On characterizing and simulating porous media

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Porous media are at the heart of many of the technology solutions that Gore offers. We have studied the performance of these media on macroscopic ($\sim cm$) lengthscales and we would like to improve our understanding of the mechanistic details of processes that occur at the microscopic ($\sim \mu m$) lengthscales within these media. For this edition of the MPI workshop we bring 3 classes of problems that are related to chemical and physical processes that occur at the microscopic lengthscale within a porous medium.

1 Modeling product transport in catalysts

Catalysts are are an integral part of many chemical processes. Catalysts are usually made of a dense but porous material such as activated carbon, zeolites, etc. that provide a large surface area. Liquids that are produced as a byproduct of a gas reaction at the catalyst site accumulate inside this porous network, slowing down transport of the gaseous reactants to the catalyst active site. Effectively transporting the accumulated liquid out of the porous structure is critical to maintain performance and durability of the catalyst assembly.

Modeling goals

Our goal in this workshop is to develop a mathematical model to understand the transport of reactants, kinetics of the reaction and the concommittant evolution of liquid within the porous structure given its material properties and structural characteristics. We are particularly interested in quantifying/predicting the timescales for flooding of the entire pore space.

2 Characterization of porous media

Characterization of porous media is fundamentally important in a variety of industrial applications. In porous filtration, for example, filter performance (particle and contaminant retention and flux efficiency) is heavily dependent on material properties such as porosity, pore size, and tortuosity. A refined understanding of microscopic structural features and how they relate to membrane permeability and particle retention efficiency can aid in design and performance optimization. A variety of experimental tools like porometry, porosimetry and capillary condensation currently aid in quantifying and understanding some of these properties. Mathematical descriptions of porous media (e.g. networks and graphs, space-filling models) have been developed and have been successfuly used in the past. One of the challenges that remains is understanding changes in the structure when external forces are applied. In this workshop, we will hypothesize, execute, and evaluate methods on how pore size characterization changes upon the application of an external force like compression.

Modeling goals

The goal of this workshop is to use mathematical characterization of porous structures and develop methodologies to quantify changes in the microscopic properties (pore size, porosity, tortuosity, etc) when external forces are applied. We hope that this problem stimulates further discussion on mathematical characterization techniques related to porous media.

3 Discrete models, optimization, and simulations

- We have a set of algorithms and python codes that simulate lattice models of transport in a porous medium (related to our problem on transport in catalysts). Our current tool is functional and works very well for small systems and for square lattices. We would like to extend the capabilities of this tool to simulate larger random graphs as well as implement new transport physics.
- Simulating a version of the cellular Potts model - we would like to know the best way to implement our algorithm in order for the code to scale to large systems.