

Master Thesis Project Proposals

Q1 2022-2023



Energy Technology & Fluid Dynamics
Department of Mechanical Engineering
Eindhoven University of Technology



Preface

This is an overview of all the Master Graduation project proposals available in Energy Technology & Flow Dynamics.

Please select 3 choices of different projects in order of preference and write a **short motivation** for your first choice to Azahara Luna-Triguero (a.luna.triguero@tue.nl).

Example:

- My first preference is project... because I am very motivated to work on...
- Second preference is... (no motivation needed)
- Third preference is.. (no motivation needed)

If you need more information on a proposal you can contact directly one of the supervisors (the emails are in each project proposal).

Supervisor	Dr.ir. Arjan Frijns
2nd supervisor	
Mentor	
Company	
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Experiments & Design

Available for ME



Project number: 01

Development of an experimental setup to measure interfacial temperature jumps during steady-state evaporation

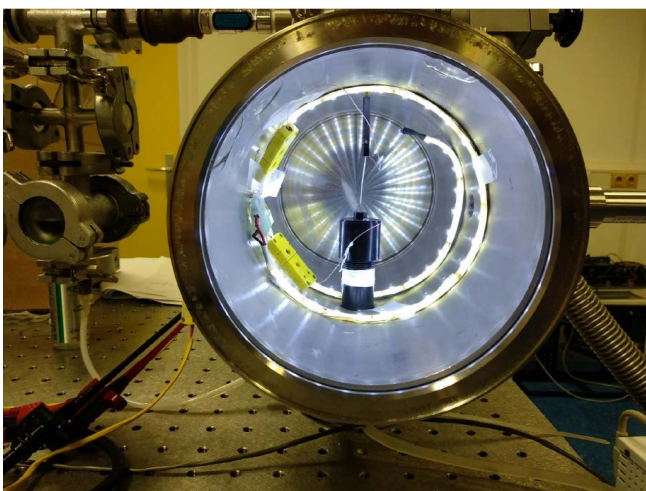
Arjan Frijns

E-mail: a.j.h.frijns@tue.nl

INTRODUCTION

Evaporation is an important phenomenon that occurs in a wide range of natural and industrial processes. Although this phenomena has been a subject of research for many years, it is still not fully understood. Experimental results of the last few decades seem to contradict with each other, and with the theory which describes this process (which are kinetic theory of gasses (KTG) and non-equilibrium thermodynamics (NET)). A remarkable example is the measurement of a temperature jump of 15 °C at the interface of a steady state evaporating water droplet at a pressure of 200Pa.

In order to determine whether this temperature jump exists and what influences this jump, an experimental setup is being developed. With this setup we should be able to measure the temperature profile at the interface of this evaporating droplet at very low pressures (in the range of 200 to 1000Pa). In a previous Master's project, we developed a set-up that is working at a pressure of about 800 Pa. However, larger temperature jumps are expected at even lower pressures (< ~300 Pa). Therefore, the setup needs to be further improved.



TASK

The developed setup consisted of an evaporating spherical water droplet in a large vacuum chamber (see photo). Purified, degassed, and temperature-controlled water (by a heat exchanger) was supplied to an evaporating geometry by a mass flow-controlled syringe. The temperature profile at the interface of this droplet was measured by a K-type thermocouple made of two 25.4μm wires, with a precision of 2μm.

Due to the occurrence of bubbles inside the syringe and the channel between the syringe and the droplet geometry, it was not possible to do an experiment lower than 780Pa and to measure the evaporating mass flow. Therefore, the experimental setup needs to be further improved such that experiments at lower pressures can be performed as well and can be compared to MD simulations.

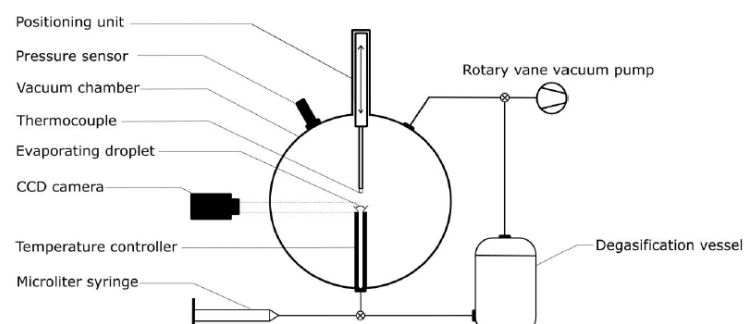
GOALS

The aim of this project is

- to develop a setup and to conduct experiments similar to the experiments as described in literature.
- to determine temperature jumps over the water droplet surface
- Compare the outcomes with empirical models from literature and with MD results

REQUIREMENTS

- Hands-on attitude and interest in performing experiments.
- Creative and solution-oriented



Supervisor	Dr.ir. Arjan Frijns
2nd supervisor	Company supervisor
Mentor	
Company	TNO, Thales, or Signify
Internal / External	External or internal (in collaboration with the company)
Starting date	Any time
Exp./Num./Design	Design/experiments/modeling

Available for ME



Project number: 02

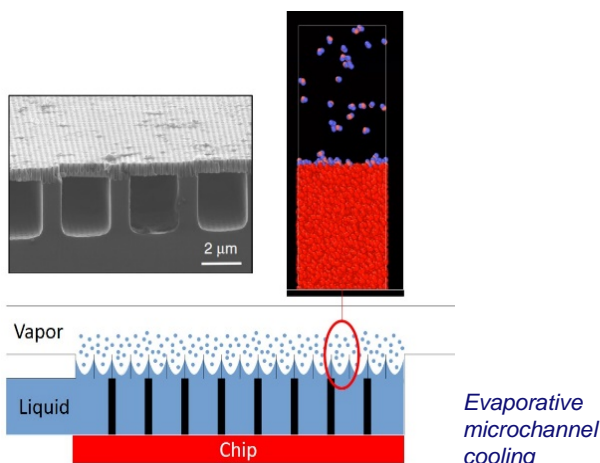
Integrated microfluidic and evaporative cooling

Arjan Frijns

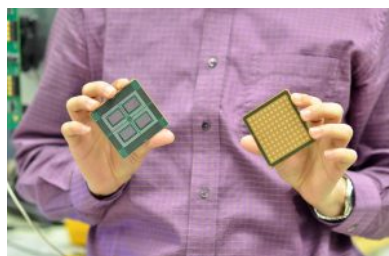
E-mail: a.j.h.frijns@tue.nl

INTRODUCTION

Moore's law is the observation that the number of transistors in dense integrated circuits doubles about every two years. This law serves as a roadmap for developments in the semiconductor industry and therefore there is a demand in the microelectronics industry to miniaturize central and graphics processing units (CPU and GPU) further. At the same time, the number of cores is increasing. Since the required (electrical) processing power does not scale down at the same pace, it results in an increase in heat flux densities that can even exceed 10 kW/cm^2 . Such power densities exceed the limits of conventional convective cooling methods (single-phase convective cooling) and controlled evaporative cooling becomes necessary. Also, in the development of the future generation telecom networks (e.g. 5G and 6G networks), similar thermal issues play a major role

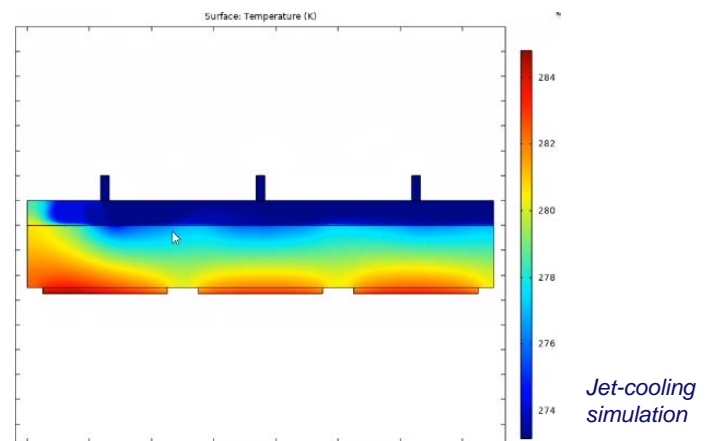


5G-antenna array



TASK

Evaporative microchannel and micro/nanopore cooling are promising techniques for (future) high heat flux cooling due to the additional evaporative heat. Adequate modeling, including surface and non-equilibrium effects, is essential for a proper system design, but are still in development.



GOALS

The aim of this project is to further develop the design of novel microfluidic cooling concepts, to model and test them. The focus is on evaporative cooling or on integrated jet cooling (single and two-phase cooling) for micro-electronics or power electronics.

The tasks in this project are:

- Numerical optimization of the microfluidic designs.
- Prototyping, testing and validation of the new designs.

The project will be done at one of the companies or in the TFE laboratory, but then in close collaboration with the companies.

REQUIREMENTS

- Hands-on attitude and interest in performing experiments and numerical simulations.
- Experience in CFD modeling and thermal network modeling (Simulink or Matlab)

Supervisor	Dr. Clemens Verhoosel
2nd supervisor	Dr. Erik Quaeghebeur
Mentor	Rodrigo Silva
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

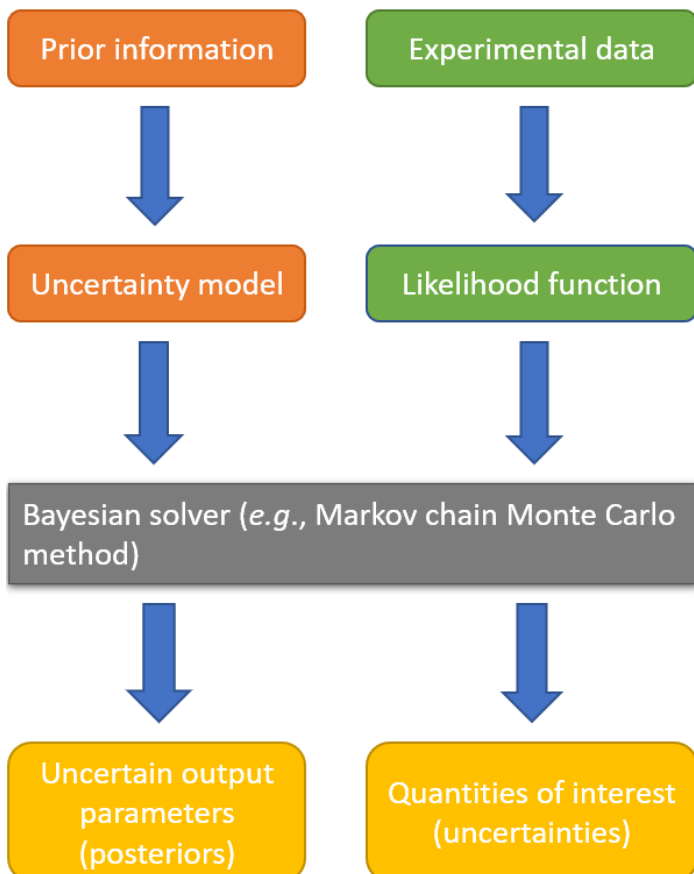
Bayesian Uncertainty Quantification in Energy Technology and Fluid Dynamics

Rodrigo Silva*, Clemens Verhoosel, Erik Quaeghebeur

*E-mail: r.lima.de.souza.e.silva@tue.nl

INTRODUCTION

Bayesian uncertainty modeling [1] provides an elegant approach to select and calibrate parameters that appear in the mathematical formulation of different engineering problems. It systematically combines physical laws, prior information and data, aiding interpretation. Uncertainty quantification (UQ) is performed by drawing inferences from Bayesian models. In practice, relations between the parameters are biased, prior information is incomplete and data is scant. In such setting, a fundamental challenge in Bayesian inference is to select an appropriate model for which there is data and prior information, thereby providing an efficient method to estimate and calibrate the parameters of interest under tolerated uncertainties [2].

