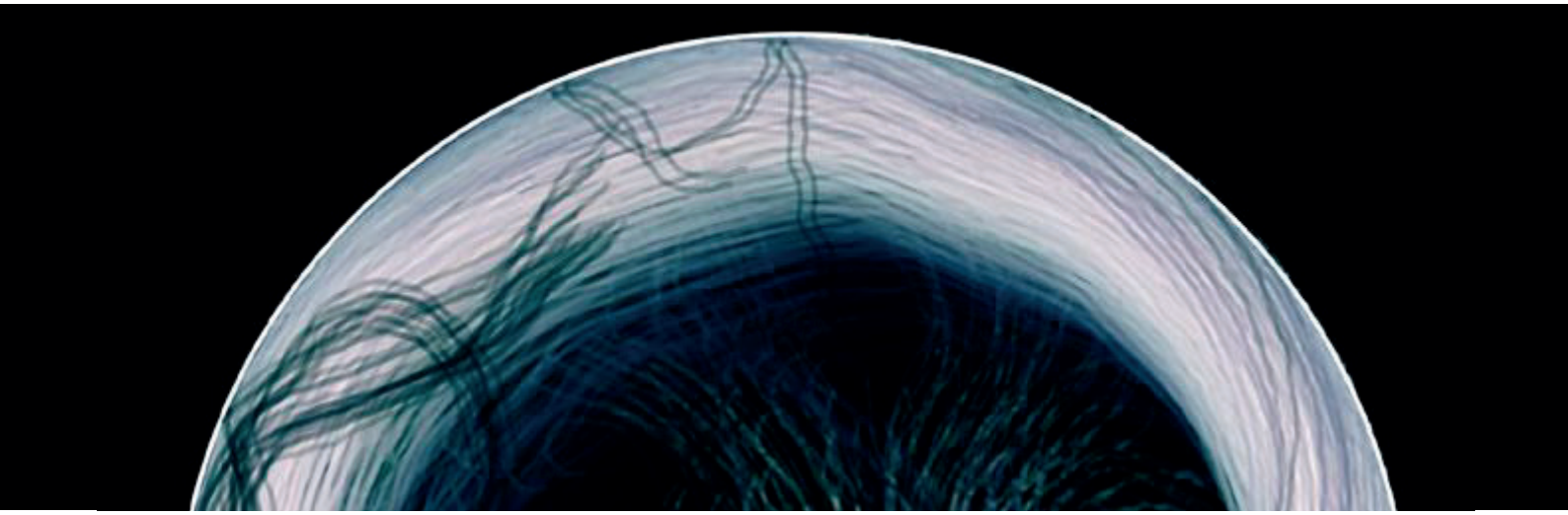
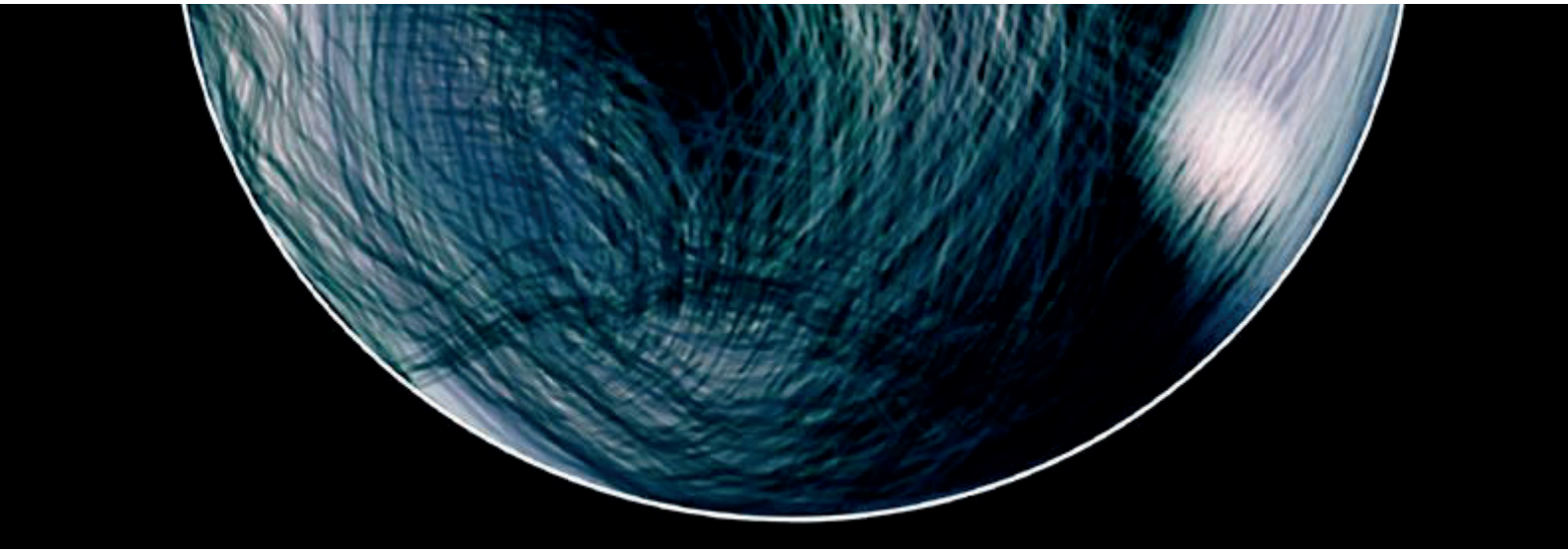
PoreLab
NTNU-UiO Porous Media Laboratory

Norwegian Centre of Excellence
The Research Council of Norway



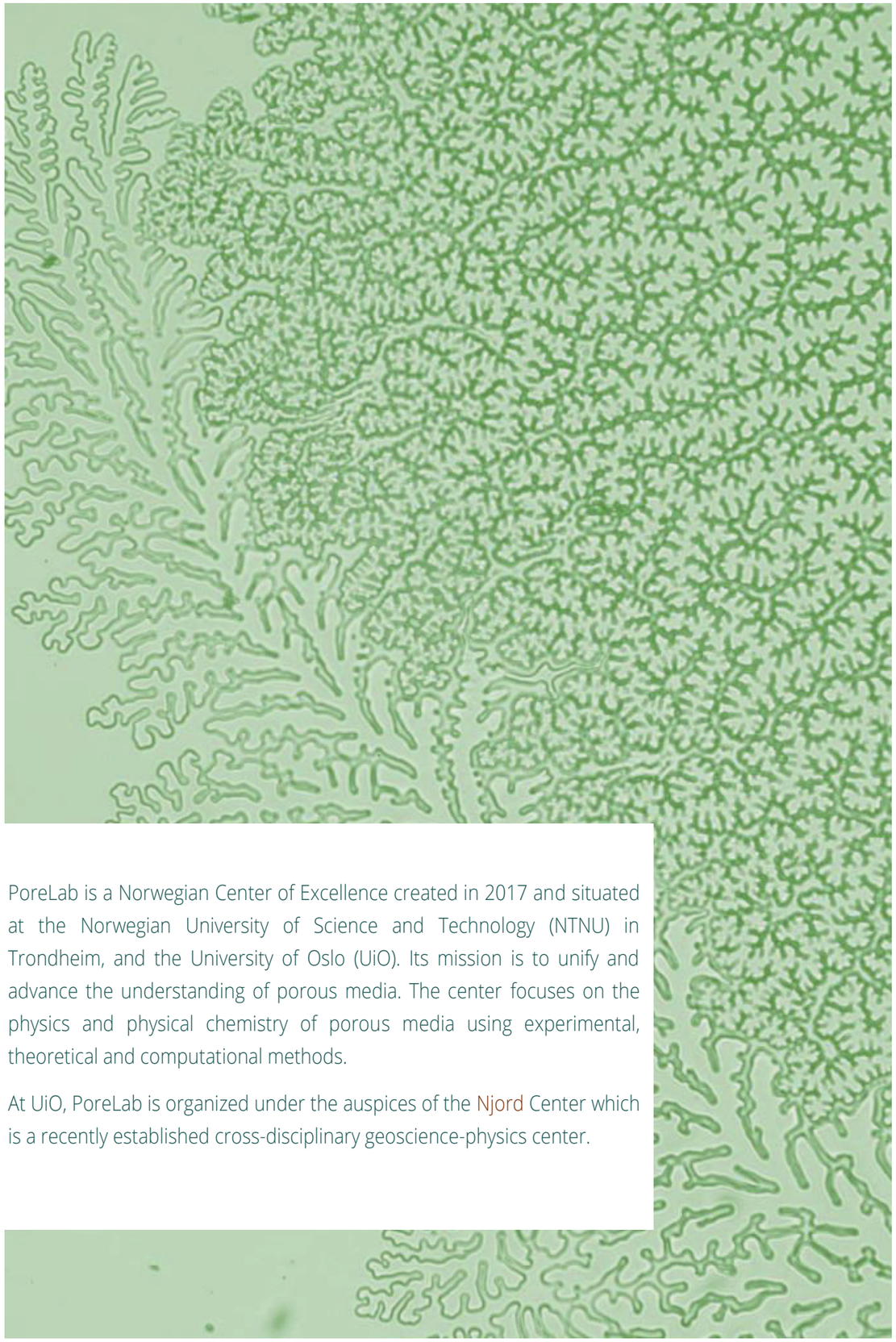
MSc at PoreLab 2020

Opportunities in 2021



NTNU
Norwegian University of Science and Technology

UiO : University of Oslo



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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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.

Overview – 2020 MSc students

Name	Title Master thesis	supervisors
Yngve Nylund Arnestad	Advanced CT Studies of Deformation Mechanics	Ragnvald Mathiesen and Dag W. Breiby
Elias Hvideberg	Molecular Dynamics Simulation of the Contact Mechanics of hydrogels	Astrid de Wijn and Alex Hansen
Marthe Brevig	Monte Carlo Simulation of Immiscible Two-Phase Flow in Porous Media	Alex Hansen and Santanu Sinha
Carlos Martínez Mingo	Ultrastructure Analysis of Gallbladder Stones using Computed Tomography	Basab Chattopadhyay and Dag W. Breiby
Martin Alexander Toresen	Swelling of Clay/Shale: A numerical investigation	Srutarshi Pradhan
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Mina Sørensen Bratvold	The Permeability of Porous Media as Studied by NEMD	Signe Kjelstrup, Michael Tobias Rauter and Olav Galteland
Peder Langsholt Holmqvist	Non-Isothermal Transport in Cation-Exchange Membranes: The Seebeck Effect in Systems of Ions Abundant in Seawater	Signe Kjelstrup and Kim Roger Kristiansen
Sebastian Nordby Price	Improving the Perturbation Theory for Mixtures Described by Lennard-Jones Potential with Large Differences in Well-Depths	Anders Lervik and Øivind Wilhelmsen
Kevin Kottakkakathu Varughese	Nanothermodynamics of a Single-Phase Fluid Confined in Complex Porous Medium	Signe Kjelstrup, Olav Galteland and Michael Tobias Rauter
Daniel Tianhou Zhan	The First Steps Towards a Perturbation Theory for Small Systems	Anders Lervik and Øivind Wilhelmsen
Gbadebo Nafiu Adejumo	Experimental Study on the Effect of Low Salinity and Ionic Composition on Wettability Alteration in Carbonates	Carl Fredrik Berg and Antje Van der Net
Fadhil Berylian	Calculation and Visualization of Energy Dissipation and Energy Balance in Reservoir Models	Carl Fredrik Berg
Anna Bjørke Kallestad	Geochemical Modeling of Low Salinity Water Flooding	Ashkan J. Ghahfarokhi
Raymond Mushabe	Effect of Water Quality on Spontaneous Imbibition into Carbonate Cores	Carl Fredrik Berg and Antje Van der Net
Shirin Safar Zadeh	Appraisal of Low-Salinity EOR on Micro-Scale: Effect of Brine Concentration on Interfacial Tension, Contact Angle, and pH	Ole Torsæter
Ådne Årevik Vikdal	Segmentation of Phases in Experimental Images of Fluid Flow using Machines Learning	Carl Fredrik Berg
Wenyu Zhou	Experimental Investigation of Osmosis and Spontaneous Emulsification Effect in the LSW Flooding	Carl Fredrik Berg
Marvin Glissner	Service Life Prediction of Concrete in Cold Climate, Benchmarking of Chloride Ingress Simulations	Mette Rica Geiker, Alexander Michel and Victor Marcos Meson
Morten Hovind and Kjetil Lien	Parametric Study of Mechanical Properties for Saline Frozen Clay	Rao Martand Singh and Chuangxin Lyu
Tonje Roås Mikalsen	Estimation of the Unfrozen Water Content Based on a Joint Electrical and Acoustic Method	Ali Amiri
Hilmar Yngvi Birgisson	Density Driven CO_2 Advection Diffusion	Knut Jørgen Måløy and Eirik G. Flekkøy
Ivar Svalheim Haugerud	Effective Diffusion in Two Dimensional Channels	Knut Jørgen Måløy, Eirik G. Flekkøy and Gaute Linga
Emily Q.Z. Moen	Active Matter in Confinement	Luiza Angheluta-Bauer and Kristian S. Olsen

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 cancerogeneous 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

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 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 aims 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.


