# Master Thesis Project Proposals Q4 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 TU/e	Dr. Michel Speetjens
2nd supervisor TU/e	Dr. Erik Steur (Dynamics & Control, ME)
Supervisor ASML	Dr. Rob van Gils
Company	ASML
Internal / External	External
Starting date	Any time
Exp./Num./Design	Num./Exp./Design



## **ADVANCED THERMAL SYSTEM IDENTIFICATION**

Michel Speetjens\*, Erik Steur, Rob van Gils
\*E-mail: m.f.m.speetjens@tue.nl

In ASML lithographic systems, silicon wafers are exposed by DUV/EUV light to create nanometer scale structures that are key to the production of semiconductor devices. During the exposure, the wafer and wafer clamp (i.e. the structure that 'holds' the wafer during exposure) heat up. A temperature increase of the wafer and clamp leads to thermomechanical deformations which reduces machine performance, see Fig 1.



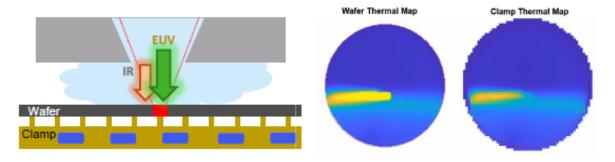


Fig 1: Wafer heating. Left: schematic picture of geometry. Right: thermal map of wafer and clamp

In current ASML systems this performance impact is mitigated in several ways. Some of those ways are model-based and require accurate thermal system identification. System to system variations, complexifies the configuration of a single model that fits all systems. Therefore, prediction models must be calibrated per system. However, classical identification methods, for example FRF measurements, come with the downside of long duration due to the thermal properties of the system.

Therefore, the objective of this MSc assignment is to investigate time efficient identification experiments that are applicable to the clamp (+ peripherals) geometry as described above. As such, the following activities are foreseen for this project:

- Study of the current model and identification techniques applied to the system
- Literature study on currently available identification techniques for thermal systems and definition of techniques to investigate in this research
- Extension of the currently available Matlab / Simulink models to validate the identification methods
- Optionally: preparing and execution of machine experiments to validate the identification method to real measurement data
- Documentation (MSc. thesis) and presentation of the results of the assignment

#### Contact information:

 dr. ir. Rob van Gils, Heat and Mass Transfer Architect / Competence leader Thermal Engineering & Control, ASML, De Run 6501, 5504 DR, Veldhoven, The Netherlands Phone: +31 (0)6 1178 6042, E-mail: Rob.van.Gils-RGIN@ASML.com

Supervisor	Dr. Stein Stoter
2 <sup>nd</sup> supervisor	
Mentor	Dr. Stein Stoter
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical



Project number: 02



# Trimmed explicit dynamics: a non-linear Kirchhoff-Love shell model

**Stein Stoter** 

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

Keywords: Explicit dynamics, Trimming, Non-linear Kirchhoff-Love shell, Isogeometric analysis

#### **INTRODUCTION**

Explicit analysis forms the backbone of impact and crashtest simulation software (see Fig. 1). These simulations often involve shell-type components. Trimmed isogeometric analysis streamlines the design-to-analysis pipeline for these types of simulations. In isogeometric analysis, the CAD-based spline geometry representation of the shells is used directly in the analysis software.



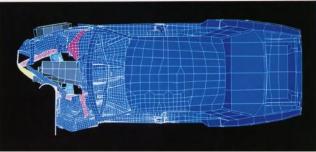


Fig 1: Crash-test simulation. Credit: Cray Research Inc.

#### PROBLEM STATEMENT

The trimming operation in CAD can lead to elements with very small support. In explicit dynamics, these small cuts may severely limit the permissible time step size. In our group, we have developed methods an analysis procedures for mitigating this adverse effect (see Fig. 2). In this MSc project, you will implement and investigate the performance of this approach for the non-linear variant of the Kirchhoff-Love shell model.

#### **WORK PACKAGE**

- Develop a familiarity with shell models and explicit time-stepping methods.
- Extend the existing linear Kirchhoff-Love shell code to a code that can handle the non-linear variant.
- Study the effect of the proposed solution method.
- Depending on the students own learning goals, subsequent research may focus on a shift to the Reissner-Mindlin shell model, or efficient implementation

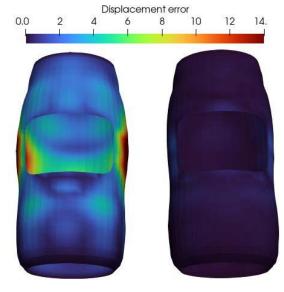


Fig 2: Error in the predicted displacement for the <u>linear</u> Kirchhoff-Love shell model, without and with the proposed solution method.

#### STUDENT PROFILE

We are looking for a MSc student who has:

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

#### REFERENCES

 Stoter, S.K.F. et al. (2022). Variationally consistent mass scaling for explicit time-integration schemes of lower- and higher-order finite element methods, Computer Methods for Applied Mechanics and Engineering, 399, 115310.

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].

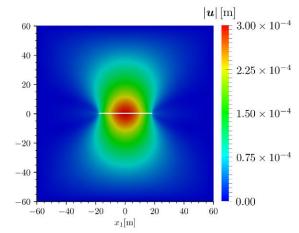
# Prior information Experimental data Uncertainty model Likelihood function Bayesian solver (e.g., Markov chain Monte Carlo method) Uncertain output parameters (posteriors) Quantities of interest (uncertainties)

#### **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.

- [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(num.) & Michiel van Gorp(exp.)
Company	N.A.
Internal / External	Internal
Starting date	Anytime
Exp./Num./Design	Experimental and numerical



Project number:



# Solving a fluid maze experimentally and numerically

Tom van Sluijs\*, Michiel van Gorp, Stein Stoter, Harald van Brummelen

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

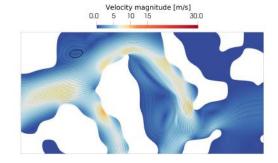
#### INTRODUCTION

Water can solve a maze under the influence of gravity, see video and image. For sufficiently small mazes the water will instantaneously follow the shortest path to the exit. This can be shown in experiments and model simulation. In this project you aim at building an experimental setup for a fluid maze and simulating an identical setup numerically.

The Cahn-Hilliard equations describe phase separation, such as water-air systems. The Navier-Stokes equations describe the motion of viscous fluids. Coupling these models gives the opportunity to describe the dynamics of multiphase flow. This Navier-Stokes-Cahn-Hilliard (NSCH) model is implemented numerically and used to simulate the fluid maze. See the figures down below or this video for a typical result.

STEVE MOULD

The experimental and numerical results can be used for cross verification. The experiments validate the model, and the model gives phenomenological insight in the fluid flow.