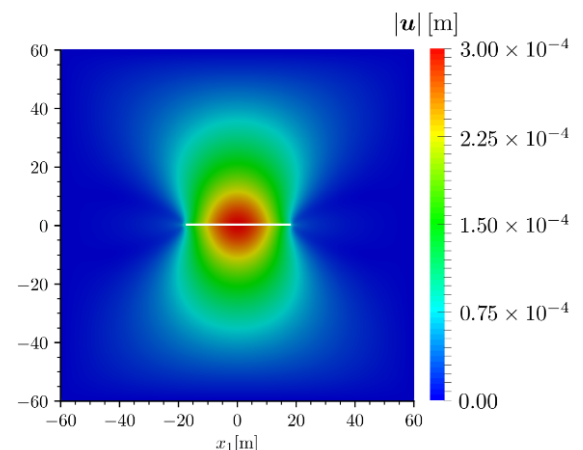


GOALS

- Apply the UQ framework to a problem of interest in energy engineering;
- Acquire experimental data or generate simulated measurements;
- Develop a Bayesian framework to explore the posterior density (e.g., Markov chain Monte Carlo methods [3]);
- Calibrate the parameters of interest under tolerated uncertainties.

REQUIREMENTS

- Affinity towards analytical and numerical solution methods;
- Good programming skills;
- Experience in MATLAB and Python.



Example: parameters of a propagating fracture model for geothermal energy applications requires calibration based on well measurements.

REFERENCES

- [1] Bernardo, José M., and Adrian FM Smith. *Bayesian theory*. Vol. 405. John Wiley & Sons, 2009.
- [2] Congdon, Peter. *Bayesian statistical modelling*. John Wiley & Sons, 2007.
- [3] Brooks, Steve, et al., eds. *Handbook of markov chain monte carlo*. CRC press, 2011.

Supervisor	Prof. Harald van Brummelen
2nd supervisor	Dr. Stein Stoter
Mentor	Tom van Sluijs
Company	Canon Production Printing
Internal / External	Internal
Starting date	2022-2023 Q1 or later
Exp./Num./Design	Numerical

Available for ME



Project number:



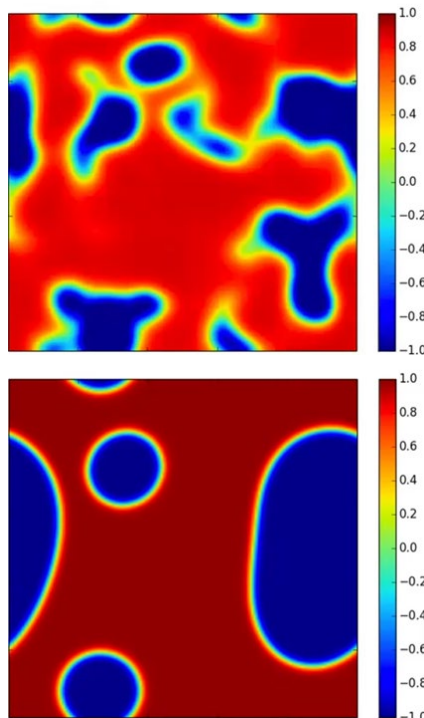
Adaptive methods for a Navier-Stokes-Cahn-Hilliard model

Tom van Sluijs*, Stein Stoter, Harald van Brummelen

*E-mail: t.b.v.sluijs@tue.nl

INTRODUCTION

The Cahn-Hilliard equations describe phase separation, such as the separation of an oil/water mixture into oil and water, as shown in the figures. Navier-Stokes equations describe the motion of viscous fluids. Coupling these models gives the opportunity to describe the dynamics of mixtures, especially the coalescence or breakup of fluid elements. This Navier-Stokes-Cahn-Hilliard (NSCH) model is implemented numerically and used to simulate for example breakup of a fluid filament.



In this model the length and time scales vary greatly throughout the domain and between different processes. Therefore, spatial and temporal adaptivity is needed to generate accurate results.

Keywords: Numerical methods, Finite Elements, Navier-Stokes, Cahn-Hilliard, Adaptivity

TASKS

In this project, you are expected to do:

- Literature review, focused on NSCH models and adaptivity
- Design an appropriate testcase to evaluate the performance of adaptive methods
- Program numerical implementation of a testcase and adaptivity methods
- Qualitative and quantitative assessment of the simulation results
- Conclusion and advise on the different adaptive methods concerning performance and computational cost

STUDENT PROFILE

We are looking for a motivated MSc student who:

- is curious about fluid dynamics, in particular multiphase flow, interface phenomena, and surface tension
- is interested in modelling, numerical methods, and programming.
- is able to present and discuss your work in a multidisciplinary group of researchers from TU/e, UT, and Canon Production Printing.
- is looking to develop his/her personal skillset: physical modelling, numerical methods, literature study, programming, and data analysis.

REFERENCES

Abels, H., Garcke, H., & Grün, G. (2012). Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities. *Mathematical Models and Methods in Applied Sciences*, 22(3). doi: 10.1142/S0218202511500138

Van Brummelen, E. H., Demont, T. H., & van Zwieten, G. J. (2020). An adaptive isogeometric analysis approach to elasto-capillary fluid-solid interaction. *International Journal for Numerical Methods in Engineering*(March), 1–22. doi: 10.1002/nme.6388

Supervisor	Prof. dr. ir. Harald van Brummelen
2 nd supervisor	Dr. ir. Arjan Frijns
Mentor	Daan van der Woude, Shahin Nejad
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME



Project number: 07



Coupling the method of moments to wall data described by a Gaussian Mixture Model

Daan van der Woude*, Shahin Nejad, Harald van Brummelen, Arjan Frijns

*E-mail: d.a.m.v.d.woude@tue.nl

Keywords: *Non-equilibrium thermodynamics, method of moments, rarefied gas dynamics*

INTRODUCTION

In many industrial applications, flows are encountered on microscopic scales. On these length scales, fluids are no longer accurately described by continuum models. On microscopic level, gases are typically described by the Boltzmann equation. This can be solved numerically in various ways, one of them is the Method of Moments (MoM)¹. There has been extensive research in this topic, but accurate description of boundary conditions remains an open topic.

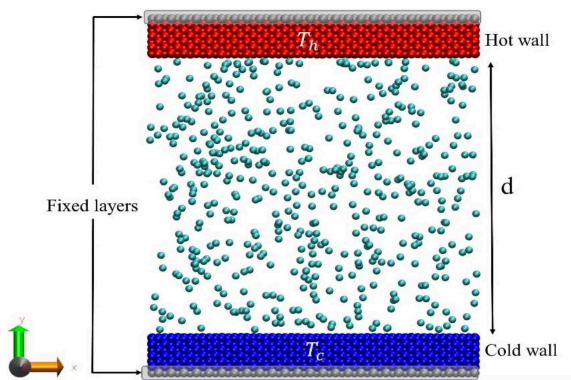


Figure 1: Schematic representation of molecular gas-wall interaction²

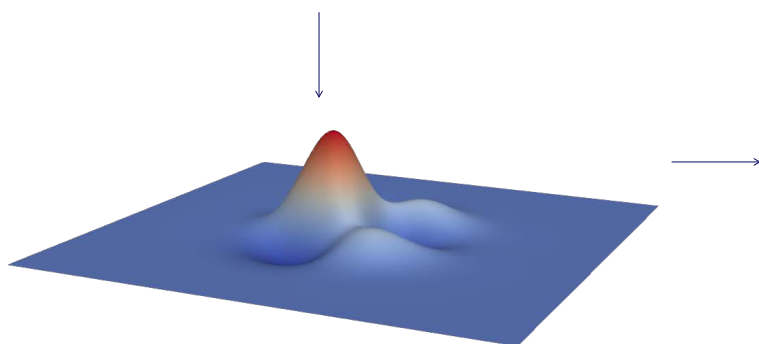


Figure 2: Computed distribution

The goals of this project are to improve the description of gas-wall interactions by using data generated by the Gaussian Mixture Model (GMM)² and investigate the influence of these interactions on the flow of rarefied gases. This will be done by setting up a method which exports data from the GMM and imports it into the MoM model. The latter will be used to solve the flow, using the GMM data as boundary conditions.

Tasks

- Develop procedure to communicate data generated by a Gaussian Mixture Model the Method of Moments model,
- Investigate the influence of the more detailed boundary description on the overall approximation properties,
- Develop an efficient method for integrating Gaussian distributions over half spaces.

STUDENT PROFILE

We are looking for a MSc student who:

- Has interest in the coupling between statistical and macroscopic thermodynamics,
- Has affinity converting abstract mathematical models to practical numerical implementations,
- Strong interest in programming and eager to improve upon their existing programming skills (e.g., Python).

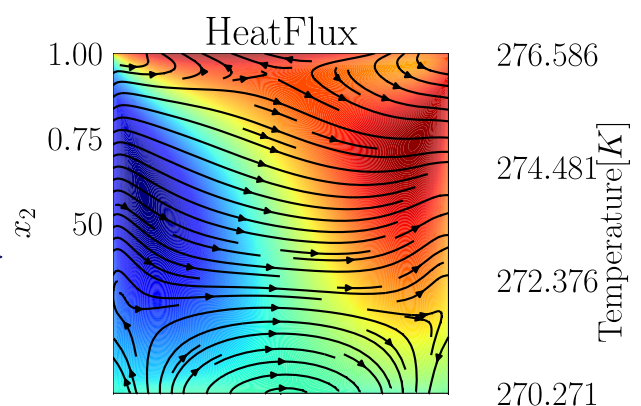


Figure 3: Computed macroscopic properties

REFERENCES

- [1] Nejad, S. M. N. et al. (2020). *The Influence of Gas-Wall and Gas-Gas Interactions on the Accommodation Coefficients for Rarefied Gases: A Molecular Dynamics Study*, Micromechanics, 11(3):319.
- [2] Abdelmalik, M. R. A. et al. (2016). *An entropy stable discontinuous Galerkin finite-element moment method for the Boltzmann equation*, Computers & Mathematics with Applications, 72(8): pp. 1988-1999.

