PoreLab is a Norwegian Center of Excellence created in 2017 and situated at the Norwegian University of Science and Technology (NTNU) in Trondheim, and the University of Oslo (UiO). Its mission is to unify and advance the understanding of porous media. The center focuses on the physics and physical chemistry of porous media using experimental, theoretical and computational methods.

At UiO, PoreLab is organized under the auspices of the Njord Center which is a recently established cross-disciplinary geoscience-physics center.

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Cover page:
Picture by Kristian Stølevik Olsen, UiO, 2020: Active matter consists of particles trying to overcome the noise in the system to move in the same direction. Inside confinements like a disc, the particles will for low noise form a cluster that moves along the system boundary.
Welcome to PoreLab

PoreLab would like to have more Master students!

We therefore invite potential students to make contact with anybody in our crew. Contact juniors to learn about our environment. Contact PIs and seniors for project possibilities!

The projects listed in the end of this booklet are only a fraction of the possibilities. We like to tailor new projects to the particular student’s wishes and can start a new topic this way. The team’s cores are presented in the Annual Report, and on our homepage. They serve also as useful starting points.

The climate crisis is a fact, and PoreLab is putting its weight behind the UN sustainability goals! With all our skills and ingenuity, we want to contribute to production of clean water and a more energy efficient world. Some of the master projects refer to that.

Norway has a high competence on transport of oil through porous media. PoreLab sees it as a mission to bring this basic competence to other fields of application.

We recently obtained a new project to study transport of nanoparticles with in cancerogenous biological tissue. This is an example of a such a change in direction.

Looking forward to seeing you in PoreLab!

Signe Kjelstrup
Leader of graduate school

Overview – 2020 MSc students

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A SCIENTIFICALLY INSPIRING AND INCLUDING WORKING ENVIRONMENT

Training of Master and PhD students, as well as Postdoctoral researchers, is a core activity at PoreLab. An essential part of NTNU’s and UiO’s mission as universities, is student and researcher education. PoreLab is a valuable contributor in this respect. A vital asset of the center from an educational point of view is that it offers each student and junior researcher a scientifically stimulating and inclusive workday, much above the level of a regular MSc/PhD/PostDoc program.

“Because we are an interdisciplinary group, we work with people from different departments and universities and fields of research, which makes it an excellent learning environment,” says Astrid Fagertun Gunnarshaug, PoreLab fellow and PhD candidate at the Department of Chemistry, NTNU. This is indeed our ambition at PoreLab, to create an interdisciplinary and international training ground for our juniors.

The aim of this catalogue is to provide an overview of the projects performed by our Master students in 2020 and inspire new students to join the team.

PoreLab is an international community. Master students at PoreLab do not only come from NTNU and UiO, but also from our international partners. The Center offers some funds that allow foreign Master students to spend some time with us, as well as to send our own students abroad. The same offer is available for Master students between NTNU and UiO.

As a PoreLab Master student, you will get an office space at PoreLab premises. Being part of the PoreLab team, you will be offered to attend and contribute to all PoreLab events, such as the Thursday Talks and the PoreLab lecture series. We host both types of events simultaneously in Oslo and Trondheim, and they are open to all.

Our Wednesday seminars - or PoreLab lecture series - are now almost always given by external lecturers. The Thursday’s talks aim to promote internal speakers who are given the possibility to present their own activities or give a lecture. It is our goal that each PoreLab member should participate with at least one presentation during the course of the year. The Thursday’s talks take place once every two weeks.

PoreLab provides a research environment that is centered for working as a team and that allows everyone’s talents to flourish. Therefore, open communication is crucial at PoreLab, and we designed the organization to achieve this goal. Srutarshi Pradhan, researcher at the Physics department, NTNU, provides a good summary: “It is easy to meet seniors and discuss and express our doubts, in scientific matters or in any other issues. This has even been encouraged and assured by our senior members”, before adding: “The wishes and constant efforts by the directors and the PIs have created a healthy and warm research atmosphere, with a family feeling among the group members”.

At PoreLab UiO, the researchers also join forces with the larger team of the Njord centre, for interdisciplinary collaboration across the fields of physics and geology, as well as larger social gatherings, conferences and other events. As postdoctoral fellow, Marcel Moura puts it: “The idea ‘Simplify it until you understand it’, is really in the nature of physics and it has given us quite a lot. However, it is important to remember that sometimes reality is bigger and more complex than our models. Therefore, being in close proximity to scientists who tackle nature at different scales of complexity – geologists, volcanologists, and rock scientists of all types – is excellent to keep our eyes open and our antennas tuned.”

Though PoreLab has dedicated, eager researchers, being at PoreLab does not only mean hard work. The Pore Buzz at PoreLab NTNU and the Junior club at PoreLab UiO are informal events that aims to strengthen connection within our group and integrate new juniors, Master students and guests. The hottest research topics in the field, as well as pizza, are on the menu of these convivial and relaxing events. For more social interaction, we all meet at 10’ every day for our coffee break, as well as at lunch time. On Mondays, fruits and cake are served. In addition, a ping-pong table became one of the most popular playgrounds for all at PoreLab NTNU.
In-house X-ray computed tomography is a well-established method for 3D imaging. Conventionally data sampling is rather time consuming, preventing the use of such methods to follow structure dynamics beyond the hour time scale in situ. However, in most cases, tomography data is vastly oversampled, opening for the possibility to reduce measurement time by various means, such as so-called compressed sensing. In the current MSc project, we have tested different sparse data sampling approaches in order to assess our ability to perform in situ tensile test experiments with our in-house CT instrument. The work has been performed in collaboration with Prof. Odd Sture Hopperstad and Prof. Arild Holm Clausen from the Centre for Advanced Structural Analysis (SFI CASA) at the Department of Structural Engineering, NTNU.

The goal of the project is to test out the viability of utilizing CT to analyze mechanical deformations, both by uncovering the advantages of using 3-4D CT compared to well-established 2-3D methods, such as DIC, and also how to limit the amount of data to enable faster computations and better time resolutions.

As experimental data, tensile stress rods with predefined geometrical shapes have been subjected to multiple stress tests, with CT scans following each deformation. To analyze the resulting 3D images a python script was used to approximate mathematical functions to the distorted surfaces of the samples.

Hydrogels are three-dimensional networks of hydrophilic polymers that are connected by cross-links. The hydrophilic structure allows the hydrogels to absorb large amounts of water, hence the name. Furthermore, hydrogels’ viscoelastic and biocompatible properties make them very interesting in the field of biomedicine. The structure of the hydrogel can be very similar to what we see in the cell walls in our body and has inspired research in tissue generation and drug delivery appliances.

The aim of the thesis is to model the contact mechanics of hydrogels using coarse-grained molecular dynamics simulations. In the human body, as well as most other physical environments, materials undergo stress by means of indentation and stretching. These processes are governed by contact mechanics and understanding more about how they apply to hydrogels will yield valuable information for improving its appliances in medicine along with many other fields of research.
In order to better understand the theory behind immiscible two-phase flow through porous media, a dynamical network model is developed. In this thesis, such a model is used to perform numerical simulations of the flow. The geometry of the model is simplified and symmetric as shown in Figure 1 and 2. The pore space is modeled by a disordered network and consists of nodes and links that are oriented with 45 degrees with respect to the average flow direction. One way to drive the fluids through the model is to time step the equations of motion, though this method is very time consuming.

The aim of the master thesis is to use Monte Carlo simulations to model the two-phase flow, in order to make the simulations less time consuming than integrating the equations of motion for the fluids.