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A glimpse of students' activities at PoreLab! The 4 pictures above date from 2019. All meetings in 2020 were organized online due to the containment measures following the virus outbreak. 1. Pore Buzz in October 2019, a gathering for the juniors with the hottest research topics and pizza. 2. Srutarshi, Hossein, Giulio and Michael take a break. 3. Internal seminar 4. Jonas, Louison, Kristian and Beatrice playing Pictionary

Yngve N. Arnestad

Department of Physics, NTNU

Advanced CT Studies of Deformation Mechanics

Fall 2019/ Spring 2020
Supervisors: Ragnvald Mathiesen and Dag W. Breiby

Background

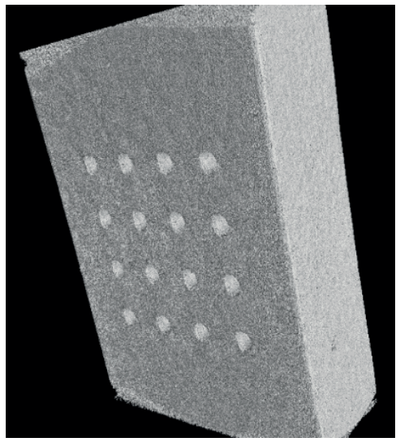
In-house X-ray computed tomography is a well-established method for 3D imaging. Conventionally data sampling is rather time consuming, preventing the use of such methods to follow structure dynamics beyond the hour time scale in situ. However, in most cases, tomography data is vastly oversampled, opening 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 Claussen from the Centre for Advanced Structural Analysis (SFI CASA) at the Department of Structural Engineering, NTNU.

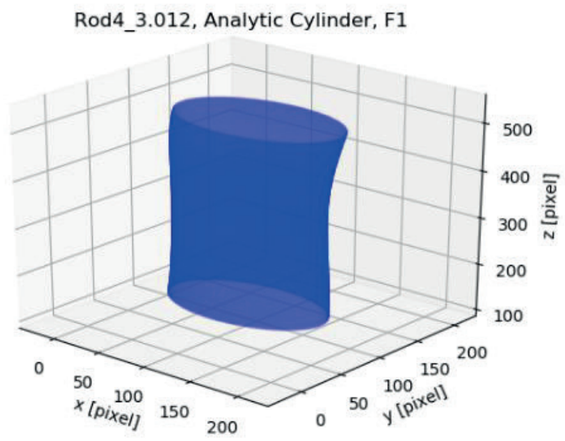
Goal

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 3-4 D 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.

Methodology

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.





Elias Nilsen Hvideberg

Department of Physics, NTNU

Molecular Dynamics Simulation of the Contact Mechanics of Hydrogels

Spring 2020
Supervisors: Astrid de Wijn and Alex Hansen

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 biocompatibile 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.

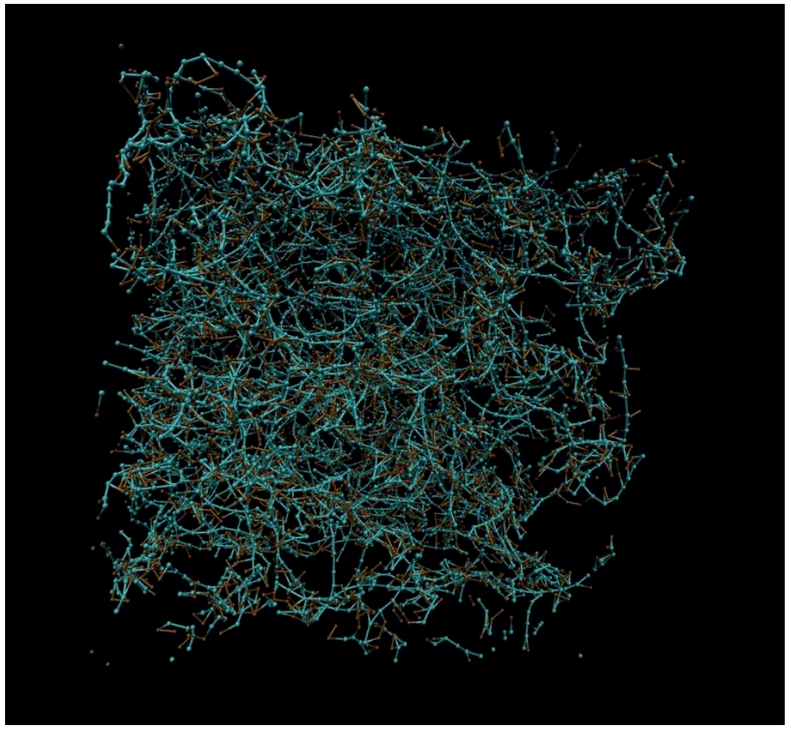


Figure 1: *Visualization of a hydrogel simulated by molecular dynamics. The visualization tool used is VMD.*

NTNU - Department of Physics

Marthe Brevig

Department of Physics, NTNU

Monte Carlo Simulation of Immiscible Two-Phase Flow in Porous Medias

Fall 2020/Spring 2021
Supervisors: Alex Hansen and Santanu Sinha

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.

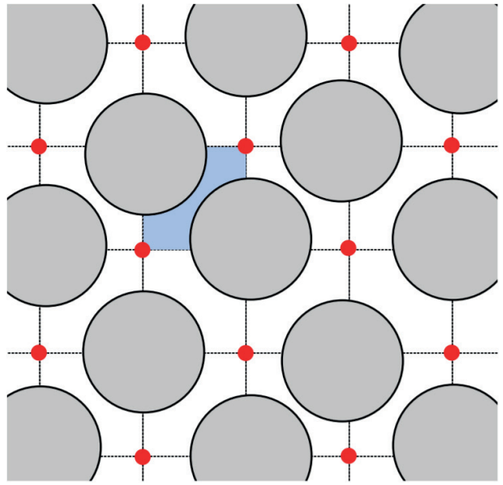


Figure 1: *An example illustration of the porous media modelled by the dynamic pore network model. The grey circles are solids while white area are hourglass shaped pore links between the solids. The red dots are the nodes connecting the links. The blue area is an example of the pore volume that belongs to one single link.*

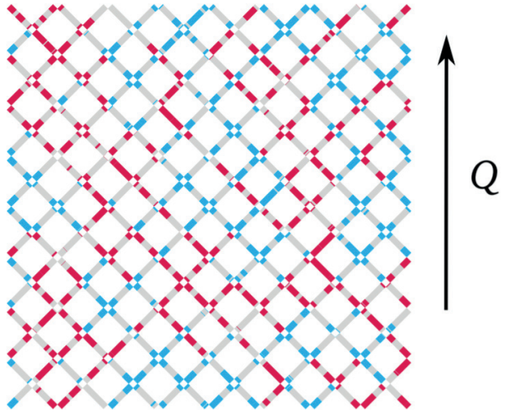


Figure 2*: An example figure of the network model with clusters of flow-highways. The links are oriented with 45 degrees and filled with wetting fluid (grey) and non-wetting fluid (red/blue). The clusters of flow-highways consist of the links in red. The fluid flow in upward direction.*

Carlos Martínez Mingo

Department of Physics, NTNU

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.

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

[1] Taton G., Rokita E., Wróbel A., Beckmann F., Thor P., Worek M. (2009) Analysis of renal calculi structure with the use of X-ray microtomography. In: Dössel O., Schlegel W.C. (eds) World Congress on Medical Physics and Biomedical Engineering, September 7 - 12, 2009, Munich, Germany. IFMBE Proceedings, vol 25/4. Springer, Berlin, Heidelberg

[2] Manzoor MAP, Agrawal AK, Singh B, Mujeeburahiman M, Rekha P-D (2019) Morphological characteristics and microstructure of kidney stones using synchrotron radiation μCT reveal the mechanism of crystal growth and aggregation in mixed stones. PLoS ONE 14(3): e0214003 https://doi.org/10.1371/journal.pone.0214003

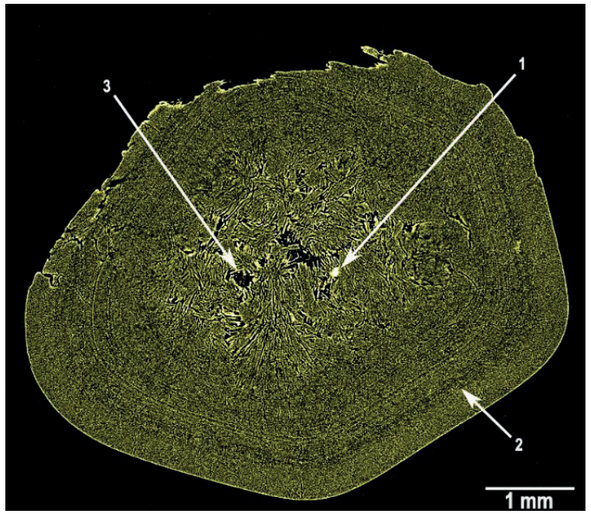


Figure 1*. Reconstructed slice of a gall bladder stone. Note the central apatite nucleation center (1), concentric outer growth layers of alternating density (2), and also cracks and pores (3).*

Martin Alexander Toresen

Department of Physics, NTNU

Swelling of Clay/Shale: A numerical investigation

Fall 2020/Spring 2021
Supervisors: Srutarshi Pradhan

Background

Swelling of Shale-rocks create several problems [1] 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 [2] 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

[1] E. Fjær, R. M. Holt, P. Horsrud, A. M. Raaen and R. Risnes, Petrolum Related Rock Mechanics (Elsevier, 2008).
[2] S. Pradhan, Swelling behavior of shale/clay: Discrete element modeling, based on Monte-Carlo technique, Interpore 2019, Valencia, Spain.
[3] M. Deriszadeh and R.C.K. Wong, Transp Porous Med (2014) 101:35–52 DOI 10.1007/s11242-013-0229-8.
[4] E. Rybacki, J. Herrmann, R. Wirth and G. Dresen, Rock Mech Rock Eng (2017) 50:3121–3140

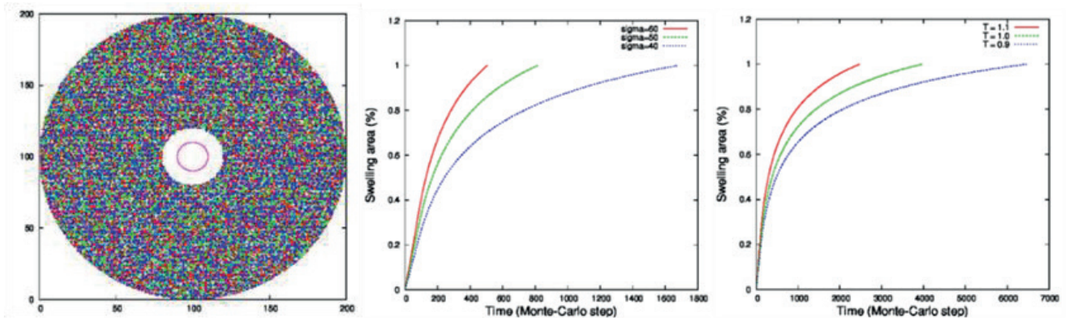


Figure: *The DEM model for Shale rock sample with clay and quartz grains (left). Swelling amount with time for different stress levels (middle) and temperature levels (right).*

Fredrik Rosenberg

Department of Physics, Department of Mechanical and Industrial Engineering, NTNU

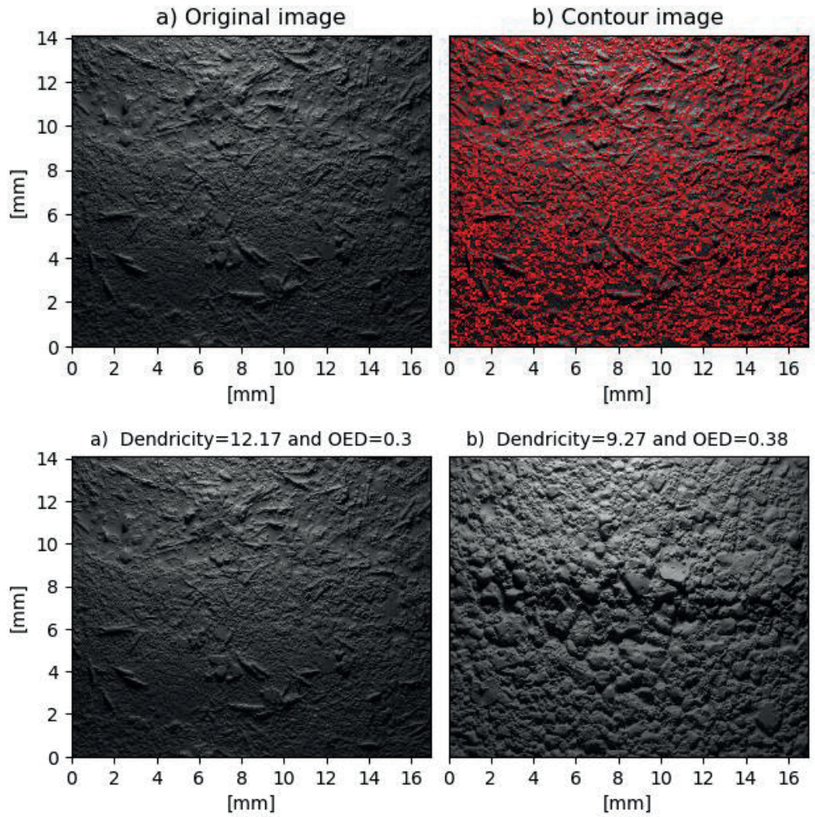
2-D Image Analysis of Snow for Cross-Country Skiing

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.