Supervisor	Dr. Michael Abdelmalik
2 nd supervisor	Dr. Timo van Opstal
Company	Sioux Technologies
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME



Project number: 08

Rarefied Heat Transfer for Next-Gen Photolithography Machines

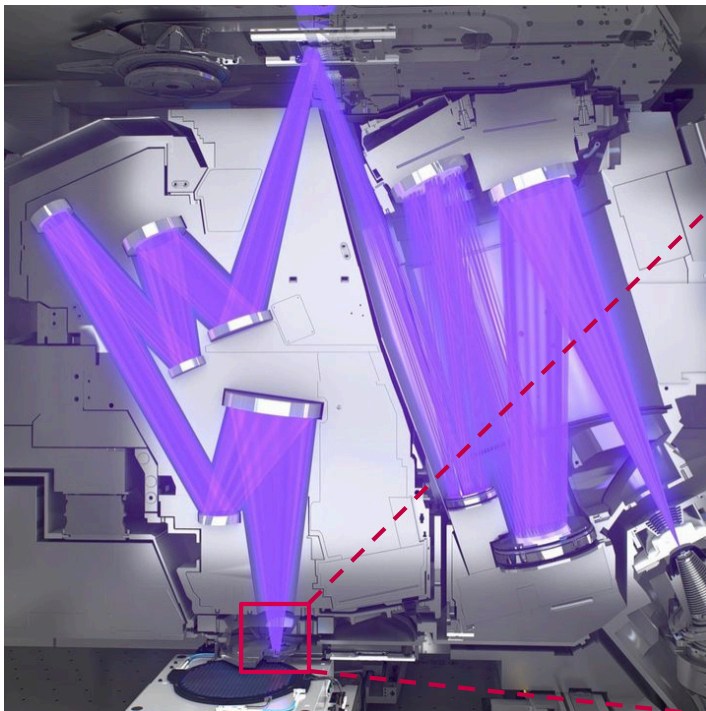
Michael Abdelmalik*, Timo van Opstal

*E-mail: m.abdel.malik@tue.nl

Keywords: *Rarefied Fluids, Finite Elements, Boltzmann Equation, Photolithography*

INTRODUCTION

Continuum/equilibrium models, such as Navier-Stokes, fail to govern gas flow in next-generation photolithography (PLM) machines because of the prevalence of rarefaction/non-equilibrium effects. In such applications, the Boltzmann equation (BE) provides a generalised flow model that bridges the continuum and rarefied regimes. Stochastic methods, such as Direct Simulation Monte Carlo (DSMC) are the mainstay method for BE in the rarefied regime. However, the stochastic nature of DSMC precludes resolution of the continuum-to-rarefied transition regime which is necessary for the next-generation PLMs.



Recently developed moment methods (MM) for BE have attracted much attention due to their deterministic nature, i.e. MM have the potential to address some key issues pertaining to DSMC in the transition regime.

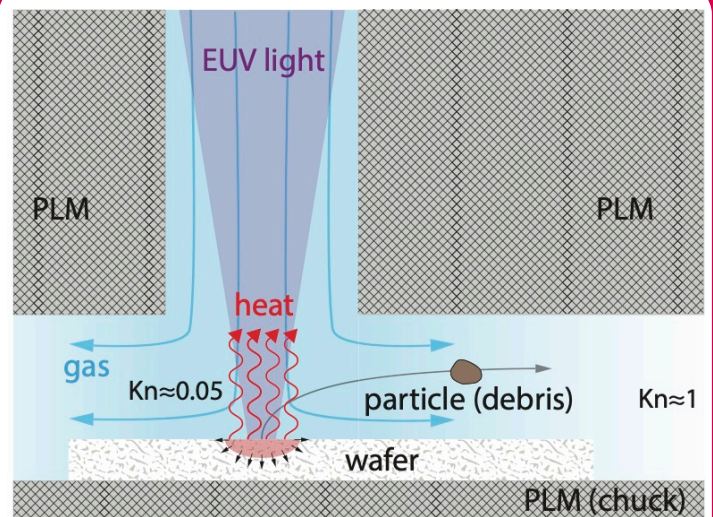
TASKS

- Set up benchmark 3D-1D problems in DSMC and MM (eg using SPARTA and NUTILS),
- Code optimization,
- Convergence analysis,
- Scan parameter space,
- 3D-3D benchmark problems,
- Experimental validation via literature data.

STUDENT PROFILE

We are looking for a MSc student who is interested in:

- mathematical multiscale modelling,
- converting abstract mathematical models to practical numerical algorithms,
- programming and eager to improve upon their existing programming skills (e.g., Python).



REFERENCES

- [1] Levermore, "Moment closure hierarchies for kinetic theories." *Journal of statistical Physics* 83.5 (1996): 1021-1065.
- [2] Abdelmalik, et.al.. "Moment Closure Approximations of the Boltzmann Equation Based on ϕ -Divergences." *Journal of Statistical Physics* 164.1 (2016): 77-104.

Supervisor	Dr. Clemens Verhoosel
2 nd supervisor	Prof. Dr. Olaf van der Sluis
Mentor	Robin Willems
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME



Project number: 09



ISOGEOMETRIC ANALYSIS OF AN ELECTROMECHANICAL BI-VENTRICULAR HEART MODEL

Robin Willems*, Clemens Verhoosel, Olaf van der Sluis

*E-mail: r.willems@tue.nl

Keywords: *Isogeometric Analysis, Finite Element Method, Cardiac Mechanics, Patient-specific*

INTRODUCTION

Computer simulations provide information that can be used by clinicians to support decision-making regarding the treatment of **Ventricular Tachycardias (VTs)**. It is the goal of this subproject to develop efficient and robust models that can be integrated into the clinical workflow.

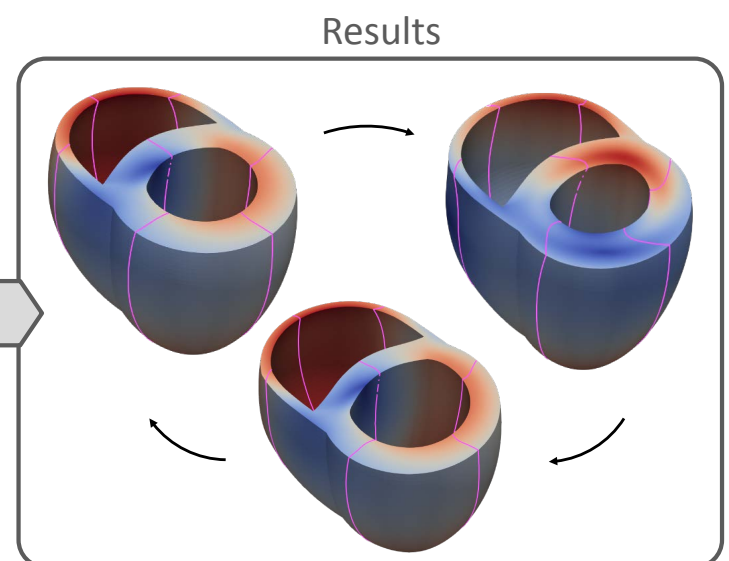
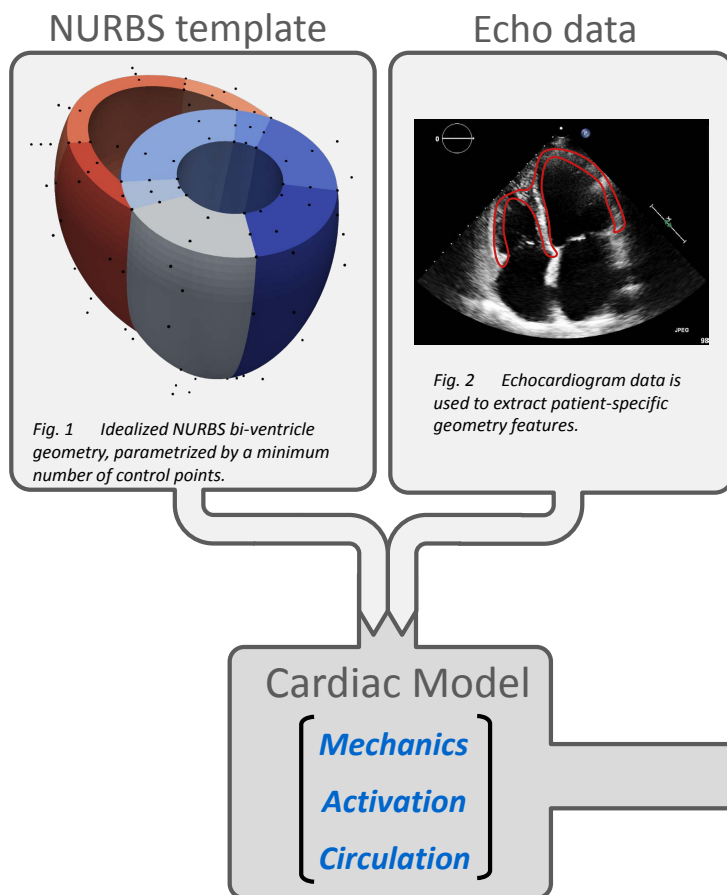
TASKS

- Develop procedure to fit NURBS template on echo data,
- Investigate parameter sensitivities using the existing IGA cardiac model (Single and Bi-ventricle),
- Uncertainty quantification analysis regarding clinical input and model output data,
- Development of an efficient Reduced Order model (ROM), suitable for clinical integration.

STUDENT PROFILE

We are looking for a MSc student who has:

- Affinity towards (advanced) numerical solution methods,
- Can operate and communicate in a multi-disciplinary project environment (Mechanical and Biomedical Engineering),
- Strong interest in programming and eager to improve upon their existing programming skills (e.g., Python).



Our simulation framework combines the Isogeometric Analysis (IGA) simulation paradigm [1] with image recognition techniques to obtain patient-specific computer models (Fig. 1 & 2).

REFERENCES

- [1] Hughes, T. J. R. et al. (2005). *Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement*, Comput. Methods in Appl. Mech. Eng., 194.39, 4135 - 4195.
- [2] Bovendeerd, P. H. M. et al. (2009). *Determinants of left ventricular shear strain*. Am J Physiol Heart Circ Physiol. 297(3):H1058-68.

Supervisor	dr.ir. Clemens V. Verhoosel
2 nd supervisor	
Mentor	dr.ir. Sai C. Divi
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME



Project number: 10



Stabilized Immersed isogeometric analysis of high Reynolds number incompressible flow problems

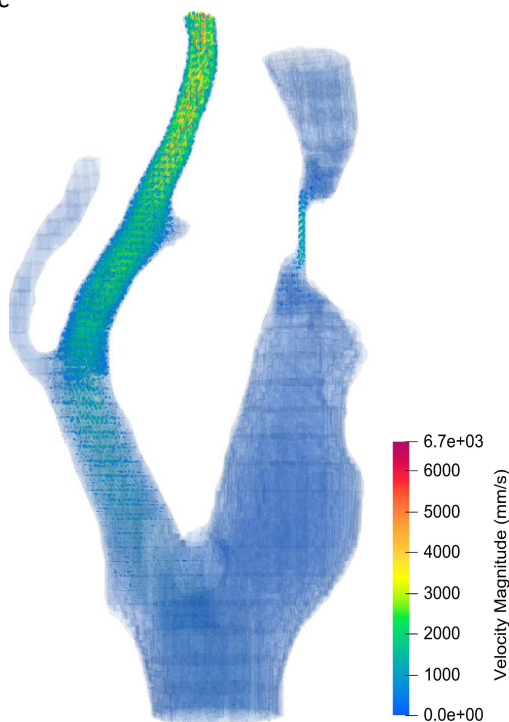
Sai C. Divi*, Clemens V. Verhoosel

*E-mail: s.c.divi@tue.nl

Keywords: *Isogeometric analysis, immersed methods, High Reynolds number flows, Turek benchmark*

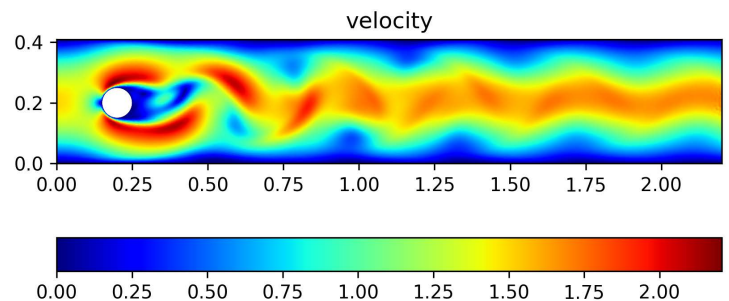
INTRODUCTION

The Finite Cell Method – a high-order immersed finite element method [1] – together with Isogeometric analysis – a spline-based finite element framework [2] – has been applied successfully in various fields, e.g., solid mechanics, scan-based analysis and in fluid-structure interaction.