### **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

#### **TASKS**

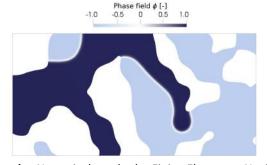
In this project, you are expected to do:

- Literature review, focused on multiphase flow, capillarity, and the NSCH model
- Building an airtight fluid maze and performing experiments
- Program a numerical implementation of the fluid maze
- Qualitative and quantitative assessment of the numerical and experimental results
- Conclusion and advise on both modelling and experimental aspects

#### **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 build an experimental setup and gather results from experiments.
- is looking to develop his/her personal skillset: physical modelling, experimental work, numerical methods, literature study, programming, and data analysis.



**Keywords**: Numerical methods, Finite Elements, Navier-Stokes, Cahn-Hilliard, Experimental setup, Image analysis

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	Dr. Michel Speetjens
2nd supervisor	
Mentor	
Company	In collaboration with TNO
Internal / External	Internal (with short visits to TNO)
Starting date	Any time
Exp./Num./Design	Num.



#### **DEVELOPMENT OF DIGITAL TWINS FOR INDUSTRIAL HEAT PUMPS**

Michel Speetjens\*

\*E-mail: m.f.m.speetjens@tue.nl

# TNO

#### INTRODUCTION

Industry is facing huge challenges to realize the transition to a nearly CO2-neutral industry in 2050. Integration of industrial heat pumps that upgrade waste heat to process heat is one of the solutions to enable this. Compression heat-pump technology for such heating purposes is in principle available and ready for market introduction. However, two main challenges hamper this market introduction. First, industrial heatpump technology has not yet reached the status of proven technology for end-users. Know-how is lacking with respect to its integration into industrial processes. Second, current industrial heat pumps are mainly developed for cooling instead of heating (Fig. 1). This leads to uncertainty at heat-pump manufacturers regarding the purpose for which to develop heat pumps and the corresponding expertise and know-how.



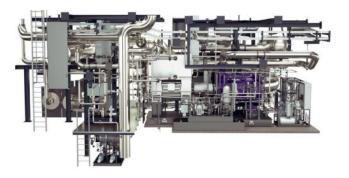


Fig. 1. Typical industrial heat pumps and their integration for cooling purposes (from Siemens Energy).

#### **PROJECT**

The main project goal is the *development of digital twins for prototype heat pumps* realized at TNO for efficient simulation of their system-level behaviour under dynamic operating conditions. The digital twins will serve as computational tool for investigating the application of the TNO heat pumps for heating purposes using waste heat so as to facilitate their integration into industrial processes. An important challenge for their development will be striking a balance between computational efficiency and prediction accuracy.

The development and validation of the digital twins involves the following steps and subgoals:

- Selection of suitable modelling approaches for heat pumps on the basis of a literature study. This may expand on previous modelling efforts at TU/e [1,2].
- Development of mathematical first-principles models for the system-level dynamic behaviour of heat pumps using (a) selected modelling approach(es).
- Implementation of these first-principles models as digital twins in programming environments such as e.g. Matlab or Modelica.
- Calibration and validation of the digital twins using experimental data from the prototype heat pumps.

#### **REFERENCES**

[1] K. Kruijt, F.J.R. Verbruggen, M.F.M. Speetjens, T. Hofman, Modeling and control of a waste heat recovery system for integrated powertrain design optimization, IFAC PapersOnLine 52-5 (2019) 598–60

[2] R. Matser, Theoretical analysis of drop-in refrigerants with a low global warming potential for chiller systems, MSc thesis TU/e-ETFD 2023

Supervisor	Dr. Michel Speetjens
2nd supervisor	Dr. Jurriaan Boon (TNO)
Mentor	
Company	TNO
Internal / External	External
Starting date	Any time
Exp./Num./Design	Num./Exp./Design



# **AMMONIA ADSORPTION FOR HYDROGEN STORAGE AND TRANSPORT**

Michel Speetjens\*, Jurriaan Boon

\*E-mail: m.f.m.speetjens@tue.nl

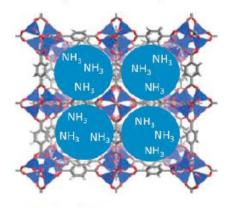
NH3 is the most important candidate energy and H2 carrier expected to arrive in European harbors and especially in Rotterdam. Import terminals are currently being planned for the import of NH3, that can be produced cheaply abroad and which can be used to fuel our industry, replacing fossil fuels.

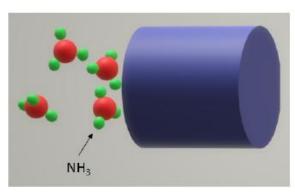






In order for the NH3 to take its role in the industry, smart processes are required for the reforming. Adsorbents (physical and chemical) can be used for the recovery of NH3 in order to create an efficient process for the production of H2.





Khabzina, 2018

In this project, the student will make a process design for several different adsorbent materials, and compare them in terms of performance. The student will perform:

- A brief literature review of processes and sorbent types
- Create a process model, including heat and mass balances
- Perform experimental campaigns to establish the performance of different materials
- Optimise the process design in terms of energy efficiency

The assignment is available at TNO, Petten, The Netherlands. For further details please contact: Dr Jurriaan Boon (<a href="mailto:jurriaan.boon@tno.nl">jurriaan.boon@tno.nl</a>) or Dr Michel Speetjens (<a href="mailto:M.F.M.Speetjens@tue.nl">M.F.M.Speetjens@tue.nl</a>).

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



Project number: 08



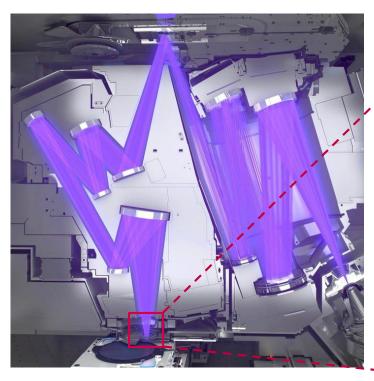
# Rarefied Heat Transfer for Next-Gen Photolithography Machines

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 govern gas flow in 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 BE in the rarefied regime. However, stochastic nature of DSMC precludes resolution of the continuum-to-rarefied transition regime which is necessary for the next-generation PLMs.



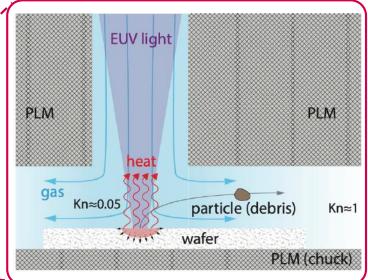
#### **TASKS**

- 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).



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.

- [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 <sup>nd</sup> supervisor	Prof. Dr. Olaf van der Sluis
Mentor	Robin Willems
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical



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.

#### **NURBS** template



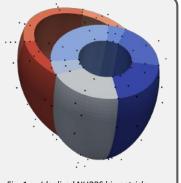


Fig. 1 Idealized NURBS bi-ventricle geometry, parametrized by a minimum number of control points.



Fig. 2 Echocardiogram data is used to extract patient-specific geometry features.