Mina Sørensen Bratvold

Department of Chemistry, NTNU

The Permeability of Porous Media as Studied by NEMD

Fall 2020/Spring 2021
Supervisors: Signe Kjelstrup, Michael Tobias Rauter and Olav Galteland

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 an ongoing effort to find a proper way to define state variables of confined media, help expand our understanding of driving forces for transport and design a method to determine the permeability.

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.

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.

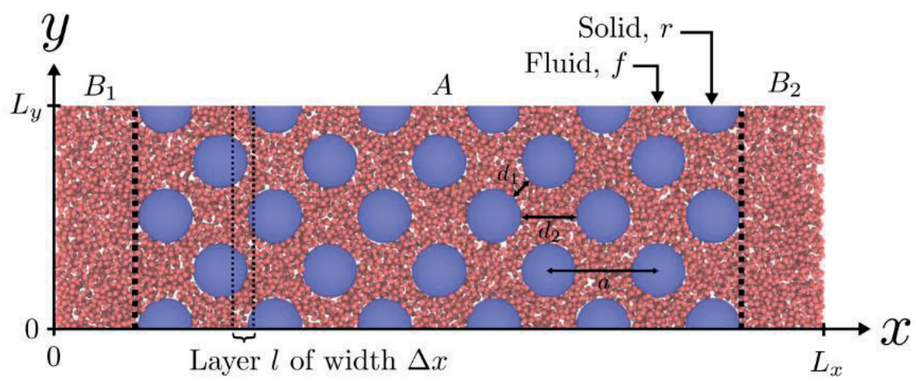


Figure 1: *System used to compute the integral pressure of a single-phase fluid in a porous medium confined in a regular lattice of spherical particles. The porous medium (blue) is surrounded by bulk fluid particles (red).*

References

1. https://www.frontiersin.org/articles/10.3389/fphy.2019.00060/full
2. https://www.frontiersin.org/articles/10.3389/fphy.2018.00150/full
3. https://www.frontiersin.org/articles/10.3389/fphy.2018.00126/full
4. https://link.springer.com/article/10.1007/s11242-014-0307-6

Peder Langsholt Holmqvist

Department of Chemistry, NTNU

Non-Isothermal Transport in Cation-Exchange Membranes: The Seebeck Effect in Systems of Ions Abundant in Seawater

Spring 2020
Supervisors: Signe Kjelstrup and Kim Roger Kristiansen

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 KCl. In this thesis, the Seebeck effect was measured in cation-exchange membranes in equilibrium with single-salt solutions of various akali- and alkaline earth chlorides, with binary NaCl-$MgCl_2$ 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-$MgCl_2$ systems, even small amounts of Mg^{2+} had relatively large, negative effects on the Seebeck coefficient. This was likely due to a high fraction of Mg^{2+} 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-$MgCl_2$ systems, and from Mg^{2+} 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 Sebeeck effect in mixed electrolytes.

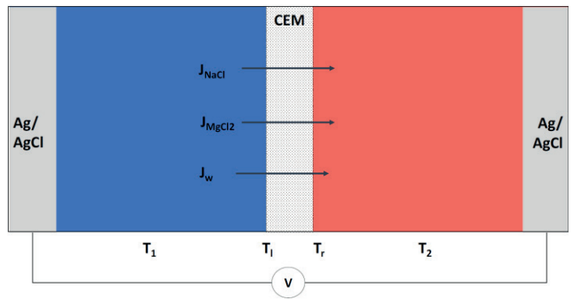


Figure 1*: Model of the thermocell*

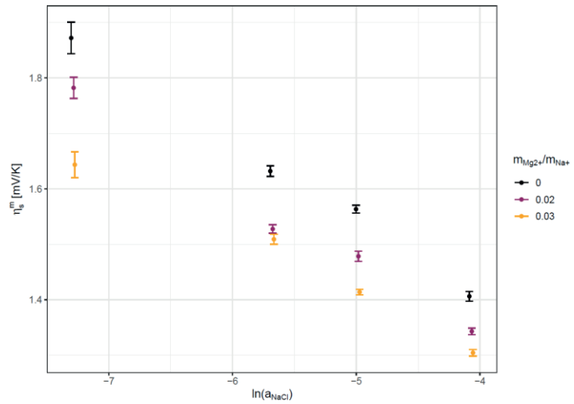


Figure 2*: Membrane Seebeck coefficients in the NaCl and NaCl-$MgCl_2$ systems, plotted against the activity of NaCl.*
The error bars indicate the double standard deviation interval of the coefficients.

NTNU - Department of Chemistry

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 monomeric, 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

[1] Cárdenas, H., Müller, E.A., 2019. Extension of the SAFT-VR-Mie equation of state for adsorption. Journal of Molecular Liquids 294, 111639.

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].

Recommended reading

1. https://www.frontiersin.org/articles/10.3389/fphy.2019.00060/full
2. https://www.frontiersin.org/articles/10.3389/fphy.2018.00150/full
3. https://www.frontiersin.org/articles/10.3389/fphy.2018.00126/full
4. https://arxiv.org/abs/2012.00562

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.

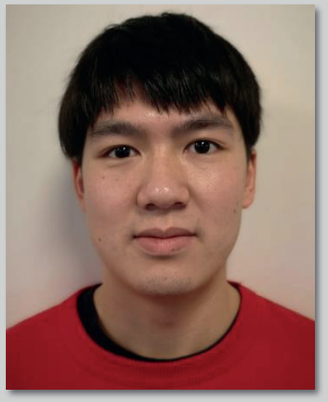
NTNU - Department of Chemistry

Daniel Tianhou Zhang

Department of Chemistry, NTNU

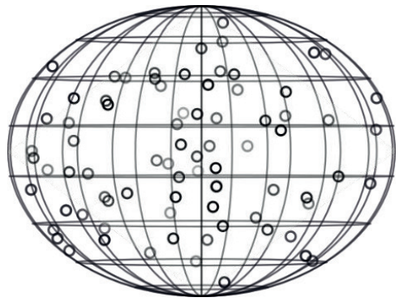
The First Steps Towards a Perturbation Theory for Small Systems

Spring 2020
Supervisors: Anders Lervik and Øivind Wilhelmsen



Background

Equation of State (EOS) developed from perturbation theory are well known in the literature and can be a very useful tool for modelling fluid behavior. While popular perturbation theories of i.e. Barker-Henderson (BH) prove to be accurate for macroscopic (bulk) pure-component fluids at high temperatures, there currently exist a lack of successful methods to obtain accurate EOS for fluids in small confinements that experience finite-size effects (small). The objective of this thesis is therefore to investigate the applicability of BH perturbation theory (BHPT) for fluids confined to small systems and to extend the first order BHPT to the specific case of the Lennard-Jones/spline (LJ/s) fluid confined to small spherical geometries with hard walls.



Results

The investigation demonstrates two major findings, 1) a difference between small and bulk hard-sphere (HS) pressure and radial distribution function g(r) (RDF) and 2) particles are depleted from the inner-core (IC) of the spherical confined HS fluid to be adsorbed on the confinement wall. For the HS RDF g(r), instead of tending toward g(r) → 1 when the pair-distance r→ ∞, 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.

By only requiring the bulk HS RDF, particle adsorption per surface area and a spherical ideal gas RDF (geometrical RDF factor), the small BHPT can predict small LJ/s properties under spherical confinement of any "relatively large" radius sizes. While this thesis has investigated the LJ/s fluid, the small BHPT should be applicable for a variety of pair potentials in addition to being able to be extended to other types of confinement geometries.

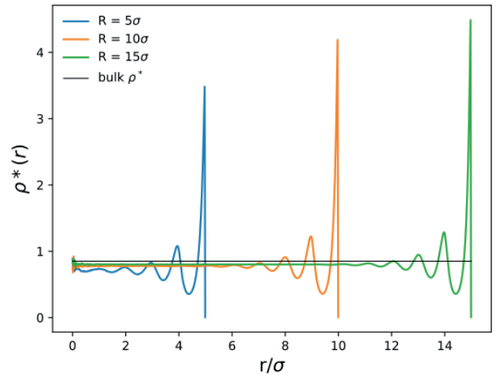


***Figure 1**: The density variation of the Psuedo HS (PHS) fluid within spherical confinements of radius R = 5σ, 10σ and 15σ for $\rho^* = 0.85$.*

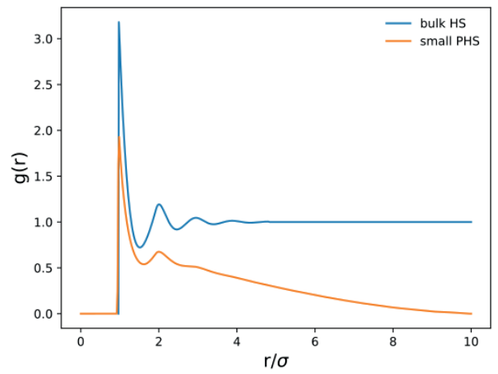


***Figure 2**: The bulk HS and small PHS RDF as a function of pair-distance r at ρ* = 0.85. In this Figure the small confinement geometry has a radius of R = 5σ.*

Gbadebo Nafiu Adejumo

Department of Geoscience and Petroleum, NTNU

Experimental Study on the Effect of Low Water Salinity and Ionic Composition on Wettability Alteration in Carbonates

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

Background

Rock wettability plays an important role in oil production. A slight change in rock wettability towards more water-wetness will have a significant change in the oil production. Carbonate rocks tend to be preferentially oil-wet or mixed wet. Altering the ionic composition of the injected brine and lowering the salinity has proven to be an efficient way to improve the water-wetness of the carbonate rocks according to several laboratory and field tests.

Methodology and Objectives

The master's thesis will study the effect of low salinity and varying ionic composition on oil recovery via spontaneous imbibition using Amott cells. Two outcrop cores from Angola (Angola cores) and Spain (Ainsa cores), which are representatives of some carbonate fields were used in this experimental study.

The objectives of this project are:

1. To build a dynamic aging set up of the same temperature as the Spontaneous Imbibition tests.
2. To build a Spontaneous Imbibition rig to adapt to an elevated temperature of 96*C.
3. To look at the possibilities of using the built Spontaneous Imbibition set up to understand the controlling factors behind the oil recovery from core materials.

Based on initial laboratory experiments on core material, the Ainsa cores have more pore volumes, and are more homogeneous than the Angola cores which are heterogeneous and tight. Both core materials are classified as limestone. From the mineralogy experiments, no traces of anhydrite were found in the Ainsa cores, but traces of dolomite were found in the Angola cores.

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].

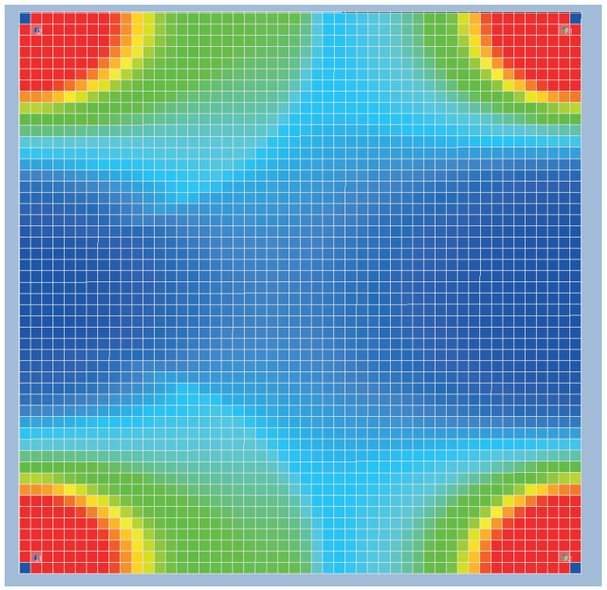


Figure 1. *Energy dissipation visualization on a simple two-dimensional reservoir with two injection wells (left side) and two production wells (right side).*

References

[1] Hassanizadeh, S.M., & Gray, W.G. 1990. Mechanics and Thermodynamics of Multiphase Flow in Porous Media Including Interphase Boundaries. Advances in Water Resources 13, 169–186.

