Master Thesis project proposals

Q1 2024-2025

Power **&** Flow

Department of Mechanical Engineering

Eindhoven University of Technology

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Preface

This is an overview of all the Master Graduation project proposals available in the Power and Flow section.

Please select 3 choices of different projects in order of preference and write a short motivation for your first choice to Giulia Finotello (G.Finotello@tue.nl). Something like:

- 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	**Asst. Prof. Claudia-F. López Cámara**
2nd supervisor	**TBD**
Company supervisor	**Prof. Hartmut Wiggers**
Company	**EMPI, University Duisburg-Essen**
Starting date	**Anytime**
Exp./Num./Design	**Experimental**

Power & Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Plasma synthesis of ultra-pure graphene for electrochemical applications

Claudia-F. López Cámara
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Introduction

Electrochemical devices (e.g., batteries or sensors) depend on the rapid exchange of charges to achieve their optimum performance. Including reduced graphene oxide or carbon nanotubes as an additive on the nanomaterials used on these devices has shown to enhance their conductivity and therefore, overall performance [1,2]. However, scalability of high performance materials is still an issue. To overcome that, plasma synthesis is shown as a promising alternative for an industrially scalable production, with the advantage of operating in continuous mode and producing ultra-pure free-standing few-layer graphene (FLG) [5-7]. Yet, the synthesis and testing of plasma-produced FLG for electrochemical applications is still limited.

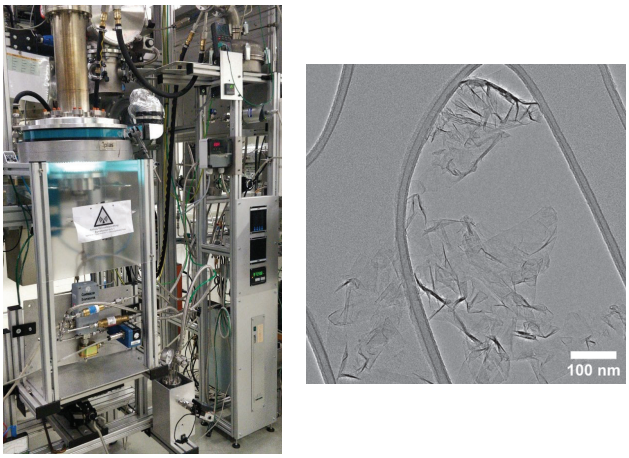

Figure 1. Left: Reactive zone of the microwave plasma reactor at the University Duisburg-Essen. Right: Few-layer graphene as seen under the transmission electron microscopy.

Project description

The focus of the proposed project is on the production of ultra-pure few-layer graphene using gas-phase microwave plasma synthesis and its further characterization and preliminary testing for electrochemical applications.

/ POWER & FLOW

Goals

1. Synthesize freestanding few-layer graphene via plasma reactor in a consistent and repeatable manner.
2. Characterizing the produced graphene and its attributes (by e.g., Raman, TEM, BET).
3. Preliminary testing of the synthesized graphene for future electrochemistry applications (e.g., batteries).

Requirements

- **The experimental part of this work will be conducted at the University Duisburg-Essen (Germany).** Thus, the student should consider commuting or living in Duisburg for most of the project period.
- The student should be motivated to learn and carry a hands-on project. No previous knowledge is required.

Benefits

The student will be working in a fast-paced collaborative environment and performing his/her work on industry-standard laboratories. S/he will be acquiring hands-on skills on:

- Operation of microwave plasma reactors.
- Safety regulations related to handling powder-form nanomaterials.
- Characterization techniques and analysis of the data.
- Basics on electrochemistry and nanomaterial electrochemical performance.

References

[1] L. Fu et al, Chem. Front. (2021)
[2] D. Pandel et al., ACS Appl. Mater. & Interfaces (2022)
[3] J. Gonzalez-Aguilar et al., J. Appl. Phys. (2007)
[4] A. Dato et al., Nano Lett. (2008)
[5] C.-F. López-Cámara et al., Combust. Flame (2023)
[6] P. Fortugno, C.-F. López-Cámara et al., Appl. Energy Combust. Sci. (2023)
[7] C.-F. López-Cámara et al., Carbon (2024)

Supervisor	Dr. Yuriy Shoshin
2nd supervisor	Dr. Viktor Kornilov
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Experimental

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

SYNTHESIS OF METAL OXIDE NANOPARTICLES BY METAL AEROSOL COMBUSTION

Yuriy Shoshin*, Viktor Kornilov

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INTRODUCTION

Nano-particles of metal oxides are widely used in industrial, biomedical, and other applications due to their high specific area and other unique properties. ***The global market of metal-oxides nanoparticles is expected o grow by ~ 9% a year and reach about US$ 10 billion by 2026.***

There are multiple chemical and physical methods exist to produce nano-oxides, and each method has its own advantages and drawbacks. The current technologies face a dilemma: To achieve high purity and well-controlled nano-particle sizes, high energy consumption and expensive equipment are required. The Power & Flow Group is now exploring a more economical way to produce metal-oxide nanoparticles of high qualities—***Generate oxide nanoparticles from vapor condensation via directly burning metal powders in air or other oxidizing gases***.