TASKS

- Apply stabilization technique (for equal-order discretization) to high Reynold number flow problems.
- Perform a thorough literature study to understand existing time-discretization schemes applicable to immersed framework.
- Study and compare different time-discretization schemes and the quantities of interest (e.g., life and drag) for a Turek benchmark problem (i.e., flow around a cylinder).
- Apply the studied schemes to a scan-based biomedical application.



STUDENT PROFILE

We are looking for a MSc student who has:

- Affinity towards advanced numerical solution methods,
- Strong interest in programming and eager to improve upon their existing programming skills (e.g., Python).

PROBLEM STATEMENT

In order to use equal-order discretization for pressure and velocity field, we need to ensure stability by the Skeleton-penalty stabilization technique [3]. The suitability of the technique is well understood for low Reynolds number flow problems (e.g., flow in carotid artery). However, immersed isogeometric analysis of high Reynolds number incompressible flow problems is still challenging.

REFERENCES

- [1] Parvzian, J., Düster, A. and Rank, E., 2007. Finite Cell Method. *Computational Mechanics*, 41(1), pp.121–133.
- [2] Hughes, T.J., Cottrell, J.A. and Bazilevs, Y., 2005. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. *Computer Methods in Applied Mechanics and Engineering*, 194(39–41), pp.4135–4195.
- [3] Hoang, T., Verhoosel, C.V., Qin, C.Z., Auricchio, F., Reali, A. and van Brummelen, E.H., 2019. Skeleton-stabilized immersogeometric analysis for incompressible viscous flow problems. *Computer Methods in Applied Mechanics and Engineering*, 344, pp.421–450.

Supervisor	Prof. Harald van Brummelen
2 nd supervisor	
Mentor	Dr. Stein Stoter
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME



Project number: 11



Higher-order time-stepping methods for spatially adaptive schemes

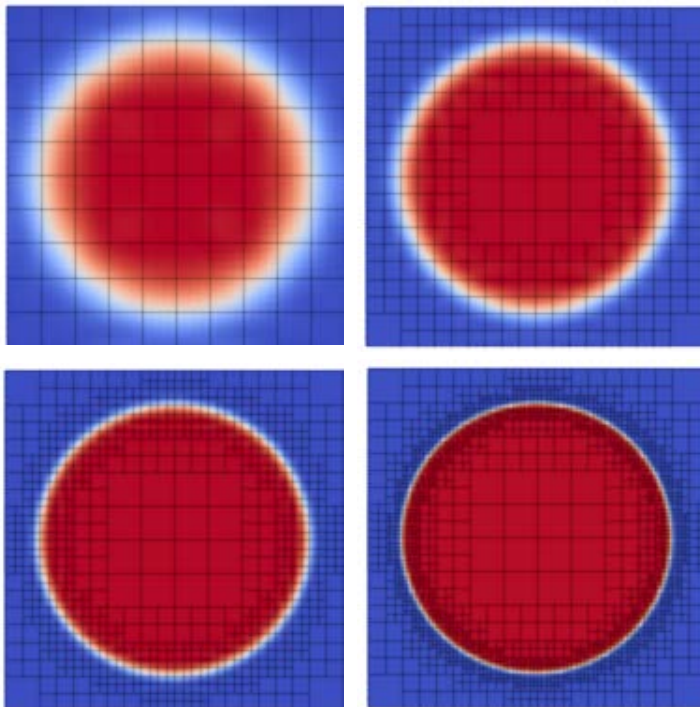
Stein Stoter*, Harald van Brummelen

*E-mail: k.f.s.stoter@tue.nl

Keywords: *Finite Element Method, Spatial adaptivity, Time-stepping, Higher-order*

INTRODUCTION

Numerical modeling always involves a trade-off between approximation quality and computational expense. Two techniques for improving quality while minimizing the increase in expense are higher-order approximation methods (e.g., in time) and local adaptivity (e.g., in space). Scenarios that particularly benefit from spatial adaptivity are physical problems that have interesting local features, such as the fluid-gas interface in the example below [1].

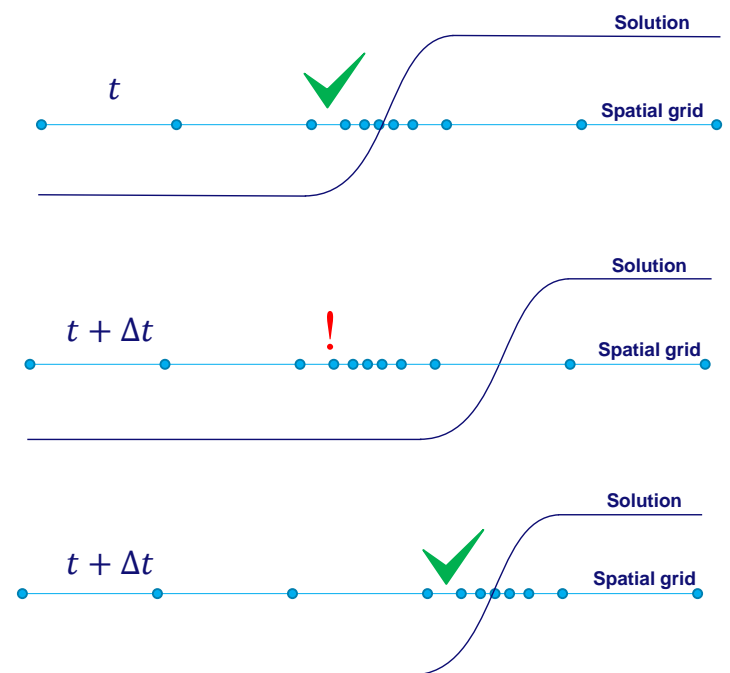


PROBLEM STATEMENT

It is challenging to design higher-order time stepping methods in a framework with spatial adaptivity. The reason is that the solution at the old and the new time-steps need to be represented on different spatial grids (see right figure).

RESEARCH TOPICS

- Perform a literature study to learn what higher-order time-stepping schemes are suitable in combination with spatial adaptivity.
- Implement a numerical approximation of a travelling shock with spatial adaptivity and different higher-order time-stepping schemes.
- Study the benefits and downsides for the different approaches.



STUDENT PROFILE

We are looking for a MSc student who has:

- Affinity towards (advanced) numerical solution methods,
- Strong interest in programming and eager to improve upon their existing programming skills (e.g., Python).

REFERENCES

- [1] van Brummelen, E. H. et al. (2022). *An adaptive isogeometric analysis approach to elasto-capillary fluid-solid interaction*, International Journal for Numerical Methods in Engineering, 122 (19), 5331-5352.

Supervisor	Prof. Harald van Brummelen
2nd supervisor	Dr. Clemens Verhoosel
Mentor	Maged Shaban
Company	Canon Production Printing
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical



Modeling and Simulation of Photopolymerization in Stereolithography Printing Process

Maged Shaban*, Clemens Verhoosel, Harald van Brummelen

*E-mail: m.m.m.shaban@tue.nl

INTRODUCTION

Additive Manufacturing (AM) has become an attractive and ubiquitous technology in rapid prototyping and in the biomedical realm. The adoption is mainly due to its free form flexibility and cost reduction during the manufacturing process.

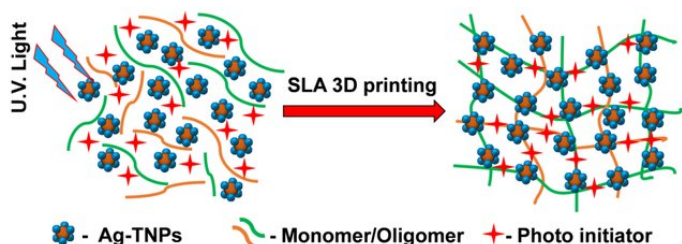


Fig. 1. The schematic illustration of the induced photopolymerization of under UV light for SLA

Stereolithography (SLA) is a sophisticated AM process that creates three-dimensional polymer and ceramic objects from a computer-aided design (CAD) file by using laser-initiated photopolymerization (see Fig. 1). SLA begins with a CAD of the desired object. The topology of the object is computationally divided into two-dimensional cross sections based on this design. The SLA device next scans a laser light throughout a vat of multifunctional photocurable monomer, drawing the cross-sectional shape on the monomer's surface. The layer is stabilized by an elevator in the monomer liquid that lowers after each laser pass. After forming a cross-section and lowering the elevator, the laser process is repeated to generate the desired object layer by layer (see Fig. 2).

Keywords: Free-radical polymerization, 3D Printing, Photopolymerization, Stereolithography

STUDENT PROFILE

- High motivation to research in the SLA process.
- Experience with Finite Element analysis and Computational Fluid Dynamics.
- Experience in COMSOL, MATLAB and Python.

TASKS

- Study Literature on photopolymerization process.
- To build a numerical model for photopolymerization process with identifying basic parameters and inter-parametric relations influencing the process.
- To develop and validate a photopolymerization model with different setups supported by essential FEM simulations (using COMSOL or Nutils)

BENEFITS

- Opportunity to be a part of state-of-the-art research into stereolithography modeling and simulation.
- This graduation project can be converted into a smaller internship project at Canon PP.
- You will get familiar with a pre-existing code and learn how to work and develop it.
- Develop programming skills in Python.
- Writing a report and collaborate on a scientific paper.

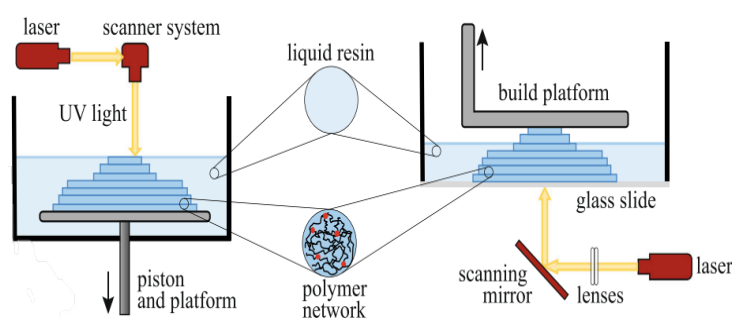


Fig. 2. Stereolithography printing process

REFERENCES

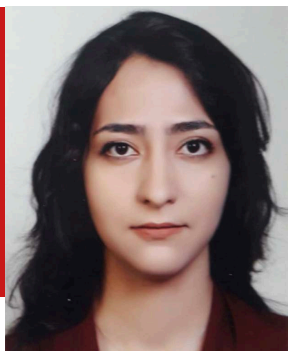
- [1] Goodner, M. D., & Bowman, C. N. (2002). Development of a comprehensive free radical photopolymerization model incorporating heat and mass transfer effects in thick films. *Chemical Engineering Science*, 57(5), 887–900.
- [2] Westbeek, S., van Dommelen, J. A. W., Remmers, J. J. C., & Geers, M. G. D. (2018). Multiphysical modeling of the photopolymerization process for additive manufacturing of ceramics. *European Journal of Mechanics, A/Solids*, 71, 210–223.

Supervisor	Dr. Azahara Luna-Triguero
Mentor	Shima Rezaie
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME-SET



Project number: 13



METASTABLE MOLECULAR HYDROGEN AT CRYOGENIC AND NON-CRYOGENIC CONDITIONS

S. Rezaie, A. Luna-Triguero

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INTRODUCTION

There are two main reasons for which hydrogen is considered the energy solution of the future; i) the highest gravimetric energy density known, ii) no carbon dioxide emissions.