A first version of the Monte Carlo method was developed as part of a PhD project some years ago. A major weakness of that version was that it could only deal with porous media where the pores form a regular lattice. Naturally occurring porous media are never like that. Hence, a new variant of the Monte Carlo method needs to be developed. This is the aim of the thesis.

Background & Motivation

Pathological mineralization inside the human body represents widely prevalent diseases such as urinary stones, gall bladder stones and atherosclerotic plaques in arteries. Although treatable, these diseases have a big socio-economic impact, and development of protocols for preventing them is an active field of research. Gallbladder stones can be removed surgically, but they can also be destroyed using ultrasonic shock waves in a process called lithotripsy. The successful outcome of this treatment depends strongly on the composition and structure of the stones [1]. Hence, obtaining the detailed microscale structure of the wide variety of these biomineralized stones along with a detailed knowledge of their chemical composition might provide better healthcare solutions.

Results

X-ray micro-computed tomography (μ-CT) has emerged as a uniquely suited technique for analyzing the inner structure of gallbladder stones non-destructively. Using the μ-CT facility of the X-ray Physics Group at PoreLab, several specimens have been analyzed. Their compositions and structures have been investigated, reflecting the different origins of the samples [2]. As an example, see Fig. 1, we present a mineral-layered sample where denser concentric nucleated layers due to the presence of the mineral apatite can be discerned. Ultimately, it is expected that one can gain insights into the nucleation and growth of gallbladder stones from a detailed view of their morphology.

Recommended reading


Carlos Martínez Mingo

Ultrastructure Analysis of Gallbladder Stones using Computed Tomography

Spring 2020

Supervisors: Basab Chattopadhyay and Dag Werner Breiby

Background & Motivation

Pathological mineralization inside the human body represents widely prevalent diseases such as urinary stones, gall bladder stones and atherosclerotic plaques in arteries. Although treatable, these diseases have a big socio-economic impact, and development of protocols for preventing them is an active field of research. Gallbladder stones can be removed surgically, but they can also be destroyed using ultrasonic shock waves in a process called lithotripsy. The successful outcome of this treatment depends strongly on the composition and structure of the stones [1]. Hence, obtaining the detailed microscale structure of the wide variety of these biomineralized stones along with a detailed knowledge of their chemical composition might provide better healthcare solutions.

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Recommended reading


Background

Swelling of Shale-rocks create several problems during underground drilling operations, such as stuck-pipe/drill-bit. However, swelling of shale-rocks can close the gaps between rock (wellbore) and casing, therefore no cementing is needed – which can save a lot of time and money and such a “natural” closing ensures “no-leakage” during further drilling and production phases. The field experience reveals that some shale-rocks are good candidate for swelling and some are not. There are several parameters that can influence the swelling behavior, such as porosity, clay-quartz contents, stress difference between field and drilling zone etc. Therefore, to plan a safe and efficient drilling through shale-rocks, we should understand the swelling mechanism of shale/clay.

Problem formation

To investigate swelling problem, we have introduced a discrete element model (DEM), based on Monte-Carlo technique. We define a probability of swelling for all the clay grains in the shale-rock sample that includes the effect of stress-difference, porosity, temperature etc. The time evolution of grain swelling results in bulk swelling behavior of the sample and the simulation result qualitatively matches with the observations of shale/clay swelling experiments. [3,4].

The aim of this Master project is to study the Monte-Carlo based DEM for the entire parameter space by varying several important inputs like porosity, clay-quartz contents, stress difference etc. The DEM simulation codes are developed in-house and are available for re-use and further improvement.

Recommended reading


Reference:
The DEM model for Shale rock sample with clay and quartz grains (left). Swelling amount with time for different stress levels (middle) and temperature levels (right).

Fredrik Rosenberg
Department of Physics, Department of Mechanical and Industrial Engineering, NTNU
2-D Image Analysis of Snow for Cross-Country Sking
Spring 2020
Supervisors: Astrid de Wijn and Antonius Van Helvoort

Motivation for the project

The motivation of this study is to characterize and classify images of snow to deduce the snow’s structure in terms relevant to the performance of skis. By creating robust image processing methods to effectively distinguish between different snow conditions, one can compare previous performances of ski preparations and snow combinations to find the optimal skis for snow with given structure.

In this project two novel image processing methods are developed. The first involves using a contour approach to calculate the Optical Equivalent Diameter (OED) and dendricity of snow grains, two metrics shown to impact the friction of skis. The second method involves using the machine learning algorithms Support Vector Machine (SVM) and Convolutional Neural Network (CNN) to classify the snow’s structure into categories, here old and new snowlogy.

Reference:
a) Original image
b) Contour image


(a) Dendricity=12.17 and OED=0.3
(b) Dendricity=22.3 and OED=0.38

In their article from 2019 [1], Galteland and coworkers used a new procedure to compute the integral pressure of a single-phase fluid in a porous medium confined in a regular lattice of spherical particles. The system is illustrated in Fig. 1. The porous medium (blue) is surrounded by bulk fluid particles (red).

The set-up was used to find thermodynamic (integral and differential) pressures and surface tension between solid and fluid, using knowledge of the geometry of the lattice.

The way to define thermodynamic properties and driving forces inside a porous medium, where the fluid is confined to very small space, is largely unknown. This project will help expand our understanding of driving forces for transport and design a method to determine the permeability.

To determine the permeability, we will use the non-equilibrium thermodynamic description of transport in porous media by Kjelstrup and coworkers [2, 3].

The thesis will expand and extend on the work done by Galteland and coworkers. We can systematically vary the thermodynamic state of the porous medium in various ways. Once we know the gradient of the pressures, we can find how the permeability varies with these variables. The aim is to see if the new way to compute the permeability can be allocated to known models like the Kozeny-Carman equation [4]. The tool will be non-equilibrium molecular dynamics (NEMD) simulations. The first goal is to compute the permeability by considering the bulk pressures outside the porous media. Next, the integral pressure will be computed locally as described by Galteland [1]. By computing the integral pressure locally, it is possible to study transient states, gradients in surface tension and gradients in porosity.

Supervisors: Signe Kjelstrup, Michael Tobias Rauter and Olav Galteland

References

Abstract
Reverse electrodialysis (RED) is a technology to produce electricity from the process of mixing fresh- and seawater. This is done by allowing the mixing to occur through ion-exchange membranes. In conventional RED, a concentration gradient across the membranes drives the mixing process. However, the process can be enhanced by a temperature gradient across the membrane, which will lead to an electric potential gradient. This is the Seebeck effect.

The Seebeck effect has previously been measured in ion-exchange membranes in equilibrium with single-salt solutions, and most extensively with NaCl and KO. In this thesis, the Seebeck effect was measured in cation-exchange membranes in equilibrium with single-salt solutions of various alkali- and alkaline earth chlorides, with binary NaCl-MgCl2 solutions, and with natural seawater. The motivation for this is to better understand how the ion species and mixtures of ions found in seawater affect the Seebeck effect.

A relation between the Seebeck coefficient and the ion species was found, in the single-salt systems. This relation is yet to be explained theoretically. In the binary NaCl-MgCl2 systems, even small amounts of Mg2+ had relatively large, negative effects on the Seebeck coefficient. This was likely due to a high fraction of Mg2+ in the membrane.