#### **TASKS**

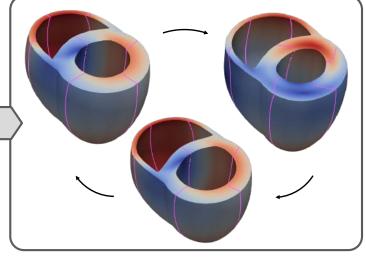
- Develop procedure to fit NURBS template on echo data,
- Investigate parameter sensitivities using the existing IGA cardiac model (Single and Bi-ventricle),
- Uncertainty quantification analysis regarding clinical input and model output data,
- Development of an efficient Reduced Order model (ROM),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

# Results



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

Cardiac Model

**Mechanics** 

**Activation** 

Circulation

- [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	prof. dr. ir. David Smeulders
2nd supervisor	
Mentor	
Company	PHILIPS
Internal / External	External
Starting date	Any time
Exp./Num./Design	Experimental & Numerical



Project number: 10

# **Gas Permeation in High Precision Vacuum Applications**

**Joris Oosterhuis, David Smeulders** 

Email: Joris.Oosterhuis@philips.com, d.m.j.smeulders@tue.nl

#### **INTRODUCTION**

High precision motion stages require air and water supply for different purposes such as cooling of actuators to achieve the desired performance. In most cases, this supply is realized through flexible hoses in the so-called cable slabs. For vacuum applications this poses an additional challenge: hoses are to a certain extend permeable. This means water, air or various hydrocarbons can be transported through the hose walls into the vacuum, which leads to molecular contamination of the vacuum environment. For design of motion stages in vacuum applications, it is essential to understand and characterize this permeation process.

**Keywords**: Gas Permeation, High Vacuum, Precision Engineering

#### **GOALS**

The goal of this MSc. project is to characterize permeation of water, air, and hydrocarbons through flexible (PTFE) hoses using a vacuum setup equipped with a mass spectrometry device (RGA). The measured data will be used to create a predictive model that is applicable in a design practice.

#### **TASK**

As such, the following activities are foreseen for this project:

- Literature study and analysis of existing measurement data
- Design and execution of a test campaign for experimental study and analysis
- Create a predictive model for the permeation process (using MATLAB or COMSOL)
- Documentation (master thesis) and presentation of results

#### **BENEFITS**

- Opportunity to work in a leading company
- Build network and experience working in a big organization
- Develop a deep understanding of the physical phenomena as well as its industrial application

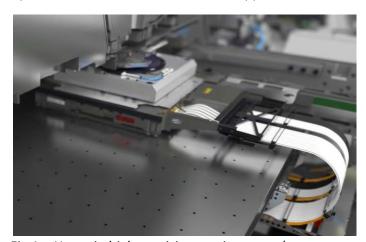


Fig 1a: Hoses in high precision motion stage (courtesy: ASML)

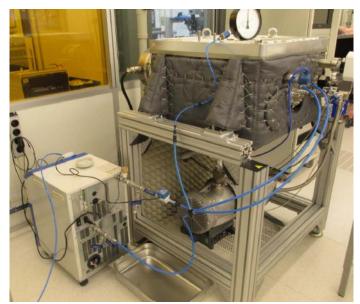


Fig 1b: Vacuum setup for characterizing hose permeation

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



Project number: 11



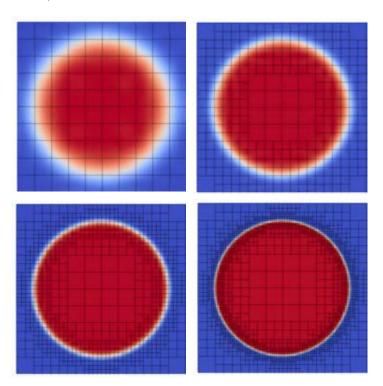
# Higher-order time-stepping methods for spatially adaptive schemes

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].

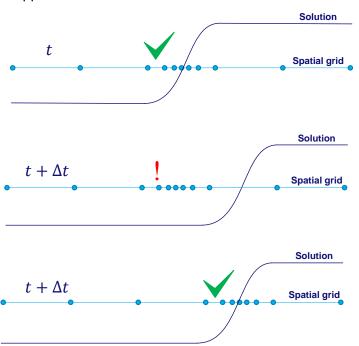


#### PROBLEM STATEMENT

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 timesteps 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.

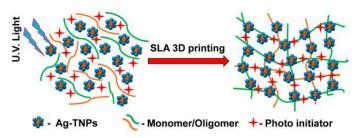


Fig. 1. The schematic illustration of the induced photopolymerization of under UV light for SLA

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 interparametric 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.

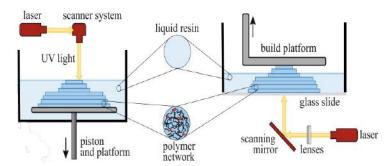


Fig. 2. Stereolithography printing process

- [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



Project number: 13



# ASSESSING METAL-EXCHANGED MATERIALS FOR HYDROGEN STORAGE

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].

In this regard, nanoporous materials are being proposed as an alternative storage solution for hydrogen. While porous materials offer the potential for this application, certain limitations, such as adsorption capacity and extreme operating conditions of temperature and pressure need to be addressed. The DOE established targets of binding energy, gravimetric and volumetric capacity, and cost [2,3].

#### GOAL

Modify porous materials to assess the effect of metal center (and other surface modifications) in the capacity and conditions of hydrogen storage in MOFs.

#### **TASK**

In this project, you are expected to:

- Review relevant literature on hydrogen adsorption in porous materials.
- Computational generate hypothetical structures based on reported materials. (Figure 1)
- Test the adsorption capacity and conditions of the new structures and the application range.

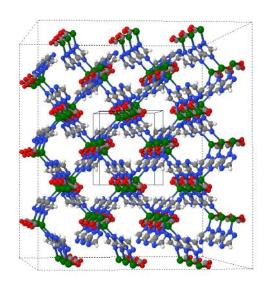


Fig. 1. Schematic representation of a Metal organic framework with original composition. Metal centers in green.

#### 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 linux os and bash command lines is desired but not mandatory

#### REFERENCES

[1] Flynn, T. (2004), Cryogenic Engineering, 2nd Ed. Taylor & Francis. ISBN: 0824753674

[2] S. I. Hwang et al., *Metal-Organic Frameworks on Palladium Nanoparticle-Functionalized Carbon Nanotubes for Monitoring Hydrogen Storage*, ACS Appl Nano Mater, 2022.

[3] H. W. Langmi, N. Engelbrecht, P. M. Modisha, and D. Bessarabov, *Hydrogen storage* Electrochemical Power Sources: Fundamentals, Systems, and Applications, 2022, pp. 455–486.