Due to its low density under ambient conditions, the storage of hydrogen is challenging energy intensive; some solutions for storing hydrogen are compressed hydrogen gas in stationary tanks or underground cavities, and cryogenic liquid [1].

Hydrogen appears to be very simple but has unique properties and a very rich phase diagram. Molecular hydrogen can be found in two isomeric forms, the most stable state, or normal state (para), and the metastable state (ortho). The mixture ratios of isomeric hydrogen depend on the external conditions, and while at cryogenic temperatures, the orthohydrogen transforms to parahydrogen spontaneously, at 300 K the ratio can reach 1:3. The transition from ortho to para is exothermic, releasing high amounts of energy (heat) which can have several implications for its storage [2].

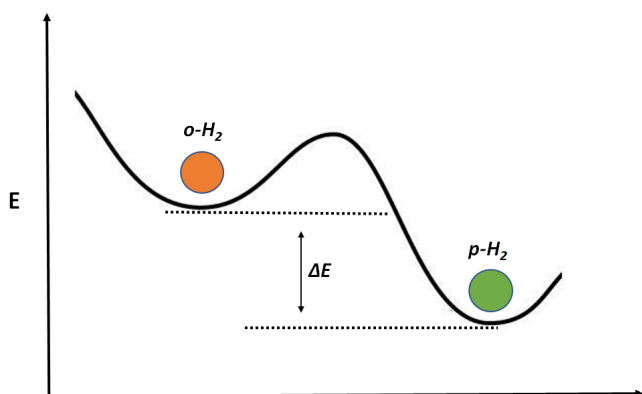


Fig. 1. Schematic representation of molecular hydrogen energy profile.

GOAL

Understand hydrogen isomeric transitions (ortho-para) and its effect in energy storage and utilization at different conditions.

Keywords: #hydrogen storage #isomers #heat release

TASK

In this project, you are expected to:

- Review relevant literature on dihydrogen phase diagram and computational methods.
- Investigate the states of hydrogen at isothermal conditions (Figure 2).
- Identify metastable states and obtain density and conductivity diagrams.

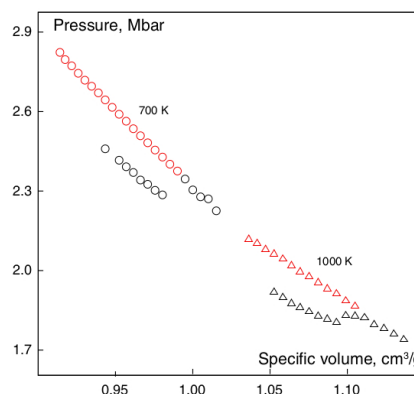


Fig. 2. Example of EoS of dense hydrogen. Metastable states in red. (adapted from reference [3]).

STUDENT PROFILE

We are looking for a high-motivated MSc student who has:

- An interest in fundamental and computational work.
- Hands-on attitude toward new challenges.
- Analytical capacity
- Eager to participate as an active member of the group
- Experience with first-principles simulations is desired but not mandatory

REFERENCES

- [1] Flynn, T. (2004), Cryogenic Engineering, 2nd Ed. Taylor & Francis. ISBN: 0824753674
- [2] Manyalibo J. Matthews, M.J., Petitpas, G., Aceves, S, M. A study of spin isomer conversion kinetics in supercritical fluid hydrogen for cryogenic fuel storage technologies, *Appl. Phys. Lett.* 99, 081906 (2011)
- [3] Norman, GE, Saitov, IM, Sartan, RA. Metastable molecular fluid hydrogen at high pressures. *Contributions to Plasma Physics* 2019; 59.

Supervisor	Dr. Maja Rücker
Mentor	Gijs Wensink
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Experimental and Numerical modeling

Available for ME-SET



Project number: 14

Digitally Enhanced Mechanical Mapping of Rough Substrates

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INTRODUCTION

From Teflon pan to professional swimming suits: many applications rely on an efficient way to repel specific fluids. The design of materials for such applications focusses on improving the repellence by using a rough material surface, mimicking e.g. the structure of shark skin or the leaves of the Lotus flower. Recent advances have enabled the usage of Atomic Force Microscopy (AFM), a tool for mapping surfaces down to the nanoscale by mechanical means (Figure 1), to assess such rough structures. Yet, the image quality is highly dependent on the probe (cantilever) used and the exact structure assessed (sample).

In this study, you will investigate the behaviour of the probe whilst it raster-scans the surface using a mix of modelling and experimental approaches to improve AFM data processing, allowing for more robust interpretation in assessing surface modification and water repellence.

Keywords: Atomic force microscopy, surface roughness

TASKS

In this project, you will be expected to complete the following tasks:

- Reviewing the relevant literature on rough surfaces, atomic force microscopy and interaction forces.
- Perform experiments with Atomic Force Microscopy on flat and rough surfaces.
- Create a numerical model describing how the important interactions influence AFM imaging.
- Compare the results of the model with the experimental measurements.

GOALS

- Identify the relation of chemical and mechanical forces acting between probe and surface during AFM measurements.
- Develop new methods for AFM data interpretation regarding surface modification and water repellence.

BENEFITS

In this project, you will benefit from:

- Improving your laboratory skills and learning how to design and carry out experiments.
- Gaining experience on creating numerical models and interpreting their results.

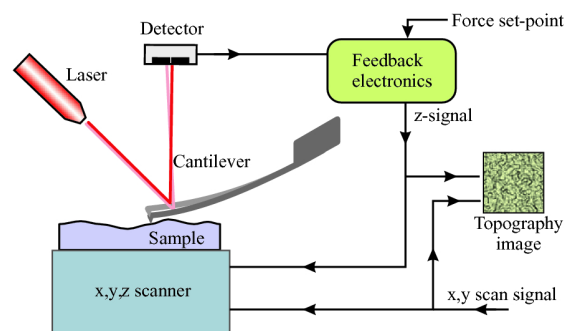


Figure 1: Principles of atomic force microscopy [1]

REFERENCES

- [1] Voigtländer, B. (2019). Introduction. In: *Atomic Force Microscopy. NanoScience and Technology*. Springer, Cham. https://doi.org/10.1007/978-3-030-13654-3_1
- [2] Yesufu-Rufai, S., Rücker, M., Berg, S., Lowe, S. F., Marcelis, F., Georgiadis, A., & Luckham, P. (2020). Assessing the wetting state of minerals in complex sandstone rock in-situ by Atomic Force Microscopy (AFM). *Fuel*, 273, 117807. <https://doi.org/10.1016/J.FUEL.2020.117807>

Supervisor	Dr Maja Ruecker
External Collaborator	Dr Pavani Cherukupally (MIT)
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Analysis

Available for ME-SET



Project number: 15

Fluid dynamics in artificial sponges used for environmental remediation

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INTRODUCTION

Oil spills polluting water reservoirs represent a major environmental problem (Figure 1). In particular, if the oil forms a suspension with the water, the separation of the contaminant represents a major challenge.



Fig. 1. Filtration of contaminated water by sponges [1]

In this study, you will investigate the fluid dynamics in artificial sponges used for the filtration of water with a focus on oil removal. You will join experiments using micro-computed tomographic imaging (Figure 2), analyse respective data (Figure 3) and assess the quality of a range of different modifications to link up the sponge design features with the response in flow dynamics and filtration efficiency.

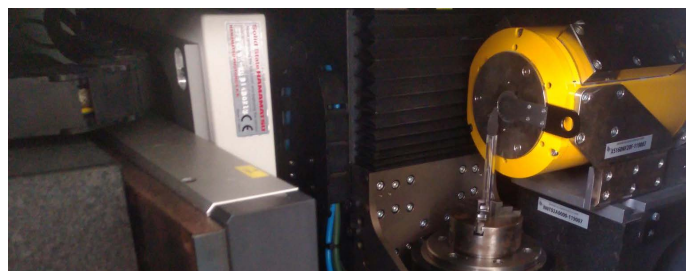


Fig. 1. Micro computed tomography equipment in the multi-scale lab.

GOAL:

Relating design features of artificial sponges for water filtration with flow dynamics and sponge efficiency

BENEFITS

- You will be working with an international team of scientists addressing current challenges for sustainable utilization of porous materials
- Gain experience in experimentation, image processing and analysis
- Advancing our understanding of fluid dynamics in porous systems

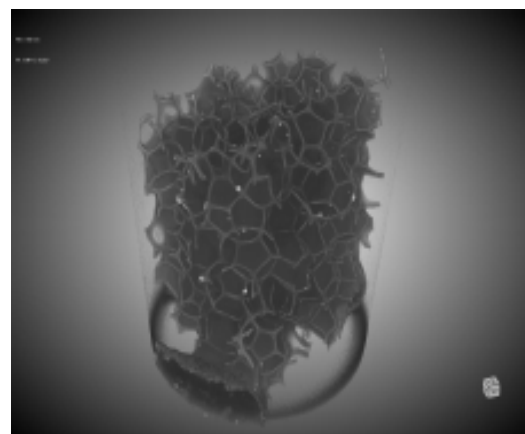


Fig. 1. 3D image of an oil saturated sponge.

REFERENCES

- [1] Abidli, A., Huang, Y., Cherukupally, P., Bilton, A. M., & Park, C. B. (2020). Novel separator skimmer for oil spill cleanup and oily wastewater treatment: From conceptual system design to the first pilot-scale prototype development. *Environmental Technology & Innovation*, 18, 100598.
- [2] van Kempen, K. D. (2016). Translating digital rock imaging techniques to the analysis of pore-scale wetting of foams to bridge the gap between molecular interactions and macro-scale wetting. MSc thesis. Eindhoven University of Technology

Study on the impact brine viscosity on CO₂ entrapment in subsurface reservoirs using 3D in-situ measurement data from the Swiss Light Source

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Fig. 2. Swiss Light Source (Villigen, Switzerland)

INTRODUCTION

The interaction of multiple fluids in the subsurface is a complex and multi-faceted problem of great importance due to its presence in a broad range of applications including carbon sequestration (Figure 1) and aquifer contaminant containment.

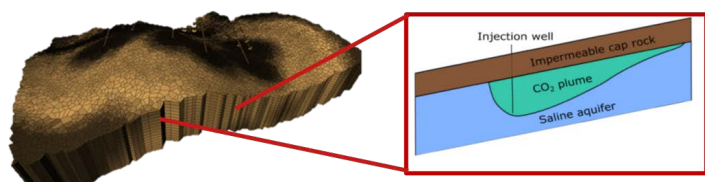


Fig. 1. Subsurface CO₂ storage.

Recent advances in X-ray imaging has allowed fluids to be imaged in-situ, and a range of flow phenomena have been identified [1-3] that will influence the propagation and trapping of fluids within a rock. These flow dynamics will control how much CO₂ can be stored safely underground, or the necessary steps to remediate groundwater contamination.

A key parameter for flow dynamics is the viscosity ratio (this is the ratio of the viscosities of the fluids present). To understand how viscosity ratio controls the change in dynamics is of great importance, and provides the potential to engineer CO₂ storage using novel injection strategies to maximize CO₂ saturation and decrease the size of the CO₂ plume in the subsurface. Fast X-ray imaging conducted at the Swiss Light Source (Villigen, Switzerland) was used to explore the role of the viscosity ratio of flow dynamics. For these experiments, two fluids were injected simultaneously into a carbonate rock sample. Then the viscosity of one of the fluids (the water) was altered to change the viscosity ratio (M). This led to a large change in the flow dynamics, qualitatively shown in Figure 2.

Quantifying the changes caused by the viscosity ratio in this state-of-the-art data set will provide a unique opportunity to understand how changes in viscosity cause flow patterns to evolve and what this means for potential trapping.