The thermoelectric potential was also measured with a seawater, and the Seebeck coefficient was higher than with pure NaCl at the same total ion concentration. This is contradictory to what we would expect from the NaCl-MgCl2 systems, and from Mg2+ being the second-most abundant cation in seawater. One hypothesis is that K+ may play a significant role, but more experimental work should be done to investigate the Seebeck effect in mixed electrolytes.
Sebastian E. Nordby Price
Department of Chemistry, NTNU
Improving the Perturbation Theory for Mixtures Described by Lennard-Jones Potential with Large Differences in Well-Depths
Spring 2020
Supervisors: Anders Lervik and Øivind Wilhelmsen

Background
The statistical associating fluid theory (SAFT) has been hugely successful in describing associating chain fluids and has recently been extended to include fluids adsorbed in cylindrical pores [1]. These SAFT-like equations of state are usually written as a sum of the Helmholtz free energy, consisting of an ideal, a monomer, a chain and an association contribution. Most of the work on these equations has been on the monomeric contribution, where the Barker-Henderson perturbation theory has shown promising results. Barker-Henderson perturbation theory is based on expanding the Helmholtz free energy from a well understood hard-sphere reference fluid into a perturbation series. Investigations of this method has shown promising results for pure fluids but has severe problems in describing the second and third order perturbation terms for mixtures with large differences in well-depth.

Objectives
The second order perturbation term has commonly been estimated using the macroscopic compressibility approximation (MCA), which combined with the mean value theorem has made it possible to obtain an analytical form. This may partly be the reason for the failure in predicting mixtures, thus the study has investigated an approach that does not utilize the MCA by using a numerical method.

Methodology
Monte Carlo simulations on the second order perturbation term has been performed over a wide range of different parameters and compared to different models for the second order perturbation term for mixtures.

Results
The numerical approach in obtaining the second order perturbation term was able to predict the general trend better than the commonly used MCA approaches but did however overestimate the slope at the higher density range.

Recommended reading

Kevin Kottakkakathu Varughese
Department of Chemistry, NTNU
Nanothermodynamics of a Single-Phase Fluid Confined in Complex Porous Medium
Fall 2020/Spring 2021
Supervisors: Signe Kjelstrup, Olav Galteland, Michael Tobias Rauter

Background
Defining the thermodynamic variables of fluids confined in porous media is necessary before we can describe transport problems. Relevant transport of fluids in porous media range from freshwater production from underground aquifers, to transport in graphitic electrodes in lithium-ion batteries as well as in the supply system of fuel cells. It is largely unsettled how to define the thermodynamic variables for porous media in general, this is because porous media can have a wide variety of sizes and shapes. In this work we will study the thermodynamic state of a single-phase fluid confined to complex porous media.

State-of-art
Kjelstrup and coworkers have developed a non-equilibrium thermodynamic description of non-isothermal transport in porous media [1,2]. This work described the driving forces for transport in terms of gradients in temperature, pressure, and chemical potential. However, it is not clear how to compute or measure these variables. Galteland and coworkers have described how to determine the integral pressure in complex geometries from the bulk pressure and geometric variables [3]. Recently the integral and normal pressure of a single-phase fluid in a slit pore have been computed directly from the mechanical pressure tensor [4].

Thesis plan
For the thesis we will study single-phase fluid confined to a complex face-centered cubic lattice of solid particles in the grand canonical ensemble [3,4]. Thermodynamic variables such as temperature, porous medium geometry and chemical potential can be varied systematically, allowing to test Maxwell relations found from the nanothermodynamic framework. Integral pressure will be computed by integrating the density as a function of chemical potential. Comparing the procedure described previously by Galteland & co [3]. Further we will attempt to compute the integral pressure directly form the mechanical pressure tensor. Essentially contributing to the development of nanothermodynamics.

Recommended reading
The investigation demonstrates two major findings, 1) a difference between small and bulk hard-sphere (HS) pressure and radial distribution function (RDF) and 2) particles are depleted from the inner-core (IC) of the spherical confined HS fluid to be adsorbed on the confining wall. For the HS RDF $g(r)$, instead of tending toward $g(r) \rightarrow 1$ when the pair-distance $r \rightarrow \infty$, the small HS RDF reduces to zero in a certain geometrical way when $r$ equals the sphere confinement diameter. For the adsorption, the depletion causes a reduction in the IC density of the small system fluid, causing the fluid to exert properties more similar to bulk fluids with lower fluid densities. By taking these small-bulk differences into account, a "small" first-order BHPT framework is developed and is observed to accurately predict the simulated small first-order perturbation term $a_1$ and the simulated small HS and LJ/s pressures.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{The density variation of the Pseudo HS (PHS) fluid within spherical confinements of radius $R = 5\sigma$, $10\sigma$ and $15\sigma$ for $\rho^* = 0.85$.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{The bulk HS and small PHS RDF as a function of pair-distance $r$ at $\rho^* = 0.85$. In this figure the small confinement geometry has a radius of $R = 5\sigma$.}
\end{figure}
Fadhil Berylian

Department of Geoscience and Petroleum, NTNU

Calculation and Visualization of Energy Dissipation and Energy Balance in Reservoir Models

Spring 2020
Supervisor: Carl Fredrik Berg

Background

Various forms of energy are involved during reservoir recovery. There are external energy, internal energy, and dissipated energy. Together, they should create an energy balance within the reservoir based on thermodynamics of multiphase flow [1].

Objective

Calculating and visualizing the energy components on a real field model should give valuable insight on the reservoir, and potential application on these could include optimum well control and placement based on energy distribution within the formation.

Methodology

This study uses open source software for reservoir simulation and visualization. The visualization software is able to connect to high-level programming languages for processing of reservoir properties data and generate new properties [2].

References


Anna Bjørke Kallestad

Department of Geoscience and Petroleum, NTNU

Geochemical Modelling of Low Salinity Water Flooding

Fall 2020/Spring 2021
Supervisor: Ashkan Jahanbani Ghahfarokhi and Ole Torsæter

Background

Waterflooding is one of the most used and successful approaches to increase oil production from oil reservoirs today. Over the years, much research has been dedicated to the investigating of ion composition and chemistry of the injected brine to optimize oil recovery. Introducing low salinity water flooding (LSWF) or smart water, the water is modified to a different ion composition than the formation water. The mechanisms responsible for the enhanced oil recovery seen in LSWF, is broadly debated in literature. However, there seems to be a consensus that the main mechanism is wettability alteration towards a more water wet state as a result of ion exchange and geochemical effects. Due to the complex interactions between oil/brine/rock, it is critical that the LSWF numerical model contains both intra-aqueous, mineral dissolution/precipitation, ion exchange and wettability alteration mechanisms. By using the equation-of-state (EOS) simulator, GEMTM by CMG, these mechanisms are included in the LSWF model.

Objective

The objective of the thesis is to investigate low salinity water flooding processes for wettability alteration and the influence of geochemical reactions. The reservoir simulation software from CMG is going to be used to develop a more realistic full-field reservoir model for low salinity water flooding.

Furthermore, a software tool that combines advanced statistical analysis, machine learning, artificial intelligence and data interpretation techniques is going to be used for both comprehensive sensitivity analysis and to find optimal solutions for different objective functions.
**Raymond Mushabe**  
Department of Geoscience and Petroleum, NTNU

Effect of Water Quality on Spontaneous Imbibition into Carbonate Cores

Fall 2020/Spring 2021  
Supervisor: Carl Fredrik Berg and Antje Van der Net

**Background**

Producing oil from a carbonate reservoir (Limestone, chalk, dolomite), is quite challenging. The main two reasons behind this difficulty are the original wettability state in the mentioned reservoir rocks that host oil, and the extent of heterogeneity, mainly fractures, that they exhibit. These rocks tend to retain oil because oil wets in preference over formation water. Also, traditional water flooding would result in the fractures acting as fast conduits to producers, and hence bypassing target residual oil. However, considering that more than a half of the oil reserves are in carbonates, there is need to produce and optimize production from them in the most economical, safe, and environmentally friendly manner. Nothing much can be done about altering the fracture state. Over the field life, the wetting state can be altered using modified versions of water or chemicals.