[2] Dale, S. I., Sjaastad, M., Hogstol, H., & Rustad, A. B. 2012. Improving Visualization of Large Scale Reservoir Models. Society of Petroleum Engineers.

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, GEM™ 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.

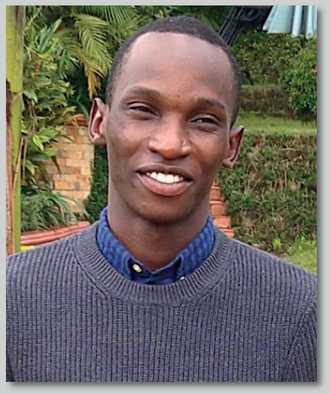
Furthermore, a software tool that combines advanced statistical analysis, machine learning, artificial intelligence and data interpretation techniques is going to be used for both comprehensive sensitivity analysis and to find optimal solutions for different objective functions.

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 study and controlled.

The second objective is to recommend probable brines that practically effective, causing higher oil recoveries, in the reservoir under study. The test is being conducted at reservoir temperature conditions.

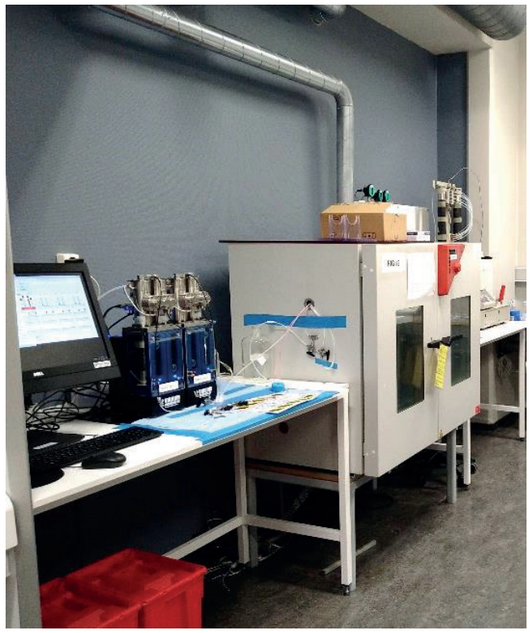


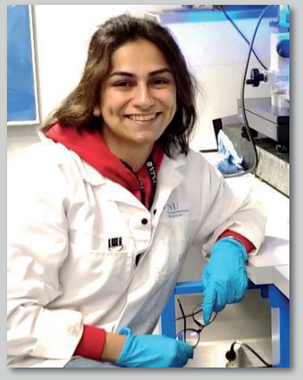
Figure *Experimental Set-up*

Shirin Safarzadeh

Department of Geoscience and Petroleum, NTNU

Appraisal of Low-Salinity EOR on Micro-Scale: Effect of Brine Concentration on Interface Tension, Contact Angle, and pH

Fall 2020/Spring 2021
Supervisor: Ole Torsæter



Background

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 micromodels to investigate the effect of invading phase salinity on oil recovery factor.

Methodology

Low salinity water (LSW) and synthetic sea water were prepared over a wide range of salinity (0-38318 ppm). For oil phase, crude oil A from one of the North Sea oil fields was used. IFT and contact angle were measured by KRÜSS DSA100S (Figure 1). For example Figure 2 and Figure 3 show visualization of IFT and contact angle measurements. During this project, two-dimensional microfluidic chips will be used to inject prepared low salinity water samples and synthetic sea water in the secondary mode.

Results

Results showed that at salt concentration of 5000 and 6000 ppm, IFT between oil and aqueous phase is minimum which means at 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.

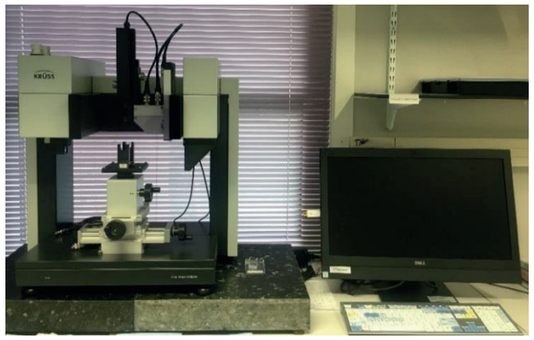


Figure 1*. Drop shape analyser, KRÜSS DSA100S, used for IFT and contact angle measurements*

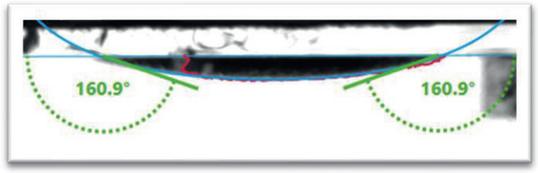


Figure 2: *Contact angle measurement*

Figure 3: *Interfacial tension measurement.*

NTNU - Department of Geoscience and Petroleum

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.

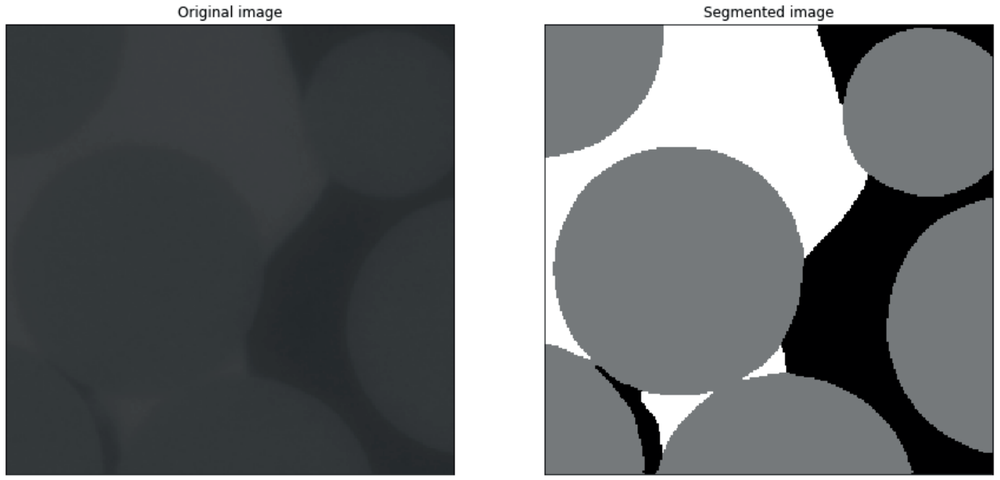


Figure: *Example of a two-dimensional image slice from a micro-CT scan of a bead pack filled with oil and water and the corresponding segmented image created with a convolutional neural network.*

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.

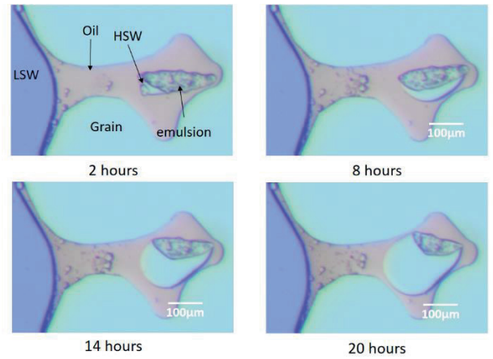


Figure 1*: Spontaneous emulsification enhances the water flow from LSW to HSW region, causing larger connate water swelling.*

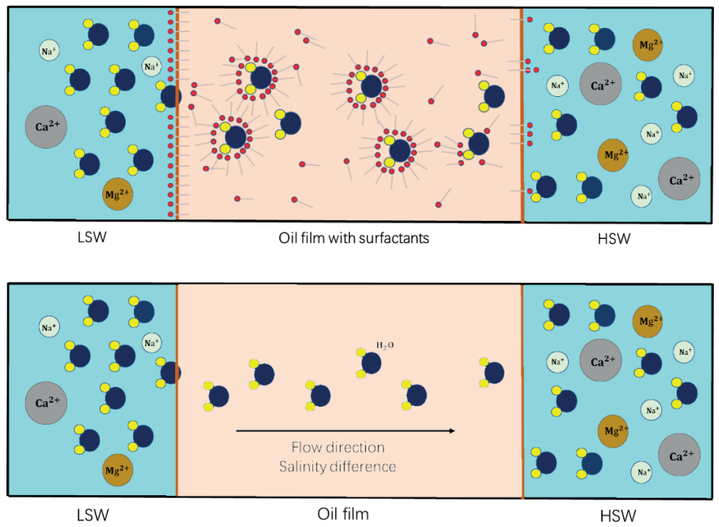


Figure 2*: Simplified schematic diagram for osmosis effect and spontaneous emulsification in LSW flooding.*

Marvin Glissner

Department of Structural Engineering, NTNU
Department of Civil Engineering, DTU (Technical University of Denmark)

Service Life Prediction of Concrete in Cold Climate, Benchmarking of Chloride Ingress Simulations

Spring 2020
Supervisors: Mette Rica Geiker (NTNU), Alexandre Michel (DTU) and Victor Marcos Meson (DTU)

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 chloride ingress into concrete and cement pastes has been an area of interest for decades. The chemical aspects of chloride binding are mostly understood and commonly agreed upon by 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.

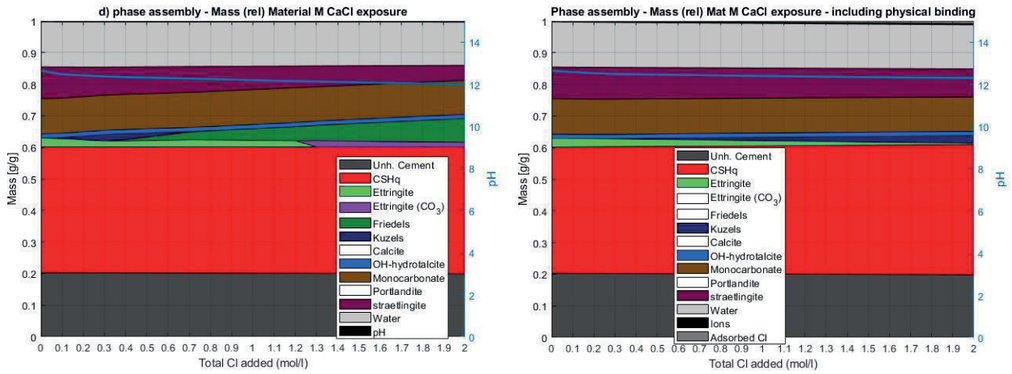


Figure: *Phase assemblage of a simulated material;*
left: no physical binding included; right: physical binding included before chemical solver is run

Morten Hovind and Kjetil Lien

Department of Civil and Environmental Eng., NTNU

Parametric Study of Mechanical Properties for Saline Frozen Clay

Spring 2020
Supervisors: Rao Martand Singh and Chuangxin Lyu

Background

Construction work in cold regions has become more common in recent decades, and along with the construction of more advanced structures, the interest relative to frozen ground engineering has greatly increased. Frozen soil is a complex material due to the phase relationship between ice and water. This causes temperature and salinity to have a major impact on soil behavior.

Furthermore, long-term design in classical geotechnics are often based on the effective stress concept. This method adds pore water pressure to calculate total stress. Investigating and understanding pore water behavior in frozen soil can enable the use of effective stress approaches in design. However, recording pore pressure in frozen soil is challenging as the ice matrix reduce hydraulic conductivity.

Objective and methodology

The first objective is to study pore water response in saline frozen clay and its correlation to different parameters. The second objective is to investigate which parameters affect the mechanical behavior of saline frozen clay, and the effect of these parameters. A triaxial testing apparatus, placed in a cold laboratory, was used to measure mechanical properties. In addition, pore water pressure was recorded using a pressure transducer connected to the bottom of the specimen.

Figure 1*. Triaxial test setup.*
Specimen prepared with membrane and O-rings.

Tonje Roås Mikalsen

Department of Civil and Environmental Engineering, NTNU

Estimation of the Unfrozen Water Content Based on a Joint Electrical and Acoustic Method

Spring 2020
Supervisors: Rao Martand Singh and Chuangxin Lyu

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 changes. 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.