GOAL:

Quantifying the changes in entrapment and flow dynamics caused by the viscosity of different fluids

BENEFITS

- You will be working with an international team of scientists addressing current challenges for sustainable utilization of subsurface resources
- Gain experience in computational image & large data processing
- Advancing our understanding of fluid dynamics in porous systems

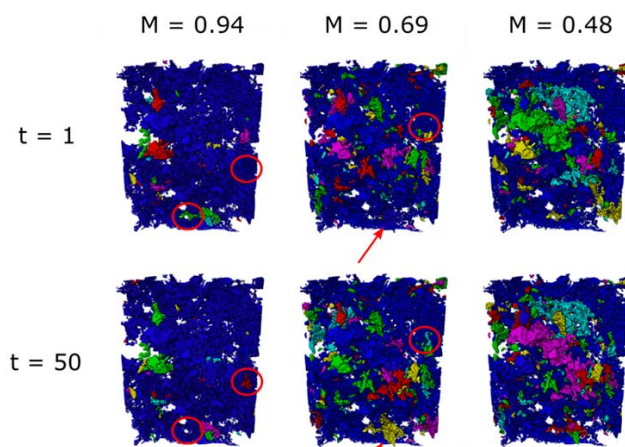


Fig. 3. The distribution of the oil phase (rock and water transparent) for different viscosity ratios (M) at two different times (t). Each connect region of oil has been assigned a different colour to show the connectivity.

REFERENCES

- [1] Spurin, C., Bultreys, T., Rücker, M., Garfi, G., Schlepütz, C.M., Novak, V., Berg, S., Blunt, M.J. and Krevor, S., 2020. Real-Time Imaging Reveals Distinct Pore-Scale Dynamics During Transient and Equilibrium Subsurface Multiphase Flow. *Water Resources Research*, 56(12), p.e2020WR028287.
- [2] Spurin, C., Bultreys, T., Rücker, M., Garfi, G., Schlepütz, C.M., Novak, V., Berg, S., Blunt, M.J. and Krevor, S., 2021. The development of intermittent multiphase fluid flow pathways through a porous rock. *Advances in Water Resources*, 150, p.103868.
- [3] Rücker, M., Berg, S., Armstrong, R.T., Georgiadis, A., Ott, H., Schwing, A., Neiteler, R., Brussee, N., Makurat, A., Leu, L. and Wolf, M., 2015. From connected pathway flow to ganglion dynamics. *Geophysical Research Letters*, 42(10), pp.3888-3894.

Borehole acoustic Stoneley wave measurement in porous sandstone

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INTRODUCTION

To accurately evaluate and predict the properties and productivity of hydrocarbon formations, permeability assessment of the formation is becoming more important. Borehole acoustic Stoneley wave plays an important role in obtaining formation permeability. This project is collaborated with PetroChina, a famous oil company in the world. For this project, we will conduct small size acoustic setup to measure pure Stoneley wave with source inside a borehole. Different rock samples (figure 1) will be used.

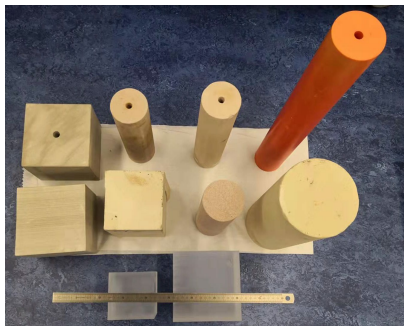


Figure 1: Rock samples for borehole Stoneley wave measurement

EXPERIMENTAL

Experiments will be conducted based on the acoustic measurement set up, which was designed by Yukai Liu. The schematic and photo are shown in figure 2 and figure 3, respectively.

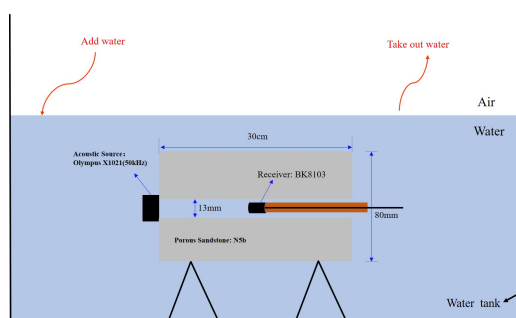


Figure 2: Schematic of borehole Stoneley wave measurement

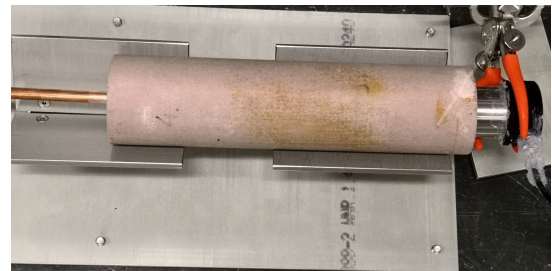


Figure 3: Photo of borehole Stoneley wave measurement setup

GOAL

The goal of this project is to measure the pure Stoneley wave excited by an acoustic source inside a borehole. The borehole size, frequency, different rock types and sound absorbing material outside borehole will be considered.

TASKS

- Conducting experiments on borehole Stoneley wave measurements with different rocks, frequencies and sound absorbing materials.
- Interpreting the experimental results.

REQUIREMENTS

- Interested in experimental studies is preferred. Especially acoustic or electromagnetic wave experiment.
- Experience in applied physics, mechanical engineering or electrical engineering.
- Knowledge on sound or electromagnetic wave generation and propagation.

Supervisor	Prof. David Smeulders
2nd supervisor	
Mentor	
Company	Bosch
Internal / External	External
Starting date	ASAP
Exp./Num./Design	Experimental and design

Available for ME



Investigating the static and dynamic behavior of airfoil bearings – Automotive Industries

d.m.j.smeulders@tue.nl

Company Description

Currently, we are looking for a Master's thesis student who will be doing research on the *"Development of a dedicated simulation model to investigate the static and dynamic behavior of airfoil bearings."*

The automotive industry is facing its biggest and fastest transformation yet. The Bosch manufacturing plant in Tilburg is showing its innovative muscles by developing and industrializing unique products that will serve the markets of now and the future. Thanks to our entrepreneurial spirit combined with the know-how and means of Bosch, we are on the verge of creating groundbreaking innovative solutions. Will you help shape the technology of the future?

Bosch Tilburg is part of the Bosch Group, a leading global supplier of technology and services, with roughly 395,000 associates worldwide. Bosch is the number one supplier in the automotive industry worldwide and is investing heavily in electrification and fuel cell technologies.

Team

You will be doing your research within a compact, multidisciplinary team (+- 5 persons) that is working on the development and (mass) manufacturing of airfoil bearings. Within this team, 1 simulation specialist is active with whom the student will closely work.

Your assignment

1. Extend an existing dynamic Recurdyn model of an air foil bearing system using a standard available Recurdyn hydrodynamic toolbox
2. Develop a custom hydrodynamic sub-solver to add compressibility to the existing model instead of the standard toolbox.

Qualifications

Need to have's

- You will start working on your master's thesis soon;
- You are studying at a technical university;
- You have good mathematical and analytical skills;
- You have knowledge of Finite Element Method;
- Your English is very well (written and verbally).

Nice to have's

- You already have knowledge of Multi-Body Dynamics;
- You are a very motivated person;
- You are able to work independently.

Additional Information

We offer

- A challenging working environment of an international and pioneering organization;
- Nice compensation for your efforts;
- Opportunity to (also) work from home.

Contact with Bosch will be initiated via prof. Smeulders. Selection process will be done by Bosch.

Supervisor	Dr.ir. Arjan Frijns
2nd supervisor	Company supervisor
Mentor	
Company	TNO, EPFL
Internal / External	External or internal (in coll. with company)
Starting date	Any time
Exp./Num./Design	Modelling/Experiments

Available for ME-SET



Project number:

Beyond the thermal comfort limits: Modelling of heat transfer throughout the human body

Arjan Frijns

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INTRODUCTION

Fast technological developments and the ever increasing complexity of new technological products require novel, intelligent ergonomic solutions. The “human factor” has become central to many of these endeavors. Over the last decades, there has been a steadily growing demand from research and industry for reliable models simulating human thermal and perceptual responses in various applications such as improved (and low-energy) individual thermal comfort in offices and dwellings, improved sleeping comfort, and optimal human performance during extreme outdoor conditions.

For optimizing individual and local thermal well-being of occupants a proper understanding of local thermal sensation and thermal comfort is essential. In close collaboration with Maastricht University, we developed the dynamic thermoregulation model ThermoSEM which is based on neurophysiological mechanisms combined with internal heat transfer mechanisms. The model is validated with human studies in climate chambers. Also, the interindividual differences of humans can be captured well for moderate conditions.

GOAL

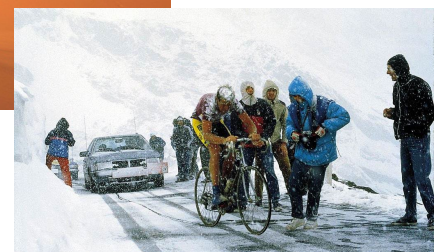
The aim of this project is to extend our thermal comfort model ThermoSEM for improved individual thermal comfort in offices and dwellings (saving energy while improving human health), improved sleeping quality and improved human performance under extreme conditions.

The focus is on numerical modelling, but it is also possible to get involved in human studies at our partners.

The tasks in this project are:

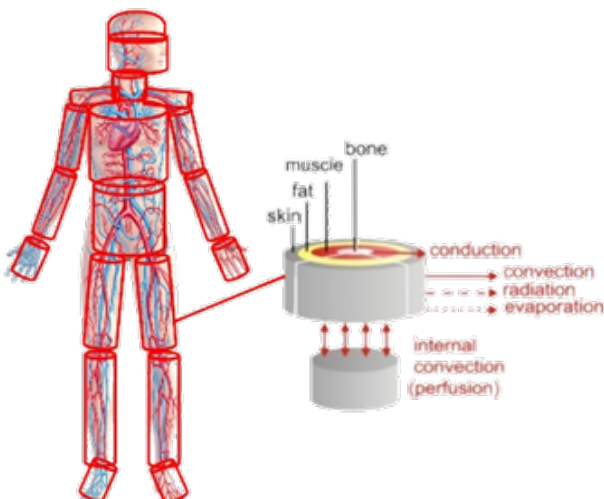
- Further development of our thermophysiological model ThermoSEM.
- Testing and validation of the improved model by climate chamber experiments and literature.

The project will be done in close collaboration with research institutes and companies.



REQUIREMENTS

- Experience in CFD modeling and/or thermal network modeling (Simulink or Matlab)
- Interest in human physiology
- Interest in working in interdisciplinary teams



Supervisor	
2nd supervisor	dr. ir. Camilo Rindt
Mentor	ir. Nico van Ruth
Company	Conico Valves bv
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME-SET



Project number: 20



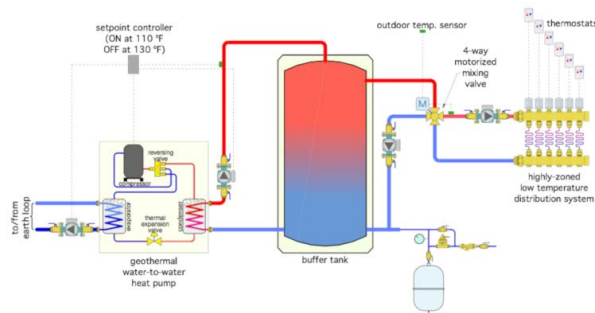
OPTIMISING HEAT PUMP OPERATING- AND STORAGE- STRATEGIES FOR FLUCTUATING ELECTRICITY PRICES

Nico van Ruth¹, Camilo Rindt²

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INTRODUCTION

Heat pumps are ever more widely used for space heating in the built environment, as the shift away from fossil fuels takes shape.