Studies on low salinity flooding or spontaneous imbibition on carbonate core plugs have showed that it is possible to alter the wetting state.

**Objectives and Methodology**

The master project that I am doing is about Low salinity imbibition experiments by studying how water quality, in terms of salinity, alters the wetting state of carbonate cores and ultimately causing changes in oil recoveries. The experiment is conducted on a heterogeneous outcrop core from Angola. The rock material is representative of the reservoir field operated by Equinor in Brazil.

Past studies have faced challenges due to experimental errors arising from core handling and change of brines during imbibition or flooding. These are being addressed with a new experimental design. The system is closed and loaded with all brines under ambient condition were analysed. Moreover, a series of low salinity water injection will be carried out on both mixed-wet and oil-wet glass microfluidic chips to investigate the effect of invading phase salinity on oil recovery factor.

**Methodology**

Low salinity waterflooding (LSWF), is one type of enhanced oil recovery (EOR) technique, in which diluted brine is injected into a reservoir to produce more oil. As it is simple, economical, and environmentally friendly method, it has received the oil industry’s attention as a promising method. However, due to the complex interactions between oil, brine, and porous media, there is no agreement about the main mechanism(s) behind this EOR technique.

**Objective**

This project work intends to garner insight into the mechanisms behind low salinity water flooding on micro scale. The interfacial tension (IFT), pH and wettability variation with brine concentration at ambient condition were analysed. Moreover, a series of low salinity water injection will be carried out on both mixed-wet and oil-wet glass microfluidic chips to investigate the effect of invading phase salinity on oil recovery factor.

**Results**

Results showed that at salt concentration of 5000 and 6000 ppm, IFT between oil and aqueous phase is minimum which means that these salinities higher recovery factor is expected. Regarding contact angle measurements, in the mixed-wet system, using water with salinity of 3000 ppm, the system moved towards water-wet state. However, in all other systems wettability remained mixed-wet. In the oil-wet system, brine concentration did not have a great impact on wettability alteration. Minimum pH was obtained with distilled water which showed the highest IFT. With adding salt to the distilled water, for all samples, pH increased whilst IFT decreased. Later it will be investigated if IFT reduction and wettability alteration are effective mechanisms behind low salinity water injection on micro-scale.
Ådne Årevik Vikdal  
Department of Geoscience and Petroleum, NTNU  
Segmentation of Phases in Experimental Images of Fluid Flow using Machine Learning  
Fall 2020/Spring 2021  
Supervisor: Carl Fredrik Berg

Background

The derivation of rock and fluid properties from high-resolution images may lead to a deeper understanding of the rock properties, pore structure and the physical processes that control the transport of fluids in porous media. The segmentation of three-dimensional CT images is a cornerstone in the creation of precise digital rock models. Traditional segmentation workflows have been tedious and have been prone to operator bias since many of the steps require manual interaction and quality control.

Due to advances in computational power and convolutional neural networks, semantic segmentation with neural networks have made tremendous progress in the last few years.

Objective

This thesis will study and develop convolutional neural networks for segmenting micro-CT images, which automates the process and eliminates operator bias.

Methodology

To ensure perfect ground truths for the machine learning process, synthetic 3D micro-CT images will be used. The images will be created by making artificial bead packs and simulate fluid flow through the pore space. Image artifacts, noise and blur will be added to make the images as similar to CT images as possible.

Several neural network architectures will be trained on the ground truths, and the results will be compared.

Wenyu Zhou  
Department of Geoscience and Petroleum, NTNU  
Experimental Investigation of Osmosis and Spontaneous Emulsification Effect in the LSW Flooding  
Fall 2020/Spring 2021  
Supervisor: Carl Fredrik Berg and Mohammad Hossein Golestan

Background

The injection of low salinity water in reservoir is considered an acceptable method to enhance oil recovery. At oil-water interface, osmosis and spontaneous emulsification are two main mechanisms contributing to connate water swelling. In dead pore structure, connate water swelling can cause oil mobilization, then increasing oil recovery. However, the inner transport mechanisms for both methods are unclear. In this study, I will mainly focus on the properties of oil as semi-permeable membrane and water transportation system during the emulsification.

Experimental approach

For these purposes, a microfluidic device is used on the experiment. By creating W-O-W structure at pore throat, we can observe the interface changes only affecting by osmosis and emulsification. Light scattering and droplets observation experiments help us better understand the interface surface shape.

Results

This study verifies the osmosis effect during the LSW flooding at direct visualization aspect. Inner transportation mechanisms are still unclear. For spontaneous emulsification, extra flows were detected by adding surfactants.

Figure 1: Spontaneous emulsification enhances the water flow from LSW to HSW region, causing larger connate water swelling.

Figure 2: Simplified schematic diagram for osmosis effect and spontaneous emulsification in LSW flooding.
Chloride ingress into concrete can lead to pitting corrosion of reinforcement steel once a critical chloride threshold is reached at the boundary of the steel surface and surrounding concrete cover. This is especially crucial in environments where a lot of chloride-containing salts are present by nature or used for e.g. de-icing operations in cold climates. Reactive mass transport model that can predict ingress of such species move more and more into the focus for reliable predictions on service life of concrete structures under specific exposure conditions where chloride ingress is of major relevance. As it is of such big interest to the scientific community. However, it has been shown by several authors that also physical binding on Calcium Silicate Hydrates, that form the binding part of a concrete matrix, is of big importance in considerations towards total chloride binding capacity of cementitious material. Reactive mass transport model built for concrete service life prediction do not consider this physical chloride binding at the present point.

**Background**

Chloride ingress into concrete can lead to pitting corrosion of reinforcement steel once a critical chloride threshold is reached at the boundary of the steel surface and surrounding concrete cover. This is especially crucial in environments where a lot of chloride-containing salts are present by nature or used for e.g. de-icing operations in cold climates. Reactive mass transport model that can predict ingress of such species move more and more into the focus for reliable predictions on service life of concrete structures under specific exposure conditions where chloride ingress is of major relevance. As it is of such big interest to the scientific community. However, it has been shown by several authors that also physical binding on Calcium Silicate Hydrates, that form the binding part of a concrete matrix, is of big importance in considerations towards total chloride binding capacity of cementitious material. Reactive mass transport model built for concrete service life prediction do not consider this physical chloride binding at the present point.

**Objectives**

1. Propose a methodology for modelling of physical chloride binding based on existing literature
2. Find existing data on the topic of physical chloride binding, review it and calibrate the chosen method with the reviewed data
3. Investigating the impact of the modelling sequence in a single step sequenced model on the results

**Results**

The results received under consideration of laboratory data obtained from published studies show that in the used model the predictions by means of a modified Langmuir isotherm would always lead to an over- or underestimation of true physical bound chlorides if physical binding is considered by a modified Langmuir isotherm approach. Therefore, a careful interpretation of results is always required. A better solution might be the implementation of a surface complexation term. No implementation by means of a surface complexation approach was included but surface complexation modelling remains interesting and promising based on the theoretical background and methodology presented in this work.

**Figure 1**

Triaxial test setup. Specimen prepared with membrane and O-rings.
Background

Frozen soils are multi-phase materials consisting of unfrozen water, ice, and soil. During freezing, when water undergoes a transition into ice, the hydraulic, mechanical and thermal properties of the soil change. Therefore, it is of our interest to know the content of both frozen and unfrozen water in the frozen soil.