**Keywords**: #hydrogen storage #DOE #porous materials

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



# **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.

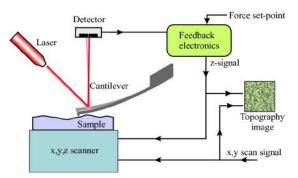


Figure 1: Principles of atomic force microscopy [1]

#### **REFERENCES**

[1] Voigtländer, B. (2019). Introduction. In: Atomic Force Microscopy. NanoScience and Technology. Springer, Cham. <a href="https://doi.org/10.1007/978-3-030-13654-3">https://doi.org/10.1007/978-3-030-13654-3</a> 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	Prof. Silvia Nedea
2nd supervisor	Prof. Ionut Tranca
Mentor	
Company	
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Modelling



Project number: 15

## **SMART Coat**

Silvia Nedea

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#### INTRODUCTION

Corrosion-induced degradation of metallic parts is a major problem for industry. It causes expensive damages to various sectors and infrastructures, with an estimated annual cost equivalent to 3-4% of the world's gross domestic product. Newer corrosion protection systems are urgently needed, as the effective but toxic treatments that use Chromium(VI) will soon be banned. The development of effective active protective coatings is time- and resource-consuming, which increases the time to market of the new products.

Within this project, which involves both academic and industry partners (e.g. Airbus), the conventional method of trial-and-error is aimed to be substituted with a smart technology, able to create and assess corrosion-resistant coatings that fulfill specific service environment demands.



#### **TASK**

Atomistic simulations are required to closely examine the performance of potential corrosion inhibitors. Access to the Dutch and Belgian supercomputer centers, as well as to the 3<sup>rd</sup> fastest supercomputer in the world, may be obtained in order to conduct these simulations.

#### **GOALS**

The aim of the project is:

- To explore the Potential Energy Surface of the inhibitor-surface and inhibitor-inhibitor interactions
- To validate the structural models obtained through comparison with the experimental data
- To predict the inhibitor effects based on reactivity descriptors

#### REQUIREMENTS

- Hands-on attitude and interest in performing modelling.
- Creative and solution-oriented
- · With interest in fundamental physical principles
- Preferably followed 4SE20ONL

Supervisor	Prof. Silvia Nedea
2nd supervisor	Prof. Ionut Tranca
Mentor	
Company	
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Modelling



Project number: 16

# THE BEST (Thermochemical Battery for Energy Storage)

Silvia Nedea

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#### INTRODUCTION

In order to tackle the modern challenges of climate change, resources depletion and geopolitical instability, the human society will have to evolve towards sustainable energy and green economy. Energy storage will play an essential role in this global energy system, in order to support the penetration of the fluctuating renewable energy sources (Sun, wind), as well as to capture the waste from various domestic or industrial processes.

Thermochemical energy storage (TCES) through reversible chemical reactions (sorption/desorption of gases like H2O or CO2) is the most promising technology for compact and lossless long-term heat storage. Its material high heat storage density is comparable to that of Li-ion batteries. The current research in this field is hampered by the scarcity of appropriate TCES materials that can store and release heat at the desired temperatures with high efficiency and storage density. Thus, novel promising candidates are required, along with means of screening the large potential structural space. Reaching this goal demands an integrated holistic approach, one that combines high-throughput computations, advanced characterisation and data driven modelling (Machine Learning/ML)



#### **TASK**

The main objective of the present project is to identify a set of novel candidate materials for TCES.

Access to the Dutch and Belgian supercomputer centers, as well as to the 3<sup>rd</sup> fastest supercomputer in the world, may be obtained in order to conduct the associated simulations.

#### **GOALS**

The aim of the project is:

- Identify features which can be used to build ML descriptors which correlate structural/electronic characteristics with thermodynamic ones. Use the ML descriptors to identify promising TCES materials.
- Use Machine Learning Potentials to understand the reaction mechanisms associated with the solid-to-solid transitions (e.g. from salt to salt hydrate).

#### REQUIREMENTS

- Hands-on attitude and interest in performing modelling.
- · Creative and solution-oriented
- With interest in fundamental physical principles
- Preferably followed 4SE20ONL and/or 4SE30ONL

Supervisor	Wout Gubbels or colleague
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: 17



# Internship within a micro-Concentrated Solar Power startup

SUNCOM energy



**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 heats a Heat Transfer Fluid running through the receiver to 425-450  $^{\circ}$  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. The insulation substantially increases the efficiency of the receiver and therefore makes it possible to utilize a smaller reflector. This allows for decentralized energy generation, on-site and nearby the end-users, such as commercial and industrial companies.



Fig. 1. Final pre-production run in operation behind our workshop in Houten. a: Receiver in focus, b: Two modules in operation

The latest version of Suncom's solar trough for lower temperatures (<100  $^{\circ}$  C) is undergoing the final tests behind our workshop in Houten, close to Utrecht. This version is being refined to be scaled up to a ~400 kWth plant which will be built in Q3/Q4 2023 in the Netherlands.

In parallel, Suncom is working on the development of a high temperature solar trough (up to ~425-450 °C) as well as a high temperature Thermal Energy Storage. Both developments provide options for internships with a combination between analytical, numerical, design and experimental work.

**Keywords**: Concentrated Solar Power, Thermal Energy Storage, Modelling, Experimental work

#### **TASK**

We are looking for entrepreneurial and enthusiastic MSc students which have interests in both modelling, experimental work and thermodynamics. We always have some potential projects available which we, in consultation, will tailor to your skills and preferences.

Suncom has a lot of experience with supervising university interns, also within the Energy Technology group. We aim to provide the best learning experience by appointing a dedicated supervisor to provide in-depth guidance, as well as communicating openly about company affairs to provide broader insights on operations in a startup environment.

#### **EXAMPLES OF PAST PROJECTS**

- Thermal analysis of a novel square heat receiver
- Aerodynamic Analysis of Novel Solar Through Design
- Analysis of the thermal boundary layer in a novel square heat receiver
- Techno-economic analysis and thermodynamic modelling of Thermal Energy Storage methods

Projects can be continuations of the outcomes of previous projects, or dive into a new aspect of our technology.

#### **BENEFITS**

- Experience working in a mission-driven start-up and join our mission to decarbonize the world's energy supply
- A flexible work environment with a lot of responsibility and ownership
- A fun office environment at a well reachable location in Houten (close to station Houten Castellum and the A27)
- The option to work from home at least two days a week
- An internship compensation of €500,- per month
- The possibility to join the company after successful completion of your internship, with the opportunity to become co-owner



# Borehole acoustic Stoneley wave measurement in porous sandstone

David Smeulders ,Yukai Liu

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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(figure1) will be used.

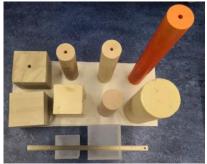


Figure 1: Rock samples for borehole Stoneley wave measurement

#### **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.

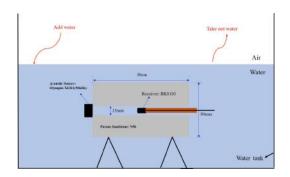


Figure 2: Schematic of borehole Stoneley wave measurement



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



# 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 fol 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. Michel Speetjens
2nd supervisor	Dr. Erik Steur (Dynamic & Control)
Mentor	
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Num./Exp.