At the same time, variabilities in supply and demand on the electricity grid are increasing, in particular due to the increasing share of intermittent electricity producers (solar-PV and wind) in the electricity supply, leading to sharp variations in short term (hourly) electricity pricing. To make use of these variations in electricity pricing, the operating strategy of a heat pump can be tailored so it operates more during hours of low electricity pricing, particularly if a significant amount of heat can be stored in a heat-buffer. The performance of such a heat-buffer for heat pumps, in terms of stratification and thermal mixing, can have a significant impact on the performance of the overall system, so careful attention to stratification is warranted [1].

Keywords: Heat pumps, thermal storage, electricity grid, energy transition, stratification

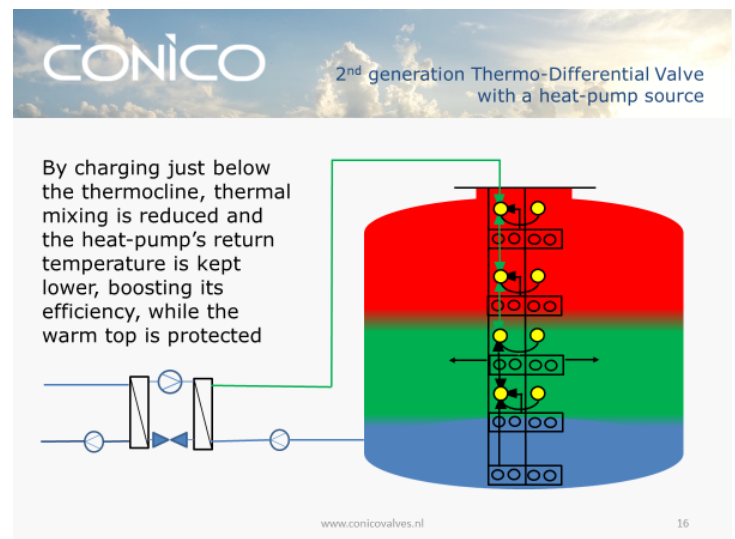
TASK

We are looking for a highly motivated MSc student with interests in energy technology and numerical modelling. In this project, you are expected to do:

- Develop a model of a heat-pump based space heating system of a building, using TRNSYS simulation studio
- Develop and test different system designs and operating strategies to optimise the performance
- Perform LCOH analysis on the modelled systems

GOALS

- To identify the optimal coupling between hourly electricity pricing and heat-pump operation
- To test different heat storage configurations to optimize the economic performance
- To investigate the role of stratification in the heat storage tank
- To investigate the economical benefit of using a Thermo-Differential [2] stratifier in the heat-buffer



BENEFITS

- Opportunity to work with a company on the design of a commercial product
- Develop a thorough understanding of heat-pumps and heat-pump storage technology
- Gain experience with developing TRNSYS modelling of built-environment energy systems

REFERENCES

- 1) M.Y. Haller et al. (2013), Hydraulic integration and control of heat-pump and combi-storage: same components, big differences. *Energy Procedia* 48, p571-580
- 2) N.J.L. van Ruth (2016), New type of valve for solar thermal storage tank stratification. *Energy Procedia* 91, p246-249

Supervisor	Wout Gubbels
Mentor	
Company	Suncom-Energy
Internal / External	External at Suncom
Starting date	Any time
Exp./Num./Design	Experimental, numerical and design

Available for ME-SET/PT/ET



Project number: 21

Thermal analysis of a novel square heat receiver

Wout Gubbels

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INTRODUCTION

Concentrated Solar Power (CSP) is a form of solar thermal energy generation where sunlight is caught on parabolic reflectors, which concentrate it onto heat receivers. This concentrated sunlight can heat a heat transfer fluid running through the receiver to over 500 °C.

The central element in Suncom's design is a square heat receiver. This heat receiver is partially insulated by a radiation heat shield and enclosed in a glass annulus under vacuum, as can be seen in figure 2. The insulation substantially increases the efficiency of the receiver and therefore makes it possible to utilize a smaller reflector, opening up new potential markets.

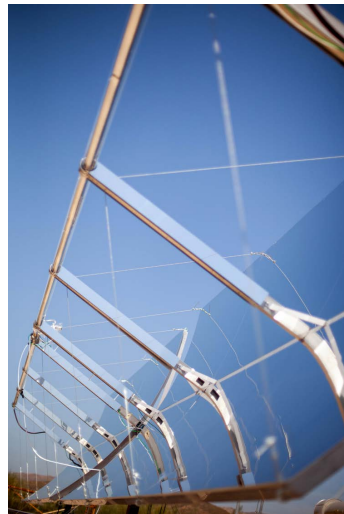


Fig. 1. Latest prototype undergoing testing in PSA, Spain

The latest version of Suncom's solar trough has been tested in Plataforma Solar de Almeria (PSA) during the summer of 2022. Currently Suncom is preparing to build their first 1MWth demonstration plant in Spain in 2023.

Keywords: Concentrated Solar Power, Thermal Energy, Testing, Efficiency.

TASK

We are looking for an entrepreneurial and enthusiastic MSc student who has interests in both modelling, experimental work and thermodynamics. In this project you are expected to:

- Construct a multiphysics model to describe the receiver.
- Model and analyse what effect insulating the receiver has on the resulting thermal boundary layer in the Heat Transfer Fluid (HTF).
- Use the model of the thermal boundary layer to predict temperatures in the receiver based on point data.
- If possible, perform experiments with the receiver to validate model predictions.

GOALS

- Provide a numerical analysis on the thermal behaviour of the receiver to complement existing experimental findings.
- Create a correlation between sensor data and resulting temperatures in the receiver.
- Determine optimal flow conditions by minimizing pressure drop whilst maximizing thermal efficiency.
- Quantify the number of sensors needed to predict extreme temperatures in the system.

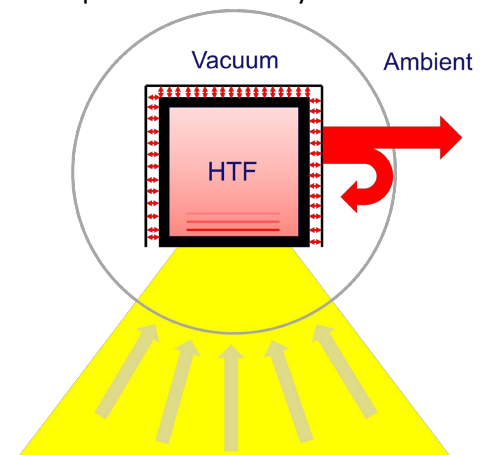


Fig. 2. Schematic cross-section of receiver in focus and insulated with radiation shield

BENEFITS

- Experience to work in a mission-driven start-up and help tackle climate change.
- A flexible work environment with a lot of responsibility and ownership.
- A fun office environment at a well reachable location in Utrecht (close to station Leidsche Rijn and the A2).
- An internship compensation of €500,- per month.
- A possibility to join the company after successful completion of your internship, with the opportunity to become co-owner.

REFERENCES

- Forristal et al. (2004), *Heat Transfer Analysis and Modeling of a Parabolic Trough Solar Receiver Implemented in Engineering Equation Solver*, National Renewable Energy Laboratory Technical Report.
- Lovegrove et al. (2012), *Concentrating Solar Power Technology*, Woodhead Publishing.

Supervisor	Camilo Rindt
Mentor	Mengting Jiang
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME-SET



Project number: 01

A data driven reduced order model for thermochemical heat storage systems

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INTRODUCTION

Thermochemical heat storage (TCHS) (see Fig.1) is among the most promising options to increase renewable energy use by bypassing the issue of the intermittence of renewable resources.

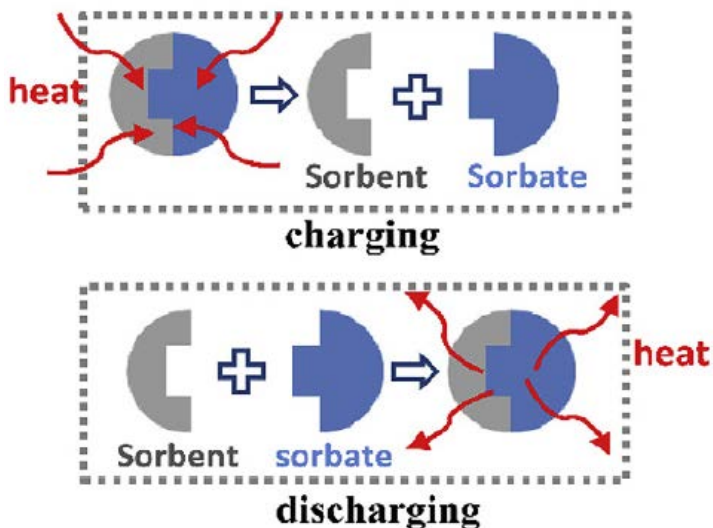


Fig.1 The working principle of a TCHS

It is based on the principle that energy is stored in the form of chemical bonds and intermolecular interactions. When a sorbent comes into contact with a sorbate, an exothermic process takes place and heat is released. The reverse process consists of applying heat to the sorbent-sorbate system to separate the components, this way the energy storage is charged. Since the components can be stored separately, there is virtually no heat loss. The sorbents that are used as materials for storing heat are also known as thermochemical materials (TCMs). Silica gel was proven to be a suitable material for the long-term storage of solar energy since it has a low charging temperature (75 °C) and it presents no thermal degradation. It is therefore selected as the TCM in this research.

PROBLEM DESCRIPTION

The successful integration of a TCHS for covering a heat demand is reliant on efficient time prediction of the heat that the system can deliver based on the current state of charge of the system and the temperature of the fluid to which the system is transferring heat. The dynamic simulation of a TCHS that concerns fluid flow, and mass and heat transfer relies on solving PDEs based on temporal and spatial discretization such as the Finite Element Method (FEM). Such simulations can provide accurate results but are computationally expensive. Reduced Order Models (ROMs) assume that most solutions of high-dimensional problems can be approximated by a lower-dimensional representation. As such, we aim at developing a ROM for the dynamic simulation of TCHSs. A Proper Orthogonal Decomposition (POD) based parametric ROM has been developed and tested on a representative section of a silica gel bed of a closed adsorption heat storage. In this project, the ROM is expected to be applied on the dynamic simulation of a real size TCHS.

TASKS

- Literature study on the topic, this includes:
 - Numerical simulations of TCHS
 - Model order reduction techniques
 - ROM for thermal energy storages
- Perform COMSOL simulations on a real size TCHS. The COMSOL simulation results will be used as the high-fidelity training data for the development of the ROM.
- Identify the most important parameters for further investigation in the ROM
- Understand the POD based ROM that has already been developed, and apply it on the real size TCHS
- Perform a district heating system simulation using the ROM for the TCHS (charged by solar thermal collector) and an in-house ROM for pipeline networks.
- Analyse the results and write a report

Supervisor	Dr. Clemens Verhoosel
2 nd supervisor	Dr. Mitrofan Curti
Mentor	Doga Ceylan
Company	Collaboration with the Dept. of Electrical Engineering
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME

TU/e EINDHOVEN
UNIVERSITY OF
TECHNOLOGY

Project number:23



An Improvement in the Cooling Structure of High-torque Permanent-magnet-free Electric Motors

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Keywords: *Permanent-magnet-free electric motor, high-torque, air gap airflow, cooling*

INTRODUCTION

High-torque generation requires a large amount of permanent-magnet usage in permanent-magnet-based electric motors. Therefore, the electrification of heavy-duty vehicles is limited by the price of the electric motor, when permanent-magnet-based motors are employed.