In this thesis, a joint electrical and acoustic measurement method is evaluated, and used to estimate the unfrozen water content based on the conducted results.

From this method, the resistivity and the P-wave velocity were obtained from the experiments, and Archie’s law and the Weighted equation were used to estimate the unfrozen water content.

It was found that when the samples froze, the resistivity and the P-wave velocity in the samples increased. At the same time, the unfrozen water content decreased. The soil type, the porosity of the soil, and the pore water salinity have a big impact on the unfrozen water content.

\[ \text{Unfrozen water content estimation based on resistivity and P-wave velocity in sand with different salinity and water content} \]

\[ \text{Unfrozen water content estimation based on resistivity and P-wave velocity in clay with different salinity and water content} \]

This effect greatly increases the rate of CO₂ dissolution compared to normal diffusion. Due to the plume dynamics, the density driven advection diffusion causes a fingering pattern, which can be realized experimentally and analyzed.

Understanding the dynamics of CO₂ advection diffusion is of great importance especially to environmental and geophysical applications. CO₂ aquifers have already been proposed as a possible candidate for long term carbon storage, so understanding their dynamics is highly relevant to today’s climate battle.
Ivar Svalheim Haugerud  
Department of Physics, University of Oslo  
Effective Diffusion in Two Dimensional Channels  
Fall 2020/Spring 2021  
Supervisors: Eirik Grude Frieckøy, Knut Jørgen Måløy and Gaute Linga

The diffusion of passive particles in the presence of a velocity field occurs in a wide range of environmental, agricultural and industrial processes. To successfully control and understand the dynamics, precise prediction of the transport is key. For such systems, one can define an effective diffusion coefficient as the proportionality of the asymptotic time scaling of the variance of the concentration. The notion of an effective diffusion coefficient has proven to be extremely useful and has therefore become the standard for quantifying the mixing properties of systems where the interplay of advection and diffusion is important. This thesis is an analytical and numerical investigation of advection-diffusion in three different scenarios.

The first is the effect of a discontinuous geometrical boundary on the effective dispersion coefficient in a two dimensional channel. Despite the ubiquity of rough surfaces and high-inertia flows in nature, it is not clear how a discontinuous boundary and an inertial fluid has on the effective dispersion. To investigate this, the effective asymptotic spreading of a passive solute in a two dimensional channel with square roughness is investigated numerically using the finite element method. The effective diffusion coefficients dependency on the boundary amplitude, Peclet number and Reynolds number is found by solving Brenner’s equations.

The second is the consequences on the effective dispersion coefficient in a channel with an oscillating body force on the fluid, and its interaction with a smoothly-varying boundary amplitude. While much is known about hydrodynamic dispersion in straight channels with an oscillating flow, there none on the effect a varying aperture will have on the mixing properties. This small geometrical change will result in much richer dynamics, with hereto unknown physics. To understand the new dynamics the investigation is both analytic and numerical. The Navier-Stokes equation is found perturbatively to second order in the boundary amplitude, and used in Brenner’s equation, for an approximate effective diffusion coefficient. The approximate result is then compared with random walk simulations, and numerical solutions of the Brenner’s equations, which we have generalized to time-dependent flows.

Lastly a completely general reciprocal relation for symmetric transport properties is investigated. In the laminar regime, flows can be reversed by inverting the external pressure. This allows for a reciprocal relation, which exactly predicts the expected concentration for specific points in the fluid. A generalization of previous work on this relationship is investigated analytically and compared to lattice-Boltzmann simulations in complex geometries. The reciprocity relation may have interesting medical, biological and industrial application, as it allows for the prediction and placement of a tracer inside an otherwise inaccessible region.

Emily Q. Z. Moen  
Department of Physics, University of Oslo  
Active Matter in Confinement  
Fall 2020/Spring 2022  
Supervisors: Luiza Angheluta-Bauer and Kristian S. Olsen

Background
The physics of active matter pertains to understanding the emergent states of matter from the coordinated dynamics of self-propelled entities. There are abundant examples of active matter across diverse biological systems from macroscopic scales, i.e. flocks of birds, school of fish, herd of sheep, etc., down to microscopic scales, i.e. bacteria colonies, tissue cells, etc. At the individual level, each self-propelled entity has the ability to consume chemical energy from the environment and convert it into motion. This gives them the property of being active and out-of-equilibrium with the environment.

In most realistic scenarios, active particles move in complex media. This complexity may range from geometric obstacles or disorder, to complete confinement. In recent studies, both of experimental and numerical nature, it has been shown that non-trivial interactions between the active particles or interactions between particles and walls give rise to interesting behaviors like particles accumulating at walls, the possibility of sorting particles with different properties or trapping particles in narrow spaces. The aim of this project is to study how self-propelled particles interact with each other and with boundaries or walls, and how confinement influences their collective behavior.

Figure: Active particles with alignment interactions that transition from a uniform state to a state of collective clockwise or anti-clockwise motion.
When two immiscible fluids flow simultaneously through a porous medium, they will self-organize into complex patterns that are describable using the language of critical phenomena. This has profound consequences for the properties of the flow. Underlying this self-organization is a competition between the viscous forces, i.e. the usual hydrodynamic forces and the capillary forces coming from the interfacial tension between the fluids and the wetting properties between the fluids and the pore walls.

When two immiscible fluids flow simultaneously through a porous medium, they will self-organize into complex patterns that are describable using the language of critical phenomena. This has profound consequences for the properties of the flow.

When two immiscible fluids flow simultaneously through a porous medium, they will self-organize into complex patterns that are describable using the language of critical phenomena. This has profound consequences for the properties of the flow.
Proposed Master Project at PoreLab NTNU (department of Physics)

**Swelling of Shale: Effect of composition and microstructure**

**Contact:** Srutarsi Pradhan ([Srutarsi.Pradhan@ntnu.no](mailto:Srutarsi.Pradhan@ntnu.no)) and Basab Chattopadhyay ([basab.chattopadhyay@ntnu.no](mailto:basab.chattopadhyay@ntnu.no))

**Background:** Swelling of Shale-rocks create several problems [1] during underground drilling operations, such as stuck-pipe or bit. The field experience reveals that some shale-rocks are good candidate for swelling and some are not. There are several parameters that can influence the swelling behavior, such as: porosity, clay-quartz contents, etc. In addition, shale-microstructure must have an important role on swelling/deformation behavior of shale.

**Problem formation:** To investigate shale-swelling problem we have introduced a discrete element model (DEM), based on Monte-Carlo technique. We define a probability of swelling for all the clay grains in the shale-rock sample that includes the effect of stress-difference, porosity, temperature etc. The time evolution of grain swelling results in bulk swelling behavior of the sample and the simulation result qualitatively matches [2] with the observations of shale/clay swelling experiments [3,4].

The aim of this Master project is to investigate the role of clay-quartz composition and clustering on the shale-swelling behavior. The student will do experimental work in the X-ray physics group (PiP) to extract the composition and microstructure [5] in representative shale rocks using X-ray computed tomography (X-ray CT). The experimental data will eventually be used directly in the DEM code. The DEM simulation codes are developed in-house and are available for re-use and further improvement.

**Other aspects:** As this project is linked to practical field operations, we would like to develop a researcher proposal for NFR next year. Results from the Master project will be used in the proposal as important ground works and the Master student will be encouraged to join the researcher project if he/she wishes to pursue a research career on this topic.

**References:**

[4] T. Risnes, “Fracturing in ice”. The Master student can be included in this project if he/she likes to pursue a research career on this topic.