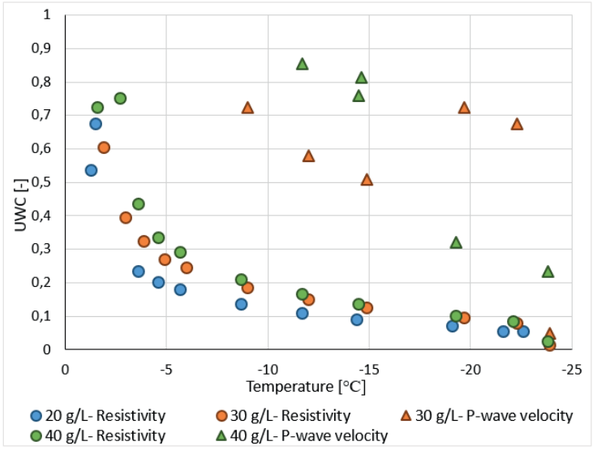


***Figure 1**. Unfrozen water content estimation based on resistivity and P-wave velocity in sand with different salinity and water content*

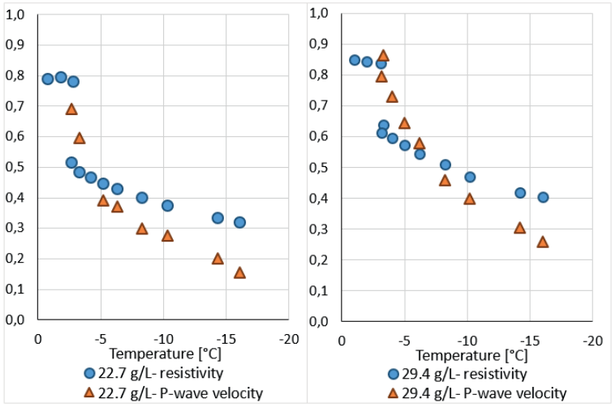


***Figure 2**. Unfrozen water content estimation based on resistivity and P-wave velocity in clay with different salinity and water content*

Hilmar Yngvi Birgisson

Department of Physics, University of Oslo

Density Driven CO_2 Advection Diffusion

Fall 2020
Supervisors: Knut Jørgen Måløy and Eirik Grude Flekkøy

Background

In general, advection diffusion is a highly complicated mechanism, where a dissolved species is transported both due to the solvent fluid flow and diffusion due to some concentration gradient. This thesis aims to investigate this mechanism in experimentally realized CO_2 porous media aquifers.

When gaseous CO_2 is introduced above the liquid surface, it will start to diffuse into the water and form carbonic acid. This increases the density of the liquid, and the densest liquid regions will start to sink due to gravity. These sinking regions, called plumes then forces new low-density water back up to the surface where it can absorb even more CO_2.

This effect greatly increases the rate of CO_2 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 CO_2 advection diffusion is of great importance especially to environmental and geophysical applications. CO_2 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.

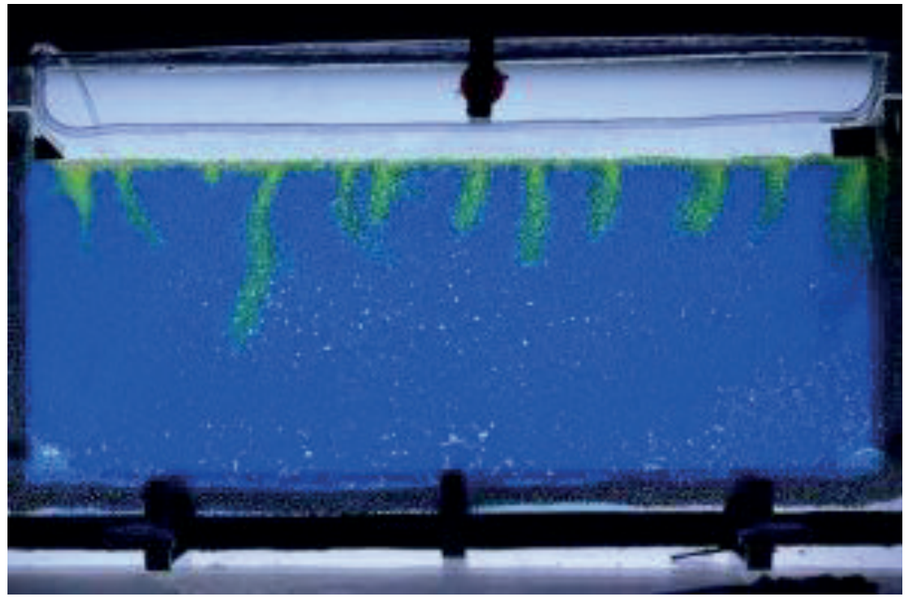


***Photo**: layer of CO_2 above a water-saturated porous medium consisting of glass beads (PoreLab UiO)*

Ivar Svalheim Haugerud

Department of Physics, University of Oslo

Effective Diffusion in Two Dimensional Channels

Fall 2020/Spring 2021
Supervisors: Eirik Grude Flekkøy, 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 coefficient's 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 inversing 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.

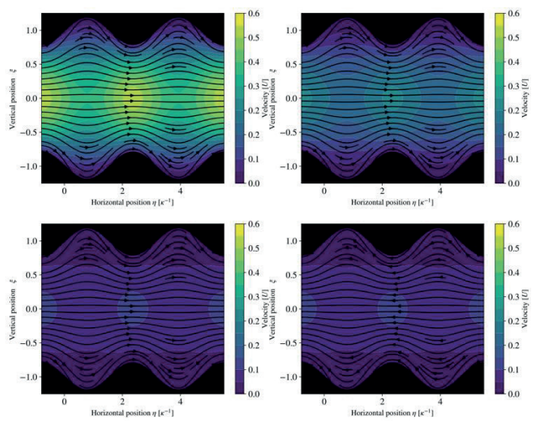


***Figure**: The analytic velocity field found from the Navier-Stokes equation with an oscillating body force.*

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.

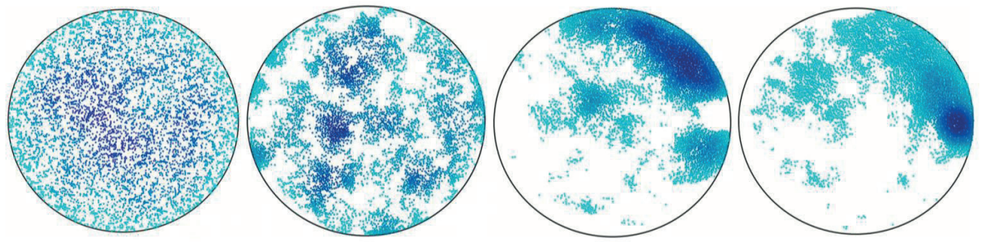


***Figure:** Active particles with alignment interactions that transition from a uniform state to a state of collective clockwise or anti-clockwise motion.*

Inspiration for Master projects

You find in the following pages a few suggestions for master projects to be performed at PoreLab

Proposed Master Project at PoreLab NTNU (department of Physics)

Shape of Clusters in Immiscible Two-Phase Flow in Porous Media

Contact: Alex Hansen (Alex.Hansen@ntnu.no)

When two immiscible fluids flow simultaneously through a porous medium, they will self-organize into complex pattern 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.

The self-organization manifests itself through how the fluids distribute themselves into clusters, which – when they move – are called ganglia. Ganglia dynamics is very rich and still rather poorly understood despite a huge effort to study these experimentally.

It is the aim of this MSc project to use a dynamic network model (i.e. a numerical model) to characterize the shape of trapped clusters and ganglia geometrically. We know, e.g. that there are length scales associated with the two types of forces involved, viscous and capillary. How do these length scales influence the shapes? To answer these questions, we will use the machinery developed in connection with percolation theory – the quintessential example of a non-thermal critical system. We will then go on to correlate the shape of the ganglia with their speed. Is there a typical shape? How does speed correlate with their size?

The findings in this project will open up for later experimental studies.

Proposed Master Project at PoreLab NTNU (department of Physics)

Phase Diagram of Mixed Wetting

Contact: Alex Hansen (Alex.Hansen@ntnu.no)

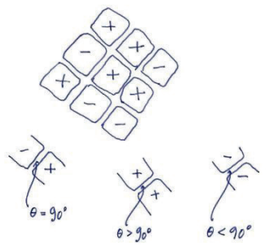
When two immiscible fluids flow simultaneously through a porous medium, they will self-organize into complex pattern that are describable using the language of critical phenomena. This has profound consequences for the properties of the flow.

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.

It is the influence of the wetting properties on the flow that is the focus of this proposal. Wetting is described by the angle the interface between the two immiscible fluids makes with the pore walls. If the interface comes in at e.g. 30 degrees, one says that the fluid in the wedge beneath the interface is the wetting fluid and the fluid in the other side the non-wetting fluid. The capillary forces will point in the direction of the non-wetting fluid. When the wetting angle is 90 degrees, the capillary forces will essentially be zero.

A particularly interesting situation is when the porous medium is *mixed wet* with respect to the two fluids. This is when the wetting angle differ between values above 90 degrees and below 90 degrees from pore to pore.

We have studied this situation using a dynamic network model (i.e. a numerical model) for the case that each pore in the porous medium has its own wetting angle drawn from some probability distribution and we have found that the flow rate goes as the pressure gradient to a power given by a critical exponent.



However, there is another situation that we have not explored, and which leads to a much richer set of behaviors than the system we have already studied. Look at the upper figure to the left. The blocks here form a porous medium in the form of a rectangular grid. The nodes are the pores and the links between them the pore throats. The capillary forces appear in the links. Now, we have denoted the blocks by "+" and "-". This means that they either has a wetting angle greater than 90 degrees or a wetting angle less than 90 degrees. When two "+" blocks meet, the pore throat between them will effectively have a wetting angle larger than 90 degrees associated with it, and if the two adjacent blocks are both of the "-" type, the effective wetting angle will be less than 90 degrees. But what happens if a "+" and a "-" block meet? The effective wetting angle is then close (or rather, for simplicity, equal to) 90 degrees. There are therefore *three* types of pore throats. Depending on the ratio between the number of "+" blocks and the number of "-" blocks, we get a very rich phase diagram. There will e.g. be two ratios, one at 0.59/(1-0.59)=1.44 and another one at a ratio (1-0.59)/0.59=0.695 at which the neutral pore throats (i.e. wetting angle equal to 90 degrees) percolate. This leads to two new critical points to be explored. How will the flow rate vs. pressure gradient behave in this system? These are completely open questions.

Proposed Master Project at PoreLab NTNU (department of Physics)

Energy Variation in LLS Fiber Bundle Model

Contact: Srutarshi Pradhan (Srutarshi.Pradhan@ntnu.no) and Alex Hansen (Alex.Hansen@ntnu.no)

Background: Fiber bundle model (FBM) is a simple and efficient model to describe the fracture-failure in composite materials under stress. NTNU physics department is involved in FBM studies since 1992. Extensive research works have been done at NTNU on equal-load-sharing (ELS) and local load-sharing (LLS) versions of FBM -both theoretically and through numerical simulations [1,2]. The NTNU fracture group has been recognized as one of the leading groups on this topic and currently this group is a part of the editorial team for a Research Topic "*The Fiber Bundle*" in the Frontiers in Physics.

Problem formation: It is obvious that if we increase stress or load on a composite material, at some point the system will collapse i.e., the material cannot bear the load and breaks into pieces. But when does this collapse point come? Is there any prior signature? Can we somehow predict this collapse point? These are some long-standing questions in the field of fracture-failure of materials. In a very recent work [3] it has been observed that in equal load-sharing (ELS) Fiber bundle model the elastic energy variation can tell us exactly when the bundle will collapse.

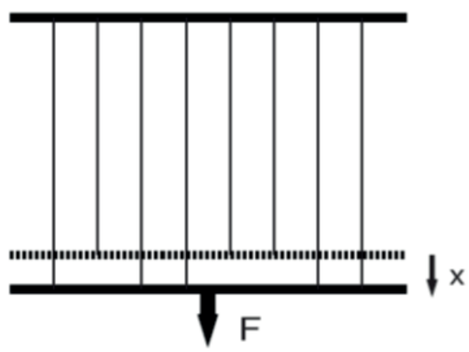
The aim of this Master project is to extend and explore the energy concept (developed in [3]) to a more realistic load-sharing scheme -the LLS model. The elastic energy and damage energy will be measured numerically as a function of external stress (stretch of the bundle) in 1-D and 2-D systems. The simulation codes have been developed (in C, C++) in-house and are available for re-use and further improvement.

Other aspects: Strength estimation and prediction of collapse point is a central issue for sustainability of composite materials and structures including buildings, bridges etc. While better understanding of the fracture-failure process can help better designing of materials and structures, new knowledge on the prior signatures of upcoming collapse will surely help mitigation plans to avoid accidents and save human lives.