In this project, a permanent-magnet-free electric motor designed for an electric tractor will be investigated, aiming at an improved cooling structure. Fig. 1 illustrates the traction motor of an electric tractor. The analyzed motor has both ac- and dc-field windings in its stator, while the rotor consists solely of electrical steel without any excitation, i.e., no heat source in the rotor. A water jacket is placed outside of the stator to cool down the stator windings.

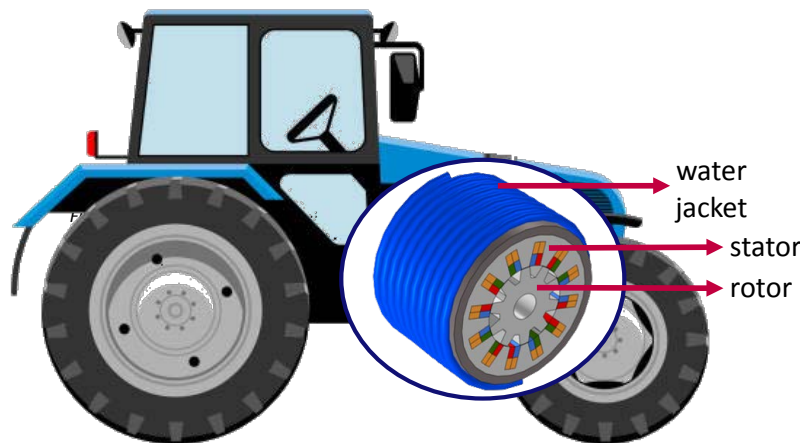


Fig. 1 A permanent-magnet-free electric motor in an electric tractor.

The water jacket transfers the generated heat from one side of the stator windings. In addition, the airflow generated by the rotation of the rotor cools down the stator windings from the other side. The objective of this project is to maximize the heat transfer done by the airflow in the air gap between the stator and rotor. The rotor slots, shown in Fig. 2, will be filled with a non-magnetic material to boost the airflow from the rotor to the stator. The material and shape of the filling will be optimized to achieve maximum heat transfer.

TASKS

- Develop analytical and numerical models to simulate the airflow between the rotor and stator due to the rotor rotation.
- Analyze the influence of filling the rotor slots with a non-magnetic material on the heat transfer from stator windings by means of developed analytical and numerical models.
- Analyze the effect of using an external fan connected to the rotor with and without rotor slot fillings.
- Optimize the shape of the filling material in rotor slots aiming at the maximum heat transfer from stator windings.

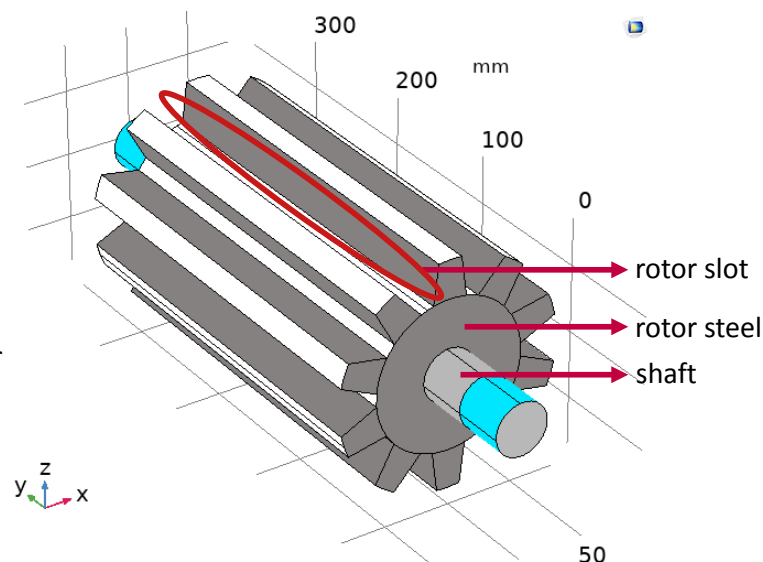


Fig. 2 The rotor of the analyzed permanent-magnet-free electric motor without any filling in its slot.

STUDENT PROFILE

We are looking for a MSc student who has:

- Affinity towards advanced analytical and numerical solution methods to compute the airflow inside electric motors,
- Can operate and communicate in a multi-disciplinary project environment (Mechanical and Electrical Engineering),
- Strong interest in simulation and optimization and eager to improve their existing modeling skills.

Supervisor	Dr. Silvia V. Gaastra-Nedea
2nd supervisor	
Mentor	
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Num. and design

Available for ME-SET



Project number: 25

NEW MATERIALS FOR ENERGY STORAGE

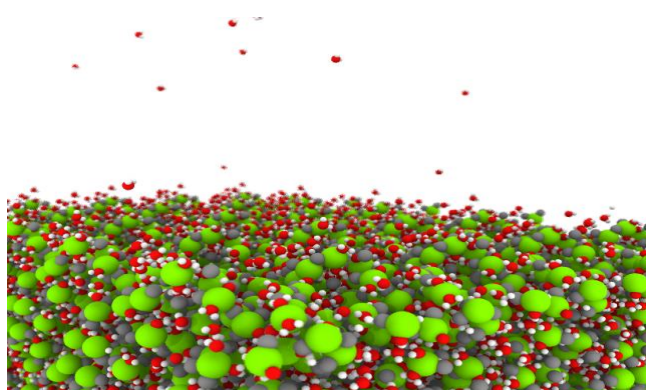
Silvia V. Gaastra-Nedea

*E-mail: s.v.nedea@gaastra.it

INTRODUCTION

In order to promote renewable resources a reliable storage system is necessary. Among different approaches to store energy, thermochemical heat storage is a highly appealing. It is based on a reversible chemical processes, like sorption of water in hygroscopic salts. Salt-hydrates are one of the most relevant materials, because of their availability, costs, operating temperature, and energy density.

The concept of storing heat in a salt hydrate is based on the following three steps. (1) In a charging cycle (endothermic reaction) the salt hydrate adsorbs solar energy and disintegrates into a lower hydrate and water vapor. (2) The water and salt are stored separately. (3) In discharging (exothermic reaction) the dried salt hydrate is recombined with H₂O, and forms a higher hydrate again, which results in a release of heat. This allows one to store heat almost without losses over long periods of time in a compact and efficient way. However, challenges remain related to the materials stabilities and kinetics.



Keywords: thermo-chemical materials, heat storage, Sorption process, material characterisation, molecular simulations

TASK

This internship/master thesis project focusses on experimental studies for characterization of new salt for thermochemical energy storage. The experiments will be done in TU/e and Lleida (Spain), where you will test the applicability of new materials for thermochemical energy storage.

The experiments can be combined with a numerical (Molecular Dynamics) study, to investigate these new salts on a nanoscale level.

GOALS

- To generate new materials based on mixing of salts hydrates.
- To characterize these materials and determine the hydration/dehydration rates
- To measure the hydrolysis output
- To develop rules to optimize the new composite materials

BENEFITS

- Experience to work in the laboratory and working both on experimental work and simulations
- Understand the challenges regarding energy storage materials and their optimization
- You will be working on multi-disciplinary approach (Mechanical Engineering & Build Environment).
- Involved in the development phase of a novel class of materials based on composite and doping of salt hydrates.

REFERENCES

Pathak et al. (2017), [Journal of Physical Chemistry C](#), 121, 38, 20576-20590, [First-principles study of chemical mixtures of CaCl₂ and MgCl₂ hydrates for optimized seasonal heat storage](#)

Supervisor	Prof. Harald van Brummelen
2nd supervisor	Dr. Clemens Verhoosel
Mentor	Maged Shaban
Company	-
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical



Photopolymerization in Stereolithography : Model Verification and Validation

Maged Shaban*, Clemens Verhoosel, Harald van Brummelen

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INTRODUCTION

Additive Manufacturing (AM) has become an attractive and ubiquitous technology in rapid prototyping and in the biomedical realm. The adoption is mainly due to its free form flexibility and cost reduction during the manufacturing process.

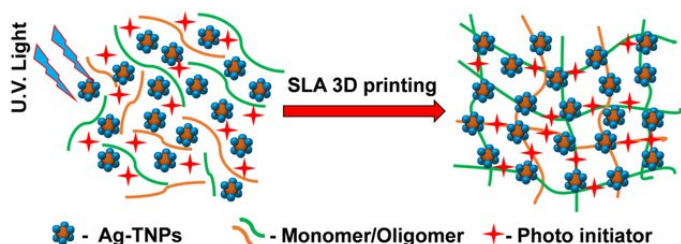


Fig. 1. The schematic illustration of the induced photopolymerization of under UV light for SLA

Stereolithography (SLA) is a sophisticated and complex AM process that creates three-dimensional polymer and ceramic objects from a computer-aided design (CAD) file by using laser-initiated photopolymerization (see Fig. 1). SLA begins with a CAD of the desired object. The topology of the object is computationally divided into two-dimensional cross sections based on this design. The SLA device next scans a laser light throughout a vat of multifunctional photocurable monomer, drawing the cross-sectional shape on the monomer's surface. The layer is stabilized by an elevator in the monomer liquid that lowers after each laser pass. After forming a cross-section and lowering the elevator, the laser process is repeated to generate the desired object layer by layer (see Fig. 2).

Keywords: Free-radical polymerization, 3D Printing, Photopolymerization, Stereolithography

STUDENT PROFILE

- Motivation to research in the SLA process.
- Experience with Finite Element analysis.
- Experience in COMSOL or MATLAB.

TASKS

- Study literature on photopolymerization process.
- To build a numerical model for photopolymerization process with identifying basic parameters and inter-parametric relations influencing the process.
- To develop and validate a photopolymerization model with different setups supported by essential numerical simulations (using COMSOL or MATLAB).

BENEFITS

- Opportunity to be a part of state-of-the-art research into stereolithography modeling and simulation.
- You will get familiar with a pre-existing code and learn how to work and develop it.
- Develop programming skills.
- Writing a report and collaborate on a scientific paper.

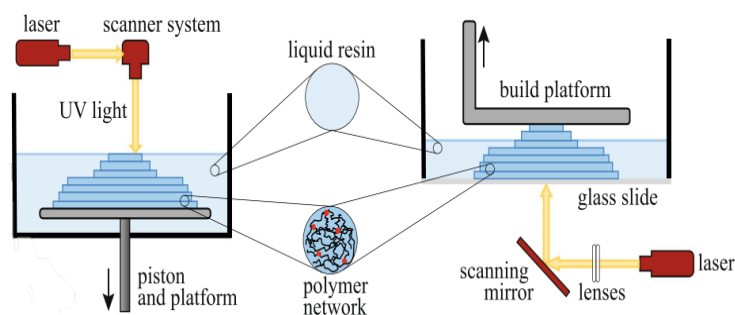


Fig. 2. Stereolithography printing process

REFERENCES

- [1] Goodner, M. D., & Bowman, C. N. (2002). Development of a comprehensive free radical photopolymerization model incorporating heat and mass transfer effects in thick films. *Chemical Engineering Science*, 57(5), 887–900.
- [2] Westbeek, S., van Dommelen, J. A. W., Remmers, J. J. C., & Geers, M. G. D. (2018). Multiphysical modeling of the photopolymerization process for additive manufacturing of ceramics. *European Journal of Mechanics, A/Solids*, 71, 210–223.