**Workload:** Master Thesis (30 ECTS)

**Requirement:** Basic knowledge of computer programming

**Resources:** None

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Proposed Master Project at PoreLab NTNU (department of Physics)

**Fracture Propagation During Fluid-Injection**

**Contact:** Srutarsi Pradhan ([Srutarsi.Pradhan@ntnu.no](mailto:Srutarsi.Pradhan@ntnu.no)) and Alex Hansen ([Alex.Hansen@ntnu.no](mailto:Alex.Hansen@ntnu.no))

**Background:** Fluid injection operations [1] are regularly done in several field case scenarios like petroleum production, geothermal installation, ground-water exploration and underground CO₂ storage. Normally fluids with high pressure are injected inside porous rocks through the injection wells and sometimes fractures open-up at the well-boundaries. We need better understanding of physical processes that guide fracture propagation in porous media and we also need to develop tools for monitoring fracture propagation. Several lab experiments [2,3] have explored the stress-induced fracturing behavior of number of reservoir rocks during fluid injection scenarios.

**Problem formation:** We have developed a discrete element model (DEM) simulation code based on Invesion percolation and distance dependent stress intensity factor (K) to mimic the stress-induced fracturing of porous rocks. Our simulation code can handle the presence of pre-existing fractures inside the sample. The simulation results agree qualitatively [4] with the experimental observations.

In this Master project, the student will study the stress-induced fracturing with several important inputs like tensile strength distribution, breaking criteria, porosity, sample size, pressure etc. The DEM simulation codes are developed in-house and are available for re-use and further improvement.

**Other aspects:** Although fractures are mostly seen as “disturbing elements” for the stability of wells and well-operations, in some cases fractures are “intended” for example, in hydraulic fracturing scenario people create fractures to increase permeability (flow channels) in the porous rocks. Creation of optimal flow channels is also the main goal for geothermal projects to enhance power production and thereby to contribute in the Green-energy-sphere. PoreLab is now developing a research proposal together with Institute of Geophysics, Warsaw on “Fracturing in ice”. The Master student can be included in this project if he/she wishes to pursue a research career on this topic.

**References:**


**Workload:** Master Thesis (30 ECTS)

**Requirement:** Basic knowledge of computer programming

**Resources:** None

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![Fig: DEM model for Shale rock sample with clay and quartz grains (left). Macrostructure-analysis shows clay-clustering (middle). Cross-section of Pierre Shale imaged by coherent diffraction imaging (5) (right).](image1)

![Fig: Fracture propagation in a DEM with no pre-existing fractures (left) and in a DEM with 6 pre-existing fractures (right).](image2)
Proposed Master Project at PoreLab NTNU (department of Physics)  
**Understanding non-Newtonian materials**  
Contact: Rafaela Cabrilo (rafaela.cabrilo@ntnu.no or raffaela.cabrilo@epfl.ch), Astrid de Wijn (astrid.dewin@ntnu.no) and Erika Eisler (ee247@cam.ac.uk)

Motivation  
Non-Newtonian fluids are ubiquitous in everyday life, but the understanding of the fundamental physical process underlying their properties still remains a big challenge [1]. Why are we able to walk (yes, you can) on a pool filled by a mixture of cornstarch and water or why toothpaste behave as a liquid when squeezed or sheared? Depending on the applied external force, yield stress materials behave solid- or liquid-like, undergoing peculiar transformations in their dynamics with increasing external load.

Your Project  
In this project you will study the stress-strain curves for a Yukawa binary colloidal system representing a typical yield stress material [2]. In particular, the effect of different friction coefficients and damping parameters on the stress-strain curves will be investigated using Molecular Dynamics simulation. The results will help rationalize complex, irreversible phenomena such as aging and creep in disordered system.

**Requirements**  
Background in Soft matter physics would be advantageous. We would like a person interested in modeling, simulation and programming able to work independently. Experience with C/C++ or Python are essentials.

**References**  

Proposed Master Project at PoreLab NTNU (department of Physics)  
**Dynamics of granular anisotropic shapes - Experiments & Simulations**  
Contact: Erika Eisler (ee247@cam.ac.uk), Astrid de Wijn (astrid.dewin@ntnu.no) and Raffaela Cabrilo (rafaela.cabrilo@ntnu.no or rafaela.cabrilo@epfl.ch)

Motivation  
Today it is possible to design and self-assemble Y- and X-shaped nanostars from DNA [1,2]. While in dilute solution they do not change their shape, in granular form they rotate freely, thus leading to a strong non-Newtonian behavior. You can work on the theoretical foundation of Soft Matter physics or do experiments and subsequently analyzing videos of these systems. The results will be used to derive dynamic information, such as the translational and rotational motion of the particles as function of concentration and other parameters. A simulation study is possible if preferred.

**Requirements**  
Background in Soft Matter physics would be advantageous. We would like an applicant who is interested in setting up the experiments and/or simulations.

**References**  

Proposed Master Project at PoreLab NTNU (department of Mechanical and Industrial Engineering)  
**Modelling of strengthening mechanisms in Aluminum alloys**  
Contact: Astrid de Wijn (astrid.dewin@ntnu.no), Inga Ringbø (ingga.ringbo@sintef.no) and Randi Homestad (randi.homestad@sintef.no)

Norway is a major producer of aluminum alloys and has several producers of aluminum products for the car industry. In this project, you will work in the nanoscale detailing of the plasticity and strengthening of aluminum alloys. To increase the strength in aluminum alloys, alloying elements are added. In addition, the material is heat treated after production. The heat treatment will result in the formation of small ordered particles coherent with the aluminum lattice. These particles can be as small as a few nanometer but are still detrimental for the strength of the alloys. During plastic deformation, dislocations travel through the aluminum lattice and will meet these particles. Depending on the size, the dislocations may either loop or shear the particle. In this project, you will study the energetics of different possible pathways for a dislocation shearing a particle in an 6xxx aluminum alloy (Al, Mg, Si) using molecular dynamics and atomistic theories. You will employ the existing open-source molecular dynamics code LAMMPS in combination with python scripting to create the models and to analyze the results.

**Required background**  
Basic material science. A basic programming course and an interest in modelling.

**Supervisors**  
Astrid S. de Wijn (astrid.dewin@ntnu.no), Inga Ringbø (ingga.ringbo@sintef.no) and Randi Homestad (randi.homestad@sintef.no)

**Research environment**  
http://syonax.net/science/research.html

**Work load**  
This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

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Proposed Master Project at PoreLab NTNU (department of Mechanical and Industrial Engineering)  
**Simulating the contact mechanics of hydrogels**  
Contact: Astrid de Wijn (astrid.dewin@ntnu.no) and Alex Hansen (alex.hansen@ntnu.no)

This project is concerned with the contact mechanics of hydrogels at the micron length scale. Hydrogels are random networks of long hydrophilic polymer chains surrounded by a water. They have many applications, especially in medicine. They are for example used in wound dressing, tissue engineering, and drug delivery.

**The goal of the project is to simulate the contact mechanics of hydrogels.** To this end, you will start from the existing molecular dynamics code written in C++ by a previous student and external collaborator Martin Møller. The code needs to be extended to include additional physical effects that are crucial for viscoelastic behavior of gels. You will then use this program to perform indentation and sliding simulations. You will study how the polymer network deforms and how the polymer concentration changes under strain. The simulations can be used to test theories how shear and normal stresses depend on crucial parameters, in particular, on the cross-link density of the polymer network.

**Required background**  
A basic programming course and an interest in modelling or programming.

**Supervisor**  
Astrid S. de Wijn (astrid.dewin@ntnu.no), Alex Hansen (alex.hansen@ntnu.no)

(Who will be the main supervisor depends on the department of the student.)