Project number: 20

# **OPTIMAL HEAT TRANSFER BY SMART FLOW CONTROL**

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#### INTRODUCTION

Thermal transport phenomena in flows is relevant to many (industrial) applications:

- heating and cooling in the processing industry;
- thermal management of power electronics;
- thermal conditioning of high-precision systems.

The common goal in such applications essentially is accomplishment of maximum heat transfer between an object and a flow via active manipulation of the flow.

#### **CASE STUDY**

Boosting of heat transfer by stirring of the fluid (Fig. 1a) is adopted as a case study. An industrial implementation of this principle exists in the heating of an initially cold fluid inside a circular container via the hot boundary (Fig. 1b, left) [1]. Stirring occurs via switching between the three flows that each are driven by a sliding wall (arrows) along apertures (heavy arcs) in the boundary (Fig. 1b, right). The key question is: "How to stir?"

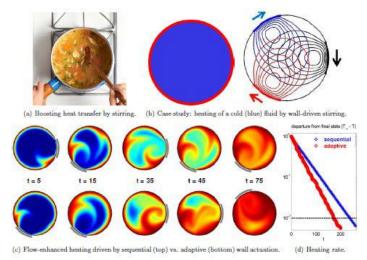


Figure 1: Accomplishing optimal heat transfer in fluid flows by "smart" flow control.

Stirring by <u>sequential</u> actuation of the sliding walls is commonly regarded the best way to boost heat transfer (Fig. 1c, top). However, this approach is sub-optimal [1].

<u>Adaptive</u> stirring by a controller that step-wise actuates the sliding walls on the basis of the most effective temperature evolution (Fig. 1c, bottom) can namely significantly accelerate the heating rate (Fig. 1d) [1].

#### **RESEARCH TOPICS**

The above findings demonstrate the potential of dedicated flow control for heat-transfer enhancement and its further exploration (by the case study of Fig. 1) is the principal goal of this research line. Specific research topics within this scope include (but are not limited to):

- Further development of the control strategy of [1] for achieving maximum heat transfer.
- Development of control strategies for other control targets (e.g. establishment of thermal fronts).
- Data-based modelling of the temperature evolution using (nonlinear) system identification.
- Development of an observer that enables state estimation from discrete sensor data.
- Experimental investigation & validation of adaptive flow control using the laboratory set-up of [2].

A multi-disciplinary approach involving expertise on heat & flow versus dynamics & control is essential to address these topics and therefore research is performed as a collaboration between research groups *Energy Technology & Fluid Dynamics* and *Dynamics & Control*.

MSc projects can be defined around any of the above topics and tailored to personal interests and preferences. We therefore invite students with an interest in these (and related) multi-disciplinary topics to contact us to discuss opportunities for MSc projects.

- [1] R. Lensvelt, M.F.M. Speetjens, H.Nijmeijer, Fast fluid heating by adaptive flow reorientation, Int. J. Therm. Sci. **180**, 107720 (2022).
- [2] O. Baskan, M. F. M. Speetjens, G. Metcalfe, H. J. H. Clercx, Experimental and computational study of scalar modes in a periodic laminar flow, Int. J. Therm. Sci. **96**, 120 (2015).

Supervisor	Dr. Stein Stoter
2 <sup>nd</sup> supervisor	
Mentor	Dr. Stein Stoter
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical



Project number: 22



# Machine learning for scale interaction in advective transport equations

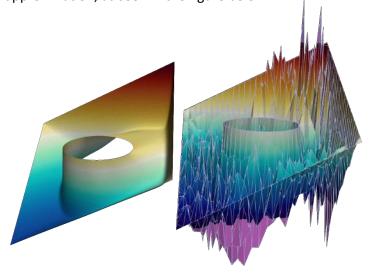
Stein Stoter

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

**Keywords**: Machine-learning, Finite element method, Scale interaction

#### **INTRODUCTION**

With the finite element method, we can approximate solutions to partial differential equations. These can be interpreted as 'coarse-scale' representations of the true solution, and the approximation error can be interpreted as the missing 'fine-scale' contribution. For transport equations, the effect of the fine scales must be taken into account (modeled) while computing the coarse scales to obtain stable results. The quality of this scale interaction model dictates the quality of the coarse-scale approximation, as seen in the figure below.



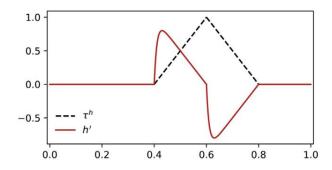
**Fig 1:** Solution to a transport equation on a unit square with a circular cut-out. Advective transport actrs from bottom left to top right. **Left:** true solution. **Right:** finite element approximation without scale interaction model.

#### PROBLEM STATEMENT

The scale interaction can be computed exactly (Fig 2.), but this costs a lot of computational power, making it unfeasible to do so during the simulation of transport phenomena. Instead, one could learn the scale interaction with a machine learning algorithm during a training phase, and then use the machine learning model during the simulation of the transport problem.

#### **RESEARCH TOPICS**

- Perform a literature study to learn about the state-ofthe-art of machine learning for scale interaction, and about the types of machine learning techniques used for similar tasks.
- Develop a code that can compute the exact scale interaction function (see one-dimensional example below).
- Develop a machine learning code that can predict these functions.
- Study the effectiveness of the machine-learned model of the scale interaction, and report on the required 'input' to the machine-learning algorithm to reliably predict correct scale interaction functions.



**Fig 2:** Scale-interaction function for a one-dimensional advective transport equation. For this particular case, the interaction function h' localizes to a single element.

#### 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

 Stoter, S.K.F. et al. (2022). Discontinuous Galerkin methods through the lens of variational multiscale analysis, Computer Methods for Applied Mechanics and Engineering, 388, 114220.

Supervisor	Dr. Clemens Verhoosel
2 <sup>nd</sup> 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



Project number:23



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

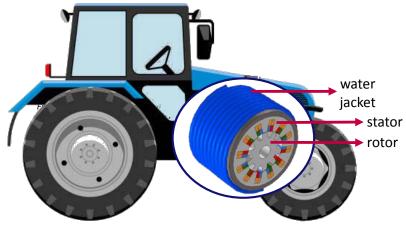
Doga Ceylan\*, Mitrofan Curti, Clemens Verhoosel
\*E-mail: d.ceylan@tue.nl

**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.



 ${\it Fig.~1} \qquad {\it A permanent-magnet-free electric motor in an electric tractor.}$ 

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.

#### / ENERGY TECHNOLOGY AND FLUID DYNAMICS

#### **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.

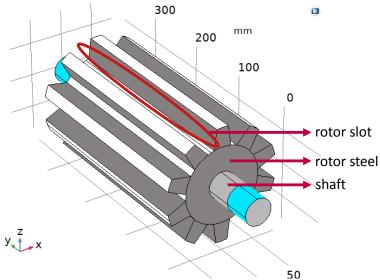


Fig. 2 The rotor of the analyzed permanent-magnet-free electric motor without any filling in its slot.