References:

[1] S. Pradhan, A. Hansen and Bikas K. Chakrabarti, "*Failure processes in elastic fiber bundles*", Rev. Mod. Phys. Vol. 82, No 1, 499-555 (2010).
[2] A. Hansen, P. C. Hemmer and S. Pradhan, "*The Fiber Bundle Model: Modeling Failure in Materials*", Wiley-VCH, Berlin (September 2015).
[3] S. Pradhan, J. T. Kjellstadli and A. Hansen, "*Variation of elastic energy shows reliable signal of upcoming catastrophic failure*", Front. Phys. Vol. 7 106 (2019)

Workload: Master Thesis (30 ECTS)
Requirement: Basic knowledge of computer programming
Resources: None



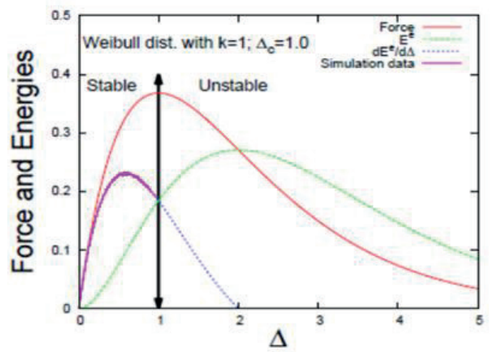


Fig: The ELS fiber bundle model (left) and the energy variations with stretch (right) for Weibull fiber strength distributions

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Proposed Master Project at PoreLab NTNU (department of Physics)

Swelling of Shale: Effect of composition and microstructure

Contact: Srutarshi Pradhan (Srutarshi.Pradhan@ntnu.no) and Basab Chattopadhyay (basab.chattopadhyay@ntnu.no)

Background: Swelling of Shale-rocks create several problems [1] during underground drilling operations, such as stuck-pipe/drill-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 (IFY) 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 problem 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:

[1] E. Fjær, R. M. Holt, P. Horsrud, A. M. Raaen and R. Risnes, *Petrolum Related Rock Mechanics* (Elsevier, 2008).
[2] S. Pradhan, *Swelling behavior of shale/clay: Discrete element modeling, based on Monte- Carlo technique*, Interpore 2019, Valencia, Spain.
[3] M. Deriszadeh and R.C.K. Wong, Transp Porous Med (2014) 101:35–52 DOI 10.1007/s11242-013-0229-8.
[4] E. Rybacki, J. Herrmann, R. Wirth and G. Dresen, Rock Mech Rock Eng (2017) 50:3121–3140.
[5] B. Chattopadhyay et el., J. Appl. Crystallogr., (2020) 53: 1562-1569.

Workload: Master Thesis (30 ECTS)
Requirement: Basic knowledge of computer programming
Resources: None

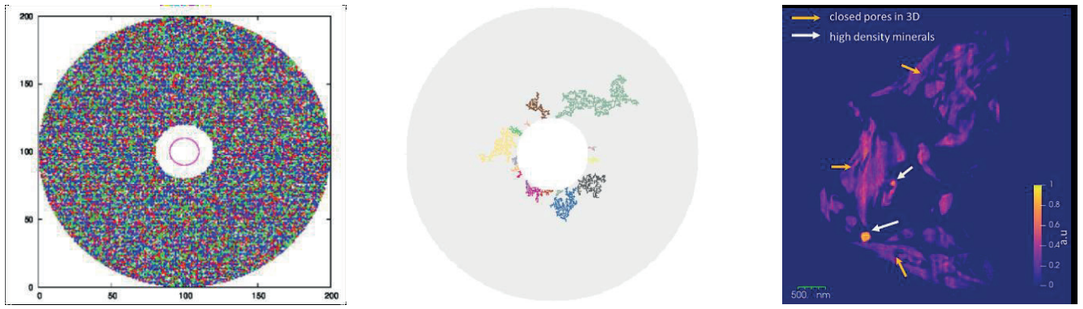


Fig: DEM model for Shale rock sample with clay and quartz grains (left). Microstructure-analysis shows clay-clustering (middle). Cross-section of Pierre Shale imaged by coherent diffraction imaging [5] (right).

Proposed Master Project at PoreLab NTNU (department of Physics)

Fracture Propagation During Fluid-Injection

Contact: Srutarshi Pradhan (Srutarshi.Pradhan@ntnu.no) and Alex Hansen (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 CO_2 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 invasion 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 likes to pursue a ***research career*** on this topic.

References:

[1] E. Fjær, R. M. Holt, P. Horsrud, A. M. Raaen and R. Risnes, *Petrolum Related Rock Mechanics* (Elsevier, 2008).
[2] S. Pradhan, A. Stroisz, E. Fjær, J. Stenebråten, H.K. Lund and E. F. Sønstebø, "Stress-induced fracturing of reservoir rocks: Acoustic monitoring and mCT image analysis", Int. J. of Rock Mechanics and Rock Engineering, DOI 10.1007/s00603-015-0853-4 (2015).
[3] S. Pradhan, A. Stroisz, E. Fjær, J. Stenebråten, H.K. Lund, E. F. Sønstebø and S. Roy, "Fracturing tests on reservoir rocks: Analysis of AE events and radial strain evolution", ARMA (2014).
[4] Invited presentation on *Fracture propagation during fluid injection: Experiment, modeling and monitoring towards field scale applications* at "Fracmeet Conference", IMSc, Chennai, India in March 2019.

Workload: Master Thesis (30 ECTS)
Requirement: Basic knowledge of computer programming
Resources: None

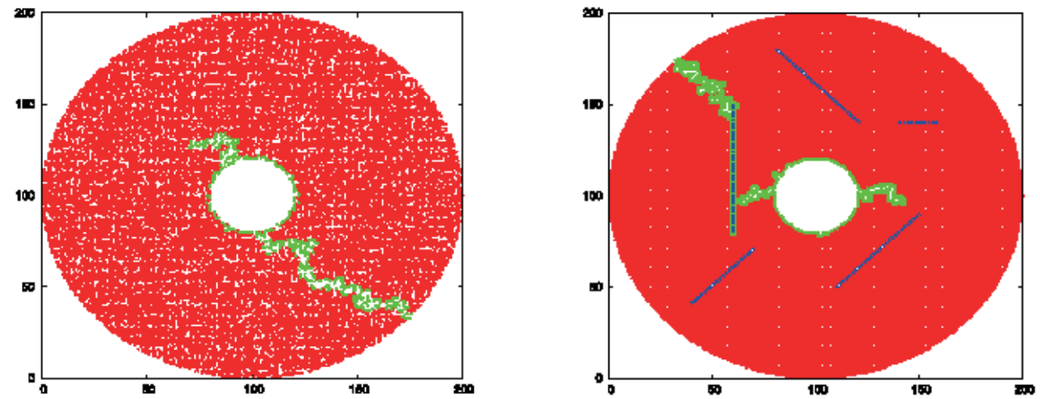
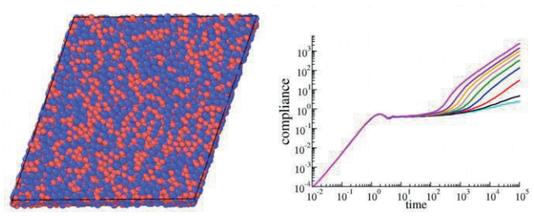


Fig: Fracture propagation in a DEM with no pre-existing fractures (left) and in a DEM with 5 pre-existing fractures (right)

Proposed Master Project at PoreLab NTNU (department of Physics)

Understanding non-Newtonian materials

Contact: Rafaella Cabriolu (raffaela.cabriolu@ntnu.no or raffaela.cabriolu@epfl.ch), Astrid de Wijn (astrid.dewijn@ntnu.no) and Erika Eiser (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 an advantage. We would like a person interested in modeling, simulation and programming able to work independently. Experience with C and/or Python are essentials.

Other aspects

Your study will be supervised by ass. Prof. Cabriolu, who has experience in simulating yield-stress materials, and by ass. Prof. de Wijn, expert in friction and modeling rheology. Your computational work will also be supported by Prof. Eiser, whose expertise includes colloidal physics, and in particular on corn-starch [3].

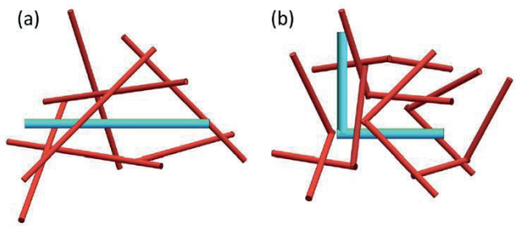
References

[1] D. Bonn and M. M. Denn , *Science*, **324** , 1401 —1402 (2009).
[2] R. Cabriolu, J. Horbach, P. Chaudhuri and K. Martens, Soft Matter, **15**, 415-423, (2019).
[3] C. Ness, Z. Xing, E. Eiser, Soft Matter **13**, 3664 – 3674 (2017).

Proposed Master Project at PoreLab NTNU (department of Physics)

Dynamics of granular anisotropic shapes - Experiments & Simulations

Contact: Erika Eiser (ee247@cam.ac.uk), Astrid de Wijn (astrid.dewijn@ntnu.no) and Raffaela Cabriolu (raffaela.cabriolu@ntnu.no or raffaela.cabriolu@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 the Newtonian nature of the aqueous solvent, however, at elevated concentrations when the particles start to overlap, they no longer can rotate freely, thus leading to a strong non-Newtonian behavior. You can view it as trying to make a large assembly of randomly placed, non-cooked spaghetti flow: Only if they are all aligned parallel to each other they can flow, but they cannot intersect and rotate. Deriving an analytical theory for the dynamics or such systems is challenging and only partially possible [3].

Your Project

In this project the student will examine the dynamics of a 2D arrangement of Y- and X-shaped granular particles, placed on a flat, vibrating table, mimicking the DNA-nanostars. This will involve setting up 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 set up a numerical model.

Other aspects

The experimental study will be supervised by the Professor Eiser, an expert in the rheology of self-assembling DNA systems. Associate Professors de Wijn and Cabriolu are experts in simulation studies of friction, rheology and yield-stress fluids.

References

[1] Z. Xing et al. “Microrheology of DNA-Hydrogels” PNAS 115, 8137 (2018)
[2] Z. Xing et al. “Structural and Linear Elastic Properties of DNA Hydrogels by Coarse-Grained Simulation” *Macromolecules*, **52**, 504-512 (2019)
[3] D. A. King, M. Doi & E. Eiser “Elastic Response of Wire Frame Glasses. I. Two Dimensional Model” arXiv:2102.02555 (2021) and “Elastic Response of Wire Frame Glasses. II. Three Dimensional Systems” arXiv:2102.02561 (2021).

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

Simulating the contact mechanics of hydrogels

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no) and Alex Hansen (alex.hansen@ntnu.no)

This project is concerned with the contact mechanics of hydrogels at the micrometer 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 Müser. The code needs to be extended to include additional physics that is 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 (MTP) (astrid.dewijn@ntnu.no)
Alex Hansen (Physics) (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.

Collaborator

Martin Müser, Saarland University

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)

Modelling of strengthening mechanisms in Aluminum alloys

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no), Inga Ringdalen (inga.ringdalen@sintef.no) and Randi Homelstad (Randi.homelstad@ntnu.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 investigate the nano-scale details concerning plasticity and strengthening of aluminum alloys. To increase the strength in aluminum, alloying elements are added. In addition is 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 final aluminum product. 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 transition state theory. You will employ the existing openly available 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.dewijn@ntnu.no>
Inga Ringdalen <inga.ringdalen@sintef.no>
Randi Holmestad <randi.holmestad@ntnu.no>
Research environment:
http://syonax.net/science/research.html
https://www.ntnu.edu/web/casa/casa

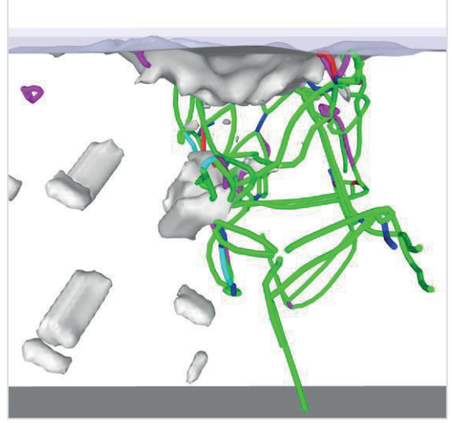


Figure: *Molecular dynamics simulation of a nanoindentation of aluminium including particles. The lines visualize the dislocations and the blobs are Mg-Si particles.*

Resources

The project will make use of high-performance computing resources that are already available through NTNU IT’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 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>
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.