**Research environment**  
http://syonax.net/science/research.html

**Work load**  
This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

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**Figure:** Molecular dynamics simulation of a nanodispersion of aluminum containing particles. The lines visualize the dislocations and the dots are Mg-Si particles.
Proposed Master Project at PoreLab NTNU (department of Mechanical and Industrial Engineering)

Modelling extremely low friction of quasicrystals
Contact: Astrid de Wijn (astrid.dewijn@ntnu.no)

In this project, you will focus on a particular class of crystalline materials that have an unusual structure: quasicrystals. The discovery of quasicrystals was awarded the Nobel Prize in chemistry in 2011. The project is concerned with how the quasi-crystal structure will affect the friction of these surfaces, through structural superlubricity. This is a dramatic effect by which friction is reduced enormously due to structural incompatibility between two surfaces at the atomic level. You will write a simple numerical simulation to compute interactions of contacts with quasicrystalline surfaces, and whenever possible do analytical calculations to accompany them.

Required background
Tribology or classical mechanics. A basic programming course and an interest in modelling or programming.

Supervisor
Astrid S. de Wijn, astrid.dewijn@ntnu.no

Work load
This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

Proposed Master Project at PoreLab NTNU (department of Mechanical and Industrial Engineering)

Numerical simulations confirming lost derivation of viscosity
Contact: Astrid de Wijn (astrid.dewijn@ntnu.no)

This project is concerned with the viscosity of fluid mixtures. The viscosity of a fluid is one of the most obvious properties when you interact with it. Consider for example the difference between air and water. Air has a lower viscosity than water, so it is easier to walk through air than walk through water. Viscosity is also an important factor in energy consumption. Of all energy generated in the world, 20% is lost to friction, and much of that is due to viscous losses in lubricants. Because of this, engineers are always on the hunt for novel ways to improve lubricants. Developing theoretical models for understanding viscosity will aid in this search. There is an extremely important expression for the viscosity of liquids that we cannot verify, because the derivation has been lost. In the 1950’s Thorne derived an expression for the viscosity of dense mixtures of hard spheres. He communicated the result to some of his colleagues, but not the derivation, and sadly passed away before publishing it. The equation was never really verified and because the theory is quite challenging, no one has ever been brave enough to try to re-derive the result. Nevertheless, Thorne’s expression is used in practical engineering applications where it is simply assumed that he didn’t mess up. The goal of this project is to verify Thorne’s expression for the viscosity of dense fluids using numerical simulations. In the first stage of this project, you will set up and perform molecular dynamics simulations of mixtures of hard spheres and compute their viscosity, to compare it to the theoretical expression. Later on, we will move on to more realistic interactions. Given the importance of Thorne’s result, it is likely that this work will lead to a publication.

Required background
Statistical mechanics or thermodynamics. A basic programming course and an interest in modelling or programming.

Supervisors
Astrid S. de Wijn (astrid.dewijn@ntnu.no)
Raffaella Cabrini (raffaella.cabrini@ntnu.no)
Christopher Fjeldstad (christopher.fjeldstad@ntnu.no)

Research environment:
http://www.mech.ntnu.no/research.html

Resources
The project will make use of high performance computing resources that are already available through NTNU’s HPC facilities and Sigma2.

Work load
This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

Proposed Master Project at PoreLab NTNU (department of Chemistry)

Thermal Osmosis
Contact: Professor Signe Kielstrup (signe.kielstrup@ntnu.no)

It has recently been found that hydrophobic membranes with pores of nanometer size will not transport water in the liquid state, but rather in the vapor state, when surrounded by water solutions at different temperatures. This opens up for a very interesting way to clean contaminated water by means of industrial waste heat. The figure illustrates an invention that puts this into practice. Water is transported against a pressure gradient by means of a temperature gradient. This is what we understand as thermal osmosis.

Problem formulation
The mechanism for water transport in the membrane that is used in the invention is little understood. The aim of the project is to help us understand how exactly (with what speed) water is passing the membrane. By understanding the transport better, we hope to improve conditions for it. The work will consist of setting up a NEMD model for water transport across a narrow pore, and study of the wall and pore shape affects the transport under relevant temperatures and pressures.

Other aspects: This study will benefit from similar simulation studies. The project will also benefit from experimental activities in our group (one Master student and partner in Spain).

Reference:
Peltier heat and Dufour effects in lithium-ion batteries

Contact: Prof. Signe Kjelstrup (Signe.Kjelstrup@ntnu.no) and Astrid F. Gunnarshaug (astrid.f.gunnarshaug@ntnu.no)

Temperature is known to be of importance for the ageing, performance, and safety of lithium-ion batteries. The heat released or absorbed inside a battery has therefore been a topic of much interest. The heat released or absorbed reversibly with the cell reaction at the two electrode interfaces, an effect known as Peltier heating. The Dufour effects in the electrolyte will also affect the electrode surface temperature. [1]

The Peltier heat is obtained experimentally by measuring the Seebeck coefficient, the reciprocal effect. The electromotive force, emf, of a thermoelectric cell (a cell with two of the same electrodes) with an applied temperature difference is measured. The Dufour effect is similarly obtained through the reciprocal Soret effect, which is simultaneously found through the time-variation of the emf in the same measurement. The setup is illustrated in the figure using the lithium metal thermoelectric cell as an example.

Project formulation

Only a few values for Peltier heats and Dufour effects has been reported. [2,3] These effects are of import for thermal modelling. [1] The aim of the project is to help mend the situation. The work will consist of making thermoelectric cells using lithium-ion battery materials and measure the Seebeck coefficient.

References

1. L. Spitzhofer, A. F. Gunnarshaug, D. Bedeaux, D. S. Burton, S. Kjelstrup, Peltier effects in lithium-ion battery modelling, accepted

Proposed Master Project at PoreLab NTNU (department of Chemistry)

Soret effects in porous media for Li-batteries

Contact: Associate Professor Anders Lervik (Anders.Lervik@ntnu.no)

Background: The heat evolution in Li batteries need to be controlled to understand why the battery sometimes overheat and catch fire in the surroundings. During the course TKJ4200, the Soret effect was investigated in an electrolyte mixture of components, LIPPP, ethylene carbonate and di-methyl carbonate. The investigation was done with LAMMPS's software. The study showed that it was likely that all components were moving in a thermal field. The results were not conclusive, however, and we would like to verify them.

Problem formulation: In order to reach valid conclusions, it is an advantage to build the system gradually and introduce new variables in a stepwise manner. It is thus interesting to study the single components, before a mixture, and a mixture before a ternary mixture. We will study all 4 cases in equilibrium in order to characterize the equilibrium state. When that is known, we apply the temperature gradient, and find the Soret coefficient for each of the systems.

Other aspects: The student will benefit from similar studies going on in the group, from experimental as well as computational activities on pore systems (one Master student, Gunnarshaug, and students working on Seebeck coefficient problems).

Fig 1. The electrolyte and electrodes in a Li battery. Sosnati et al: Li-batteries, 2013

Proposed Master Project at PoreLab NTNU (department of Geoscience and Petroleum)

Fluid distribution simulation

Contact: Carl Fredrik Berg (carl.berg@ntnu.no) and Hamidreza Erfani Gahrooei (hamidreza.erfani@ntnu.no)

In this project the candidate should simulate fluid distributions in digital images of porous media. From micro-CT imaging, we have images of fluid distribution at different wetting conditions inside the pore system. The candidate should use the software package “surface evolver” to simulate fluid distributions inside the same pore space at different wetting conditions and compare the simulated results to the images.