#### 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



Project number: 25

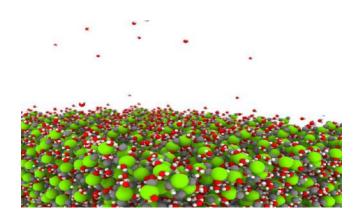
# **NEW MATERIALS FOR ENERGY STORAGE**

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), <u>Journal of Physical Chemistry C.</u> 121, 38, 20576-20590, <u>First-principles study of chemical mixtures of CaCl2 and MgCl2 hydrates for optimized seasonal heat storage</u>"

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

\*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.

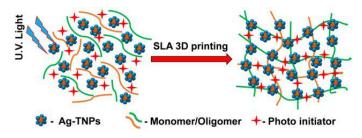


Fig. 1. The schematic illustration of the induced photopolymerization of under UV light for SLA

Stereolithography (SLA) is a sophisticated 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 interparametric 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.

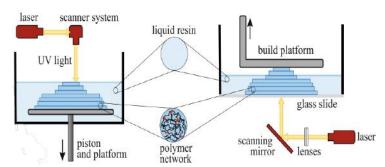


Fig. 2. Stereolithography printing process

- [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.

# Voltgoed~



# Internship or Graduation Project

Clemens Verhoosel - TU/e

E-mail: CVerhoose@tue.nl

Stan Hoppenreijs – Voltgoed<sup>~</sup> E-mail: stan@voltgoed.nl

#### INTRODUCTION

Voltgoed is a multiple award-winning Heat as a Service (HaaS) startup company founded by three TU/e alumni. Our mission is to reduce the environmental impact of our energy consumption. We develop, realize and operate innovative all-electric heating and cooling systems that are sustainable, energy-efficient and have low operational cost. Our projects include real estate developments that range between 200 and 1200 apartments. Voltgoed is headquartered at the High Tech Campus in Eindhoven.

#### **INNOVATIONS**

Within Voltgoed we innovate the technical performance of our heating and cooling systems in terms of energy efficiency, uptime and durability. This not only increases the technical performance but also increases customer satisfaction. For example, we use data from the heating and cooling systems and heat meters to detect anomalies at an early stage, inform our consumers about their heat consumption and provide them with insights to reduce their environmental impact.





#### **RESEARCH OPPORTUNITIES**

- Develop analytical and numerical models to simulate the performance of heating and cooling systems. Since we have access to many systems in the field it is also possible to validate these models.
- Develop algorithms to detect anomalies in the performance of heating and cooling systems at an early stage.
- Analyze and develop smart grid solutions that can be applied to our systems to prevent congestion and help balance the grid.
- Design and develop innovative heating and cooling concepts for large apartment buildings or area developments.
- Any other innovative ideas that you would like to work on. ©

#### STUDENT PROFILE

We are looking for an MSc student who has:

- Affinity with all-electric heating and cooling systems, i.e., heat pump technology.
- A strong drive to challenge the status quo.
- Interest in simulation and optimization and eager to improve your modelling skills.
- A team player that can operate and communicate in a multi-disciplinary team.

If you have any thoughts on other innovations that we could apply, feel free to reach out as well. We are willing to set up an innovative project just for you!

Supervisor	Dr. Michel Speetjens
2nd supervisor	Ir. Hette de Vlieger (IF Technology)
Mentor	
Company	IF Technology
Internal / External	External
Starting date	Any time
Exp./Num./Design	Num./Exp./Design



#### SUSTAINABLE HEATING FOR THE BUILT ENVIRONMENT

Michel Speetjens\*, Hette de Vlieger \*E-mail: m.f.m.speetjens@tue.nl

#### INTRODUCTION

The engineering & consultancy company **IF Technology** (<a href="https://iftechnology.nl">https://iftechnology.nl</a>) specializes in development of sustainable energy systems. One area of application concerns sustainable heating & cooling of the built environment using technologies such as e.g. geothermal or aqua-thermal systems and heat pumps.

#### **RESEARCH TOPICS**

#### 1. Performance of thermal-energy storage systems

Two promising forms of thermal energy for heating & cooling of the built environment are:

- Aqua-thermal energy (Fig. 1);
- Acquifier Thermal Energy Storage (ATES).

Both systems rely on the seasonal availability of energy, which results in "charging" and "discharging" of a reservoir (i.e. a body of water or a subsurface porous rock layer) either directly by exchange of water or indirectly via a heat pump. Efficient design and operation is essential for an optimal and sustainable performance of such systems.



Fig. 1. Heating & cooling of the built environment by aqua-thermal energy (from IF Technology).

/ Energy Technology & Fluid Dynamics

Challenges within this scope include:

- Thermal and hydraulic modelling of the seasonal heat exchange of the thermal-energy reservoirs.
- Optimization of the seasonal (dis)charging for both technical and economic performance.
- The impact of variable operating temperatures on the COP of the heat pump and the overall efficiency.

#### 2. Integration of power-to-heat (P2H) systems

Intermittency and fluctation due to weather is a major challenge for sustainable electricity generation by e.g. solar panels and wind turbines. Electricity storage in e.g. Li-ion batteries can mitigate this yet is a costly option. The fact that a substantial part of the generated electricity is eventually used for heating naturally advances storage of electricity in the form of thermal energy via heat pumps (so-called "power-to-heat" or P2H) as a promising alternative. Challenges include:

- Integration of the P2H concept in existing thermalenergy systems & energy networks.
- Techno-economic optimization of such integrated energy systems for certain ranges of energy prices.
- Techno-economic feasibility of heat pumps for P2H applications: dynamic response to electricity variations; economic viability of P2H units; optimal P2H operation on basis of predicted heat demands.

#### **MSc PROJECTS**

MSc projects can be defined for both research topics and tailored to personal interests and preferences. We therefore invite students with an interest in these topics to contact us to discuss opportunities for MSc projects.

Supervisor	Dr. Clemens Verhoosel
2 <sup>nd</sup> supervisor	TBD
Mentor	TBD
Company	TouchWind BV.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical



Project number: 28

# Numerical study on the wake behavior of wind farms with tilted turbines

Clemens Verhoosel
\*E-mail: Cverhoose@tue.nl

Keywords: Wind farm modelling, CFD, Rotor tilt, Wake steering

#### **INTRODUCTION**

Climate change is a big problem facing us today. There is a strong need for renewable energy sources and it is increasing each year. TouchWind is developing a floating offshore wind turbine. As a startup, it is hard to compete with the already existing turbine manufacturers. However, with the design of a tilting one-piece rotor, TouchWind believes that the cost per kWh can decrease. Furthermore, TouchWind estimates that tilted turbines can be placed closer to each other and thus occupy less space.





Figure 1: TouchWind rotor during normal operating conditions.