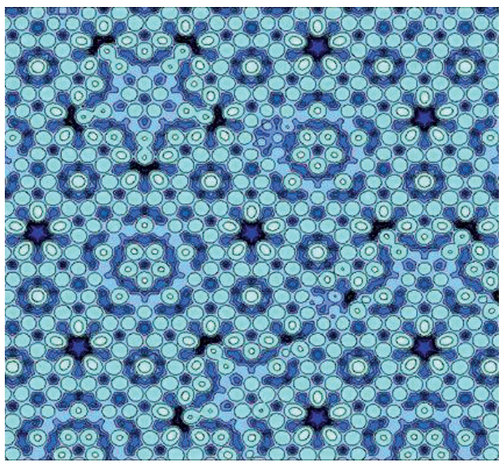


Figure: *Example of a quasicrystal surface, atomic model of fivefold icosahedral-Al-Pd-Mn. (Picture from Wikimedia Commons)*

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

Simulating mechanical properties of 2d materials

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no)

In this project, we will investigate the mechanisms of solid lubrication using Molecular-Dynamics simulations. In lubrication with a solid powder, small, nm-thin flakes of the solid slide easily past each other. While we have some understanding of the behavior of single sliding flakes, we are only beginning to explore the effects of having multiple flakes that can act collectively, or how multiple layers interact with each other [1].
This project will focus on possible effects of tearing of layers, as well as the interactions between layers. Another possible line of inquiry is the interactions between flakes. You will employ the existing openly available molecular dynamics code LAMMPS in combination with python scripting to create the models and to analyze the results.

[1] *Understanding the friction of atomically thin layered materials*, David Andersson and Astrid S. de Wijn, Nature Communications **11**, 420 (2020).

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

Supervisor
Astrid S. de Wijn <astrid.dewijn@ntnu.no>
Research environment: http://syonax.net/science/research.html.

Resources
The project will make use of high-performance computing resources that are already available through NTNU IT'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.

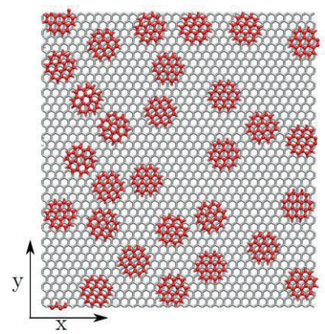


Figure 2: *A top view of a simulation of a single layer of graphene flakes acting as a solid lubricant*

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 wade 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)
Raffaela Cabriolu (raffaela.cabriolu@ntnu.no)
Christopher Fjeldstad (christopher.fjeldstad@ntnu.no)
Research environment:
http://syonax.net/science/research.html

Resources
The project will make use of high-performance computing resources that are already available through NTNU IT'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

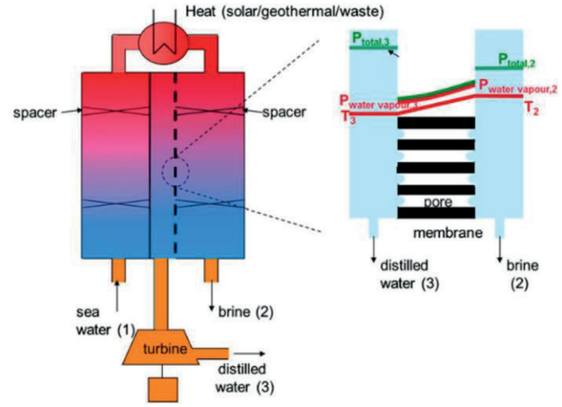
Contact: Professor Signe Kjelstrup (Signe.Kjelstrup@ntnu.no)

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 :
[1] Keulen et al. J. Membr, Sci. 524 (2017) 151 2. Lee et al. Nature Nanotechnology 9 (2014) 31



Proposed Master Project at PoreLab NTNU (department of Chemistry)

Peltier heats and Dufour effects in Lithium-ion batteries

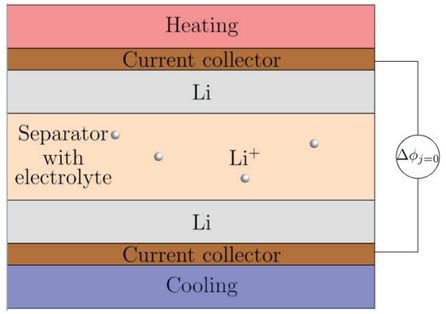
Contact: Prof. Signe Kjelstrup (Signe.Kjelstrup@ntnu.no) and Astrid F. Gunnarshaug (astrid.f.gunnarshaug@ntnu.no)

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 set-up 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. Spitthoff, A. F. Gunnarshaug, D. Bedeaux, O. S. Burheim, S. Kjelstrup, Peltier effects in lithium-ion battery modelling, *accepted*
2. Q. Huang., Y. Manming and J. Zhiyu, Thermal study on single electrodes in lithium-ion battery, *Journal of Power Sources* 156 (2) (2006) 541-546.
3. A. F. Gunnarshaug, S. Kjelstrup, D. Bedeaux, F. Richter, O. S. Burheim, The reversible heat effects at lithium iron phosphate-and graphite electrodes. *Electrochimica Acta*. 337 (2020) 135567

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, LiPF6, ethylene carbonate and di-methyl carbonate. The investigation was done with LAMMPS 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 thus is 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 ionic systems (one Master student, Gunnarshaug, and students working on Seebeck coefficient problems).

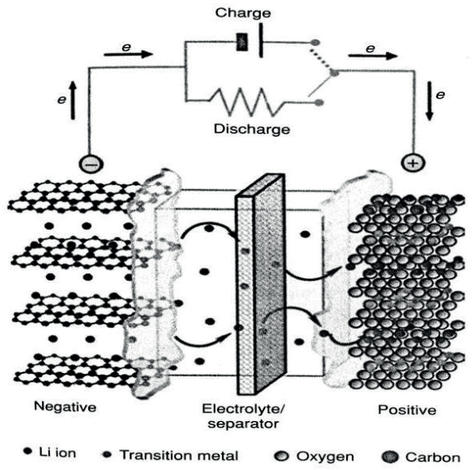


Fig.1 *The electrolyte and electrodes in a Li battery. Scrosati et al: Li-Batteries, 2013*

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

Fluid distribution simulation

Contact: Carl Fredrik Berg (carl.f.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 porous media. 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. Further, the candidate should compare a displacement process simulated by the "surface evolver" to a displacement simulated using a morphological approach (simulated using an already exiting script).

Supervisors: Hamidreza Erfani Gahrooei and Carl Fredrik Berg

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

Simulation of single-phase flow

Contact: Carl Fredrik Berg (carl.f.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.

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

Micro-CT imaging on low salinity flooding

Contact: Haili Long-Sanouiller (haili.long-sanouiller@ntnu.no) and Carl Fredrik Berg (carl.f.berg@ntnu.no) and

This study is going to evaluate the effect of low salinity water (LSW) and high salinity water (HSW) on the remaining oil saturation at pore-scale employing X-ray microtomography. It investigates the connectivity of the residual oil phase after brine flooding under different flow rate. It also compares the remaining oil phase saturation and topology after LSW flooding to HSW flooding at same capillary numbers. The aim for this study is to see the effect of low rate on the performance of LSW recovery. There is also an ambition to observe if there is a relationship/effect on the wettability of the surfaces measured by area of surface in contact with water/brine. The drainage-imbibition experiments will be performed via using a core-flooding setup integrated with a high-resolution X-ray micro-tomography scanner to capture the pore-scale fluid configuration. The 3D images will be processed and analyzed to quantify the remaining oil saturation, oil recovery.

Supervisors: Haili Long-Sanouiller and Carl Fredrik Berg

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

Pore-scale investigation of low salinity waterflooding in Sandstones

Contact: Tomislav Vukovic (tomislav.vukovic@ntnu.no), Hamidreza Erfani Gahrooei (hamidreza.erfani@ntnu.no), Antje van der Net (antje.van.der.net@ntnu.no)

The parameter *zeta potential* statically characterizes the transition zone between rock and liquid regarding the surface charge and fluid interaction. In this project, the objective is to proof whether the zeta-potential measurements of rock-brine system can be used to predict the surface characteristics behavior during low salinity waterflooding and consequently additional oil recovery. Detectable with zeta-potential measurements are double-layer expansion and surface force modification, parameters recognized as important mechanisms of low salinity waterflooding. These mechanisms can result in wettability alteration, which is one of the main principles applied to increase oil production. The zeta-potential measurements of glass beads/crushed sandstone are used to investigate the sandstone-brine surface properties at different salinities and pH. Afterwards, the optimum chemical condition of the injection brine is examined in two-phase displacement micromodel experiments for a better understanding of pore-scale mechanisms of low salinity waterflooding EOR method.

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

CDC curve- structure dependence in water wet porous media

Contact: Antje van der Net (antje.van.der.net@ntnu.no)

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.

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

Improvement of unsteady state relative permeability measurements by the use of partitioning tracers

Contact: Antje van der Net (antje.van.der.net@ntnu.no)

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 insitu 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.

Proposed Master Project at PoreLab UiO (department of Physics)

Pressure fluctuations in porous media flows

Contact: Knut Jørgen Måløy (K.J.Maloy@fys.uio.no)

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.

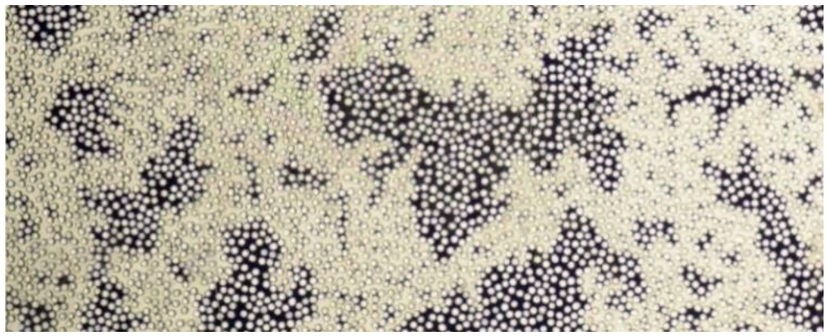


Figure: *Detail of the trapped liquid clusters (blue) left behind after air (white) is slowly injected from the left in a quasi-2D porous network previously saturated with the liquid*

Proposed Master Project at PoreLab UiO (department of Physics)

Influence of the flow speed on the pore invasion dynamics

Contact: Knut Jørgen Måløy (K.J.Maloy@fys.uio.no)

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. 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.

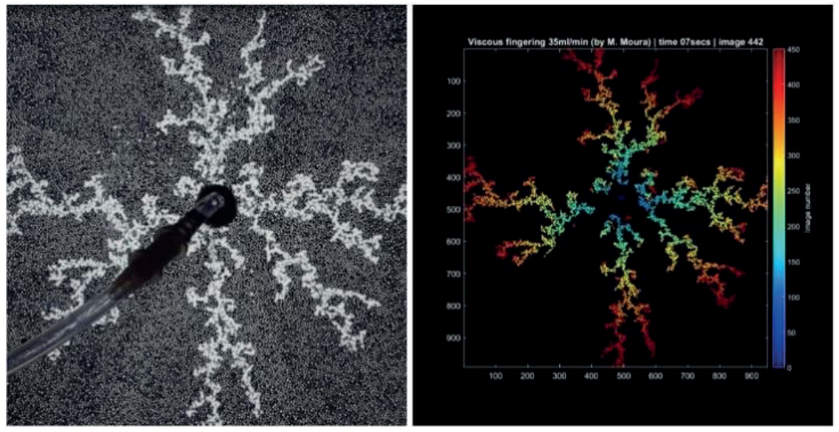


Figure: *Viscous fingering pattern (left) observed when air is injected fast in a porous medium previously filled with a viscous liquid (blue). The image analysis (left) shows the time (image number) of injection of each pore*

Education

Why Study Porous Media and What Courses to Choose?

Porous media are all around us. In the ground, water fills the pores of aquifers, and oil is found in porous medium. Pollutants may follow rainwater into the ground which is a porous medium; where do the pollutants end up? When underground water rises during earthquakes, they may push the soil particles apart so that it loses it strength with the results that building topple. Less dramatically, but extremely importantly, the physics and chemistry of nanoporous media is at the core of fuel cells, batteries, and in heterogeneous catalysis. They make up concrete and biological tissue. A better understanding of the flow patterns in these materials will make them much more efficient – an important goal in a world that needs to become greener.

In PoreLab we study phenomena of these and related kinds, aiming to understand, improve and use the porous materials in ways that are more environmentally friendly, and more effective than now. An interdisciplinary PoreLab-environment has been constructed to facilitate contact between different disciplines and speed up this development.

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 physics.

PoreLab Course 1 - Theory and Simulation of Flows in Complex Media

FYS4465/FYS9465 (Dynamics of Complex Media) at UiO or KJ8210 (Flows in Porous Media) at NTNU

PoreLab course 1 covers hydrodynamics where capillary and viscous forces play a role. It also covers simulation methods, thermodynamics and statistical physics relevant to porous media. The course content is motivated in terms of ground water flows, biological tissue, hydrocarbon management, fuel cells, electrophoresis, building materials and the quest for the governing equations. PoreLab course 1 is open for students from both NTNU and UiO. Professor Eirik Flekkøy is the lecturer for this course.