Supervisors: Hamidreza Erfani Gahrooei and Carl Fredrik Berg

Simulation of single-phase flow

Contact: Carl Fredrik Berg (carl.berg@ntnu.no) and Per Arne Slotte (per.slotte@ntnu.no)

In this project the candidate should compare methods for simulating single-phase flow on digital images of porous media. These images are obtained by micro-CT scanning, and are regular grids where each grid cell is either a pore or solid. There are several software packages available, with a range of underlying solution methods and grid complexity. As we will solve the problem on a regular grid, the candidate will determine if the added complexity of more versatile grid models leads to different results. Further, the solutions should be compared to analytical solutions.

Supervisors: Carl Fredrik Berg and Per Arne Slotte.
The capillary desaturation (CDC) curve correlates how the residual oil saturation depends on the capillary number (ratio of viscous and capillary forces), mainly for water wet systems. This concept is applied in simulation tools to adapt the end point saturations of the relative permeability curves, dependent on how either viscous or capillary force are changing e.g. by implemented EOR methods. The CDC curves are measured in the lab, determining residual oil saturation as a function of flow rate. The question is when this concept of CDC curves is applicable.

How to use this concept if the wettability changes? Can variations in CDC curve tell anything on the wettability distribution within the core? To start answering these questions, a literature study shall collect knowledge available. The study shall explore the use and dependencies of CDC curves measured, e.g. dependencies on wettability. Micromodels and core-flooding will be used to further explore the effect of wettability on the CDC curve.

Relative permeability curves can be determined by performing unsteady state relative permeability measurements. The determination of the core saturation is hereby critical. The production monitoring of core flooding experiments often comes with a large uncertainty. The use of partitioning and none partitioning tracers can potentially be used as a second additional method for saturation determination. The idea is that by monitoring the arrival of the different tracers and the use of tracer modelling more accurate instat saturations can be derived.

Simulations in CMG stars or a similar modelling tool shall verify the possibility of use of partitioning tracers in core flooding. Experiments with modelling of unsteady state flooding experiments shall show the proof of concept in the lab.

The invasion of porous media flows is a topic of pivotal importance for several aspects of human activity. The extraction of water from natural reservoirs and the recovery of oil from subsea rocks are two examples where the knowledge of porous media physics brings immediate economical and societal impact. Since the visualization of flows in porous media can be very challenging, numerical simulations have been used to study the morphology and dynamics of flow structures both in fast and slow injection processes. With the development of modern high-resolution and high-speed imaging techniques, we are now in position to address experimentally questions, that previously could only be accessed via numerical simulations. In this project we will investigate, both experimentally and analytically, how the invasion dynamics of a pore is affected by speed of the flow.

The investigation of porous media flows is a topic of pivotal importance for several aspects of human activity. The extraction of water from natural reservoirs and the recovery of oil from subsea rocks are two examples where the knowledge of porous media physics brings immediate economical and societal impact. One point that makes experiments in porous media particularly challenging is the fact that natural porous media, such as soils and rocks, are never transparent. By using artificial micromodels, one can overcome this challenge. In this project we will perform experiments in which one fluid will displace another in a quasi-2D porous network. We will take pressure measurements and images of the flow simultaneously and we will try to correlate the outcomes of these two measures. One of the main objectives is to try to use the fluctuations in the pressure signal to obtain indirect information about the properties of the porous network (such as its porosity) and the fluids involved (such as their viscosity contrast). This can provide the means for the development of new measuring techniques based on the pressure signal only, which can be further employed in the investigation of natural porous media.

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PoreLab offers a range of courses open for all students at our host universities. The two first courses, PoreLab course 1 and PoreLab course 2 are jointly organized between NTNU and UiO. They were adapted to PoreLab with a special focus on porous media.

**PoreLab Course 1 - Theory and Simulation of Flow in Porous Media**

The course aims at giving the students basic knowledge of numerical simulation of fluid flow in petroleum reservoirs. Students will understand partial differential equations for single phase and multiphase flow in porous materials, and numerical solution methods of these using finite difference and finite element methods. Students will be able to use common modeling tools for numerical prediction of reservoir behavior. They will be able to do derivation of equations for flow in porous media, and numerical solution of these equations.

**PoreLab Course 2 - Experimental Techniques in Porous and Complex Media**

The course aims at giving the students basic knowledge of numerical simulation of fluid flow in petroleum reservoirs. Students will understand partial differential equations for single phase and multiphase flow in porous materials, and numerical solution methods of these using finite difference and finite element methods. Students will be able to use common modeling tools for numerical prediction of reservoir behavior. They will be able to do derivation of equations for flow in porous media, and numerical solution of these equations.

**PoreLab Course 3 - Chemical Engineering Thermodynamics**

The objective of the course is to teach fundamental techniques as an aid for further studies in reservoir engineering and related subjects. The students learn basic theory to determine reservoir properties on one- and two-phase flow in subsurface reservoirs and will be able to do reservoir simulation and conduct basic measurements in a core lab.
Numerical Methods in reservoir Simulation
PG8607, NTNU
The course gives an introduction to the various numerical formulations applied in reservoir simulators. The course contains:
- Difference methods.
- Control-volume method.
- Time integration.
- Linear equation solvers.
- Stability and numerical dispersion
By completing the course, the candidate will have a deeper understanding of the mathematical building blocks that goes into various reservoir simulators, different numerical representations and solution methods.

Disordered systems and percolation
PYS4460/PYS4460, UiO
The course provides an introduction to methods and problems in modern statistical physics with emphasis on algorithmic and computational methods. The applications addressed and the computational methods introduced are relevant for material science, complex systems, chemistry, solid-state, molecular, and bio-physics.
The course aims to build understanding for the macroscopic effects of microscopic interactions using numerical simulations of microscopic models, coupled with a concurrent development of a relevant theoretical framework.

Statistical Mechanics
FY54130, UiO
This course will give the student a thorough introduction to thermodynamics and statistical physics, with an emphasis on the fundamental properties of gases, liquids and solids. The course also gives a theoretical foundation for further studies of systems with many particles or degrees of freedom.
By completing the course, the student will be able to compute (numerically and analytically) thermodynamic quantities and correlation functions for quantum mechanical and classical models in statistical mechanics using various techniques and approximations. The student will gain experience with models of gases, liquids, electrons in materials, lattice vibrations, and magnetism as well as being able to deduce and mathematically transform thermodynamic identities. The student can also use thermodynamic stability criteria, and you can characterize phase transitions. The student will have knowledge about terms and concepts related to the renormalization group (RG) and use it to construct various Monte Carlo algorithms.

Condensed Matter Physics II
FY59430, UiO
The course presents an overview of some functional materials and their properties, mainly seen from an experimental viewpoint. Some central theories, which describes the properties of the materials and their response to external impact, will be discussed. Topics that will be covered include dielectric materials, magnetic materials, superconductors as well as selected topics within micro- and nanostructured materials.
The subject will be useful for gaining an understanding of the interplay between classical and quantum mechanical phenomena and clarify how microscopic/atomic processes give rise to the typical properties of different materials.
By completing the course the student will have a broad knowledge of the core areas of condensed matter physics and materials science, as well as a good understanding of the physical basic principles behind the properties of different types of functional materials and some micro/nanostructured materials.

Photo on the right: PhD candidate Astrid Fagertun Gunnarshaug at the Department of Chemistry, NTNU, working with thermoelectric cells for lithium-ion battery research in the laboratory with glovebox.
Porous Media Laboratory
NTNU, UiO

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