Figure 2: TouchWind rotor during storm conditions.

Both beliefs arise from the so-called 'Park effect' of the TouchWind turbines. The TouchWind rotors can tilt. This means that the rotor will be, as visible in Figures 1 and 2, positioned at an angle relative to the wind. This has a lot of benefits for one turbine itself, but with multiple turbines placed in a row, more benefits can arise. The benefits that arise by placing multiple turbines are called the TouchWind park effects.

Wind turbines form wakes downwind of the turbines. Wakes are the more turbulent and less energy-rich flow that forms due to the energy extraction of wind turbines. By applying tilt to a rotor the wake gets redirected downwards creating a new fresh stream of energy for the downwind placed turbines. These phenomena is visualized in Figure 3. Research has shown that with a wind gradient present, even higher energy outputs can be reached for a wind farm with tilted turbines than for a conventional wind farm.

However, tilted rotors are not commonly used and so only a little information is known about the airflow/wake behavior of these turbines. With the use of CFD simulation, TouchWind wants to get a better insight into the wake behavior. This involves numerical modeling problems used for analyzing or optimizing wind farm behavior. The goal of these simulations is to use rotor tilting to maximize the power output of the wind turbines.

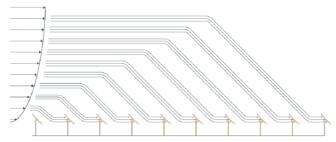


Figure 3: TouchWind rotor during storm conditions.

#### **TASKS**

- Develop and use analytical and numerical models to simulate wake behavior in a wind farm.
- Analyze the influence of tilted rotors on power outputs.
- Tackle problems that are faced in a starting company.

#### STUDENT PROFILE

We are looking for an MSc student who has:

- Affinity towards advanced analytical and numerical solution methods to simulate wind farms.
- Interest in working in a start-up. This involves working in a small team, but also working independently.
- Interest in working in the sustainable energy market and contributing to creative energy solutions.



https://touchwind.org/

Supervisor	Dr. ir. Camilo Rindt
2nd supervisor	
Mentor	
Company	PHILIPS & ASML
Internal / External	External
Starting date	Any time
Exp./Num./Design	Experimental & Numerical



Thermal Contact Conductance in Vacuum

Joris Oosterhuis, Rob van Gils, David Smeulders, Camilo Rindt

 $\textbf{Email:} \underline{\textit{Joris.Oosterhuis@philips.com}}, \underline{\textit{Rob.van.Gils-RGIN@ASML.com}}, \underline{\textit{d.m.j.smeulders@tue.nl}}, \underline{\textit{c.c.m.rindt@tue.nl}}$ 

#### INTRODUCTION

In thermal design in high precision applications in vacuum (e.g. ASML EUV machines) the thermal contact conductance (TCC) between metallic surfaces often plays a dominant role, see Fig 1a. Previously, tools and values from literature have been employed to model this heat transfer at a contact. Also, an experimental setup and testing procedure, see Fig 1b, was set up to investigate the thermal contact conductance in vacuum. Especially for contacts between low thermally conductive and hard metals the thermal contact resistance can be significant.

**Keywords**: Thermal Contact Conductance, Precision Engineering

#### **GOALS**

Objective of this MSc-project is to investigate methods to increase the TCC in both vacuum and atmospheric conditions between samples on this experimental setup. Solution directions can be searched in the application of coatings and/or thermal interface materials. But a literature survey on possibly other solution directions should be done as well.

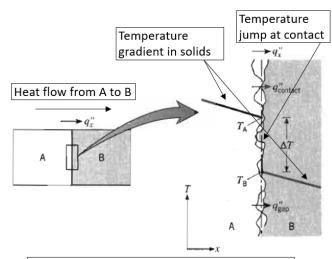
#### **TASK**

The following activities are foreseen for this project:

- Study of previous work: design of experimental setup, found results and peculiarities, etc.
- Literature survey on possible techniques to improve TCC and definition of techniques to investigate in this research
- Optionally: updating testing procedure using advanced identification techniques and modelling
- Performing a series of measurements on the setup to derive the TCC for a set of coatings and/or interface materials
- Documentation (MSc. thesis) and presentation (at Philips + ASML) of the results of the assignment

#### **BENEFITS**

- Opportunity to work in a leading company
- Build network and experience working in a big organization
- Develop a deep understanding of the physical phenomena as well as its industrial application



Thermal Contact Conductance; [Incropera2006]

Fig 1a: Thermal Contact Conductance

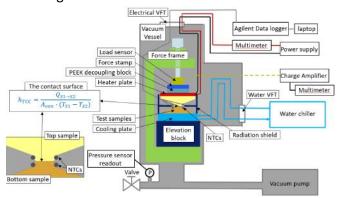


Fig 1b: Schematical representation of test setup

Supervisor	Prof. David Smeulders
Mentor	Ruben D'Rose
Company	N.A.
Internal / External	Internal
Starting date	01-02-2023
Exp./Num./Design	Numerical and experimental



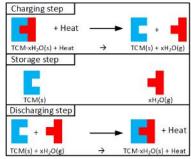
Project number: 30

# MODELLING HYDRATION OF A TCM PARTICLE USING IMPLICIT AND EXPLICIT GEOMETRIES

Ruben D'Rose\*, David Smeulders
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#### INTRODUCTION

Thermochemical materials (TCMs) are used to store energy in chemical bonds. Hydration of a salt is an exothermic reaction used to discharge the TCM of heat.



TCM tablets are fabricated by pressing powder together, creating a random porous structure, which resembles a network of mostly connected, but also isolated pores. Transport of water and heat occurs parallelly through the solid TCM and the pores, of which the medium is air. Understanding the transport physics on the micro (particle) scale is crucial for understanding of transport on macro (reactor bed) scale.

**Keywords**: Heat storage, porous media, TCM hydration, transport phenomena.

#### **TASK**

We are looking for a highly-motivated MSc student who has interest in numerical and experimental work, 3D modelling and fluid dynamics. In this project, you are expected to:

- Conduct literature review, focus on 3D modelling of porous media.
- Write a script to generate random porous structures.
- Use micro-CT to scan a porous TCM tablet and reconstruct a 3D digital geometry.
- Use the random and scanned geometries in commercial FE software to model TCM hydration, along with heat and water transport (explicit model).
- Compare the explicit model with an implicit model that uses the continuum approach.

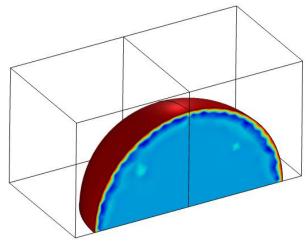
#### **GOALS**

- Develop a method to digitally construct random porous structures.
- Scan and reconstruct a physical porous structure.
- Develop a model for TCM hydration.
- Make recommendations regarding the use of the continuum approach for TCM hydration.

