
- Familiarity with image processing is an advantage
- Independent, structured and interdisciplinary work
- Very good knowledge of English (spoken and written)

Contact:

For more information you can contact with
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