PoreLab Course 2 - Experimental Techniques in Porous and Complex Systems

FYS4420/FYS9420 (Experimental Techniques in Porous and Complex Systems physics) at UiO or PG8605/TPG4565 (Dual porosity reservoirs/Petroleum engineering) at NTNU

PoreLab course 2 covers experimental techniques related to porous media and is open for students from both NTNU and UiO. The course is adapted to PoreLab with a special focus on porous media physics. It contains projects that will give students introduction to important experimental techniques in the field porous media and complex systems. The teaching consists of 4 projects and approximately 4 hours of lectures for each project. The lab part of each project will take a total of 1-2 full days. Finally, a research report will be written on each of the projects. PoreLab course 2 is offered on both Ph.D. and Master level and is open for domestic and visiting students. Contacts are: Professor Knut Jørgen Måløy, UiO, and Professor Ole Torsæter, NTNU.

Additional courses offered at either NTNU or UiO are relevant for porous media.

Irreversible Thermodynamics

TKJ4200, NTNU

In this course we learn to describe energy conversion and the efficiency of this conversion using irreversible thermodynamics. The entropy production (the energy dissipation) will be constructed for systems with transport of heat, mass and charge. It covers as well: concentration cells, liquid junctions, membrane transport, electrokinetic effects, Soret, Duffour, Peltier and Seebeck effects. The fundamental properties will be connected to renewable energy technologies, like thermoelectric effects, salt power plants, batteries, thermal osmosis or fuel cells. The underlying molecular mechanisms for coupled transport processes are discussed. The energy efficiency of the mentioned processes is in focus. The students take part in a project, theoretical or experimental, formulated in collaboration with the teacher. The purpose is to obtain hands-on experience to use irreversible thermodynamics with the purpose of contributing to the UN goals of sustainability. The purpose is also to train collaboration skills and presentation techniques

Statistical Physics

TFY4230, NTNU

The course provides an introduction to statistical physics, mainly for systems in thermal equilibrium. The student should understand quantum and classical statistical mechanics for ideal systems and be able to judge when quantum effects are important. The student should understand the connection between microphysics and thermodynamics.

Mass and Heat Transfer in Porous Media

EP8208, NTNU

The course content is as follow: Fick´s, Navier-Stokes, Euler´s, Bernoulli's and Newton's second equations and conservation laws in transport processes. The Chapman-Enskogs, two-film, Eyrings, hydrodynamical, penetration, and varying interface renewal theories. The models and concepts of Dufour, Soret, Onsager, Kingery, Luikov and Stamm. The analogy of micro and macro transport processes. Criteria of similarity, model and object equations. Equations for steady state and transient convective and molecular diffusion in gases, liquids (ionic or not), concentrated solutions and porous solids. The gradients of concentration, moisture, temperature, pressure and phase change. Dimensionless groups and experiments on internal and external transport in laminar and turbulent flows. Transport properties in multicomponent mixtures. Transport in bubbles, droplets, cellular, capillary and porous solids. Quasi-steady method and mass transport in equally accessible surfaces. The development of transport rates in with chemical reaction, diffusion and convection. Sorption isotherms and spacial polytherms equations with effect of temperature. Sorption inflection points and distribution of micro and macropores and related equations. Experimental application of transport equations and correlations.

Applied Heterogeneous Catalysis

KP8132, NTNU

The course is given every second year, next time in the fall term 2021. The course aims to give an understanding of the relation between modern theories of catalysis and the industrial application for the most important groups of heterogeneous catalysts, metals, metal oxides and zeolites. Assessment of the potential developments and limitations of catalysts will be analyzed through examples from industrial applications or processes under development. This includes the catalyst synthesis, a kinetic description of the different processes involved in a catalytic cycle (adsorption, surface reaction and desorption), mass and heat transfer issues, as well as interpretation of results from experimental and theoretical investigations.

Catalysis, Specialization Course

TKP4515, NTNU

The specialization consists of modules giving a total sum 7,5 credits. Modules are chosen from the following list:

1. Environmental catalysis - (3.75 credits).
2. Heterogeneous catalysis (advanced course) - (3.75 credits).
3. Industrial colloid chemistry - (3.75 credits).
4. Reactor modelling - (3.75 credits).
5. Chemical engineering, special topics - (3.75 credits).

Modules from other specializations can be chosen given the approval of the coordinator.

Chemical Engineering Thermodynamics

TKP4107, NTNU

Chemical engineering thermodynamics forms one of the basic pillars for understanding chemical engineering process. In this course, we build on basic principles and learning objectives from subjects such as basic thermodynamics and process engineering. The syllabus is based on updated international standards and it will enable the students to calculate thermodynamics properties of ideal and non-ideal pure component systems as well as mixtures. Furthermore, the students will learn to calculate phase and chemical equilibria. The attained knowledge will help the students to model and simulate existing industrial processes as well as analyzing novel solutions in research and technology development. This competence is needed in order to develop and implement new and possibly more complex technologies, which are necessary in order to achieve future sustainable industry development.

The students will be able to understand and apply basic thermodynamic concepts, select and apply suitable thermodynamic models, calculate thermodynamic properties of components and mixtures, in ideal and non-ideal systems, use standard chemical potential, fugacity and activity in practical calculations, explain the limitations and assumptions in presented thermodynamic models, calculate simple phase equilibria and phase equilibria in multi-component systems.

Energy and Process Engineering, Specialization Project

TEP4550, NTNU

The topic will be closely linked to the ongoing research activities. The following subjects are offered:

1. Industrial heating and refrigeration processes in all parts of society. 2. Processing, transport and utilization of natural gas and hydrogen. Multiphase flow. Thermal power production. gas-fired power plants, fuel cells. Safety, environment, economy and management. 3. Combustion processes, industrial burners, boilers and gas turbines, emissions of polluted materials from combustion. Exhaust cleaning. Safety regarding fire and explosion. 4. Turbines for water and wind power. Transport of liquid and gas in pipe systems. Pumps and compressors. Aerodynamics of buildings, transport vessels and sports. Hydraulics, hydraulic control systems for control of various machinery. Energy and Indoor Environment. District heating and other hydronic processes. Energy conservation and energy monitoring. Solar heat utilization. 5. Components, processes and plants regarding refrigeration and food processing. Cooling / freezing, dewatering / drying, heat pumps and environmentally secure working fluids.

The specialization topic consists of two subjects (tema), each 3,75 study points. Choice of themes is done in consultation with the responsible teacher of the chosen project work. Further info regarding the subjects and teachers is given by the specialization topic at one of the 4 department groups.

Reservoir Property Determination by Core Analysis and well testing

TPG4115, NTNU

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 by well testing and core analysis. They study the influence of reservoir properties on one- and two-phase flow in subsurface reservoirs and will be able to do well test interpretation and conduct basic measurements in a core lab.

Geomechanics and Flow in Porous Media

TPG4112, NTNU

The subject should give basic knowledge about flow in porous media related to reservoir engineering and hydrogeological applications, and basic understanding of geomechanics and its importance in mining operations, tunnel constructions and exploitation of petroleum resources.

The course consists of two parts, one flow part (50%) and one rock mechanics part (50%).

The flow part deals with porous media characteristics: Porosity, permeability, flow equations for single- and multi-phase flow, capillary pressure, relative permeability and applications in earth sciences and petroleum engineering.

The rock mechanic part deals with tensions and pore pressure in the earth crusts, tectonic tensions, normal and abnormal pore pressures, tension determination, rock mechanic field and laboratory experiments, mechanical properties of rocks, tensions close to wells and subsurface holes. Other topics are: Stability of wells during drilling, sand/particle production, hydraulic fracturing, reservoir compaction and surface setting, significance of rock mechanics in reservoir control and use of rock mechanics in relation to rock installations

Reservoir Simulation

TPG4160, NTNU

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 methods. They will be able to use common modeling tools for numerical prediction of reservoir behavior during production of oil and gas and will be able to do derivation of equations for flow in porous media, and numerical solution of these by using finite difference methods.

The course content is as follow: partial differential equations for one-phase and multi-phase flow in porous materials, and numerical methods for solving these.

Topics are as follow: Summary of rock and fluid properties; derivation of PDE's; numerical solution of PDE's using finite differences; methods for solving linear and non-linear equations; discussion of different types of reservoir simulation methods; practical sides of reservoir simulation applications.

Applied Computer Methods in Petroleum Science

TPG4155, NTNU

The course addresses methods for numerical differentiation and integration, numerical solution of ordinary differential equations, numerical solution of sets of linear equations, numerical solution of partial differential equations, and numerical optimization useful for petroleum engineering and geoscience.

The course aims at giving the students experience in use of computers to solve numerical problems in petroleum engineering and geoscience.

The students will acquire knowledge about basic numerical techniques applied to problems from petroleum engineering and geoscience. They will be capable of writing programming routines for the numerical solution of problems in petroleum engineering and geoscience.

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
FYS4460/FYS9460, 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
FYS4130, 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. S(he) 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 deduce critical exponents. S(he) will be able to deduce the master equation and use it to construct various Monte Carlo algorithms.

Condensed Matter Physics II
FYS9430, 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

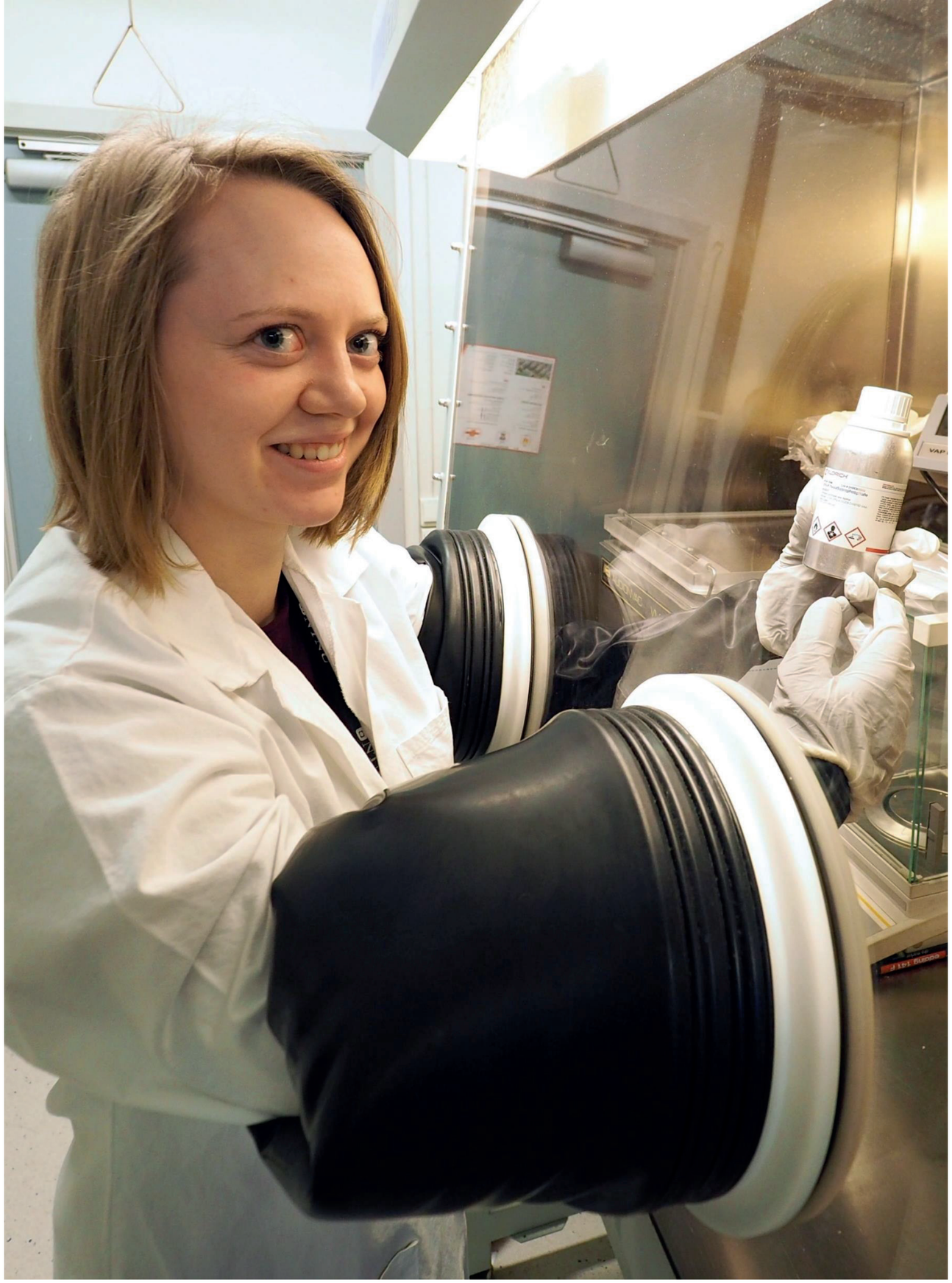


***Photo on the right**: PhD candidate Astrid Fagertun Gunnarshaug at the Department of Chemistry, NTNU, working with thermoelectric cells for lithium-ion battery research in the laboratory with glovebox*

Porous Media Laboratory
NTNU, UiO

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