#### **Student profile**

We are looking for a student who:

- is interested in transport phenomena.
- has affinity or is interested in developing affinity towards multi-physics modelling.
- has interest in programming using a language of choice and wants to improve upon their existing programming skills.
- is interested in using experimental equipment.



#### **REFERENCES**

Nemati et al., (2020), A stochastic approach for predicting tortuosity in porous media via pore network modeling.

Bedell et al., (2021), Open-Source Script for Design and 3D Printing of Porous Structures for Soil Science.

Chen et al., (2022), Pore-scale modeling of complex transport phenomena in porous media.

Xu and Zhang, (2022), Research on modeling method of porous air bearing materials based on random particles.

Aarts et al., (2022), Diffusion limited hydration kinetics of millimeter sized salt hydrate particles for thermochemical heat storage.



# Borehole acoustic Stoneley wave measurement in porous sandstone

David Smeulders ,Yukai Liu

Email: d.m.j.smeulders@tue.nl , y.liu3@tue.nl

#### 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. For this project, we will conduct small size acoustic setup to measure pure Stoneley wave with source inside a borehole. Different rock samples(figure1) will be used.

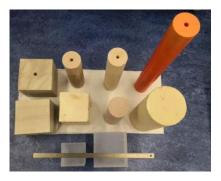


Figure 1: Rock samples for borehole Stoneley wave measurement

#### **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.

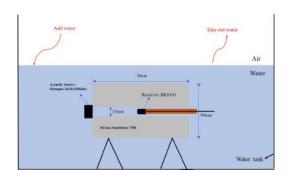


Figure 2: Schematic of borehole Stoneley wave measurement

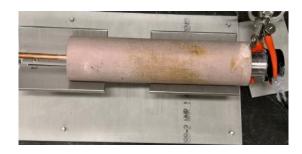


Figure 3: Photo of borehole Stoneley wave measurement setup

#### **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	Dr. Azahara Luna-Triguero
2nd supervisor	Dr. Maja Rucker
Mentor	Mohammad Hossein Khoeini
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical and Experimental



Project number: 32

# Estimation of the adsorption energy distribution of the solid surface by inverse gas chromatography

Mohammad Hossein Khoeini\*, Azahara Luna-Triguero, Maja Rucker

\*E-mail: m.h.khoeini@tue.nl

#### INTRODUCTION

In the establishment of hydrogen as an alternative carrier gas, the porous media which facilitates the hydrogen flow and storage need to be optimized in terms of reactivity and transport properties. Two main parameters governing the transport properties are surface area and surface energy of the porous media's surface. These two parameters determine the extent and strength of the interaction of the fluid with the solid's surface.

In this context, Inverse gas chromatography (iGC) is proposed as a sensitive and relatively fast technique for characterizing these two physiochemical properties of materials [1]. In this technique, different probe chemicals are injected at different concentrations into the column which is packed with the porous sample under investigation (Fig. 1). The retention data of the different probes are used to determine the surface energy.

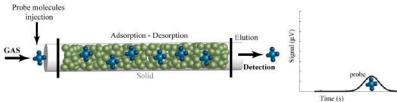


Fig. 1. principle of inverse gas chromatography

#### **Problem statement**

From the theoretical perspective, the surface of a solid is not composed of interacting sites with a unique energy, but of sites with a range of energy of interaction (figure 2) [2]. On the contrary, the surface energy measured by inverse gas chromatography with different probe chemicals reflects only the average energy of all interacting sites [3].

In this study, we want to develop an inverse method to obtain the distribution of interacting sites from the average surface energy which is measured by IGC. The developed inverse method will be used to assess reference solids (glass beads).

**Keywords**: Surface energy distribution, Inverse gas chromatography, sorption technique

#### **Task**

We are looking for the high-motivation student who has creative, solution-oriented, and interest in performing experiments and numerical simulations. In this project, you are expected to do:

- Literature review, focusing on different configuration of interacting sites on the surface, and inversion methods of calculating energy distribution functions.
- Developing an inversion method and model the method in MATLAB
- Conducting the experiments on the reference solids (20% of project)
- Assessing the validity of the developed inverse method by measured experimental data.

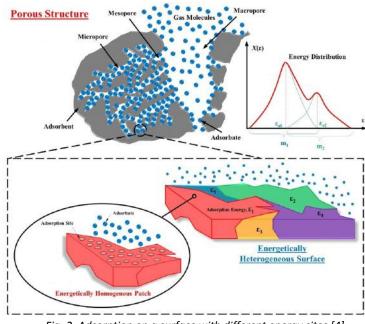


Fig. 2. Adsorption on a surface with different energy sites [4].

- [1] Thielmann F., 'Introduction into the characterisation of porous materials by inverse gas chromatography', Journal of Chromatography A, 2004, 1037, 115-123.
- [2] H. Balard, Estimation of the Surface Energetic Heterogeneity of a Solid by Inverse Gas Chromatography, Langmuir 1997 13 (5), 1260-1269.
- [3] Smith, R., Williams, D., Burnett, D., Heng, J., A New Method To Determine Dispersive Surface Energy Site Distributions by Inverse Gas Chromatography, Langmuir 2014 30 (27), 8029-8035.
- [4] Ng, K.C., Burhan, M., Shahzad, M.W. et al. A Universal Isotherm Model to to Capture Adsorption Uptake and Energy Distribution of Porous Heterogeneous Surface. Sci Rep 7, 10634 (2017)..

# TU/e HEATPOWER

#### Experimental set-up for turbine volute testing to increase RCG-turbine output

#### **Background**

Heat Power & TU/e developed a compact, fast responding and Steam and gas turbine: the Rankine Compression gas turbine (RCG). A 5kWe industrial prototype was realized in a wood milling factory in Schijndel (fig right). The RCG implements a radial free power turbine that drives a high-speed generator in direct drive. The maximum allowable speed of the generator is 21000RPM. However, this is still a relatively low speed for the turbine, that limits the pressure ratio and therefore the power output.





Numerical studies showed that altering the size of the housing of the expansion turbine, can improve the turbine power output at lower RPM's. An experimental set-up at TU/e was realized to be able to experiment with different turbine housing designs (fig below). The set-up is operated with cold air to make it possible to perform experiments with non-metallic 3D printed turbine houses.

#### Goals

- Realize an improved experimental set-up that comprises a centrifugal blower so that the turbine volutes can be tested with larger air flows
- Design alternative turbine volutes & realize the designs by 3D printing.
- Implement the printed turbine volutes in the set-up and perform experiments.
- Advise on future steps for altering the turbine housing to increase the turbine output at lower RPM's.



#### **Assignment**

Pursue goals as described in the above. Note that the scope is flexible and that there will be support of staff with turbo technology, power electronics, utilities, data-acquisition and control. The supervisor and Master student together will assess which of the above goals are feasible within this assignment and where the focus of this assignment will be.

Contact: Henk Ouwerkerk (H.Ouwerkerk@tue.nl) & Rick de Lange (H.C.d.Lange@tue.nl)