Keywords: *Metal combustion, nano-particles synthesis, metal oxides*

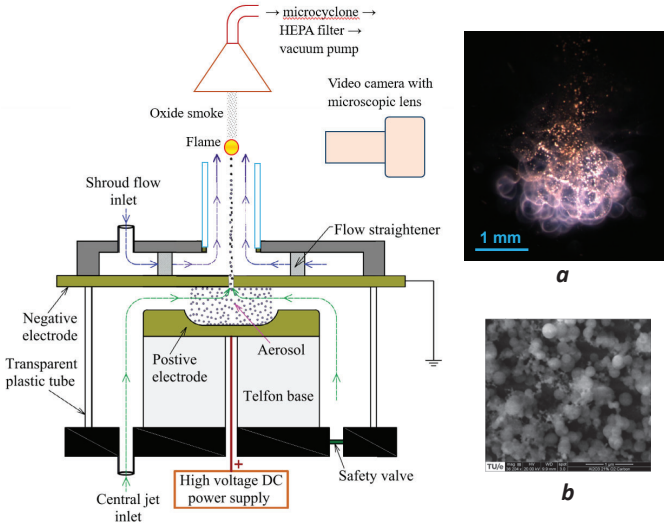

Fig 1. ***a)*** *Schematic of the electrodynamic burner.* ***b)*** *Al aerosol* ***c)*** *Al_2O_3 nano-particles generated by the flame.*

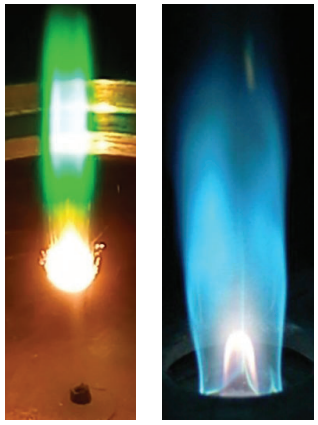

Fig 2.
a) *Iron aerosol micro-flame burning in oxygen. Combustion products (iron oxide nanoparticles) are illuminated with a green laser.*
b) *Hybrid propane-oxygen-zinc dust flame. The blue luminous zone is produced by the own thermoluminescence of condensing ZnO nanoparticles.*

GOALS

- To explore the possibility of synthesizing metal-oxide nanoparticles by direct combustion of (micrometric) metal powders. The prime focus is on iron oxide, while other metals can also be considered.
- To modify the existing micro-burner so that nano-oxide synthesis in hybrid hydrogen-oxygen-metal aerosol flames can be studied.
- To determine the properties (e.g., morphology, size distribution, phase, and elemental composition) via material characterization techniques including X-ray Diffractometry (XRD) and Scanning Electron Microscopy combined with Energy Dispersive Spectroscopy (SEM-EDS).

Achieving all the above goals is not necessary, while the proposed project assumes performing a significant step toward these goals. The proposed project is flexible and the concrete project plan can be adjusted to the preferences of a candidate.

BENEFITS

- Opportunity to get thorough training for material characterization—a highly demanded skill set by many industries.
- Well prepare you for a PhD research on combustion and material synthesis.
- International collaboration opportunities.

Supervisor	**Asst. Prof. Claudia-F. López Cámara**
2nd supervisor	**TBD**
Company supervisor	**Prof. Hartmut Wiggers**
Company	**EMPI, University Duisburg-Essen**
Starting date	**Anytime**
Exp./Num./Design	**Experimental**

Power & Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Spray-flame synthesis and performance testing of cathode materials for sodium ion batteries

Claudia-F. López Cámara
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Introduction

Batteries are crucial for the energy transition and helping on creating a more sustainable future. Sodium ion batteries emerge as an alternative to lithium ion batteries. Moreover, the electrode materials in any battery play a critical role on the battery performance and feasibility, having shown that polyanion structures are promising cathode material for sodium ion batteries.

Given the potential large battery materials demand, industrially-scalable methods should be considered when creating electrode materials. Hence, spray-flame reactor processes are considered as a suitable method as they can produce polyanionic-based materials in a highly-reproducible and scalable manner, continuously, and in a cost-effective way. The standardized SpraySyn burner also permits for using a wider variety of reactants, facilitating the investigation of multiple polyanion-based compositions.

Figure 1. Top: Spray-flame from the University Duisburg-Essen. Bottom: T-battery for performance testing.

Project description

The focus of the proposed project is on the production, characterization, and testing of cathode material for sodium ion batteries using spray-flame synthesis.

Goals

1. Synthesize polyanion-based materials in powder form via spray-flame reactor in a consistent and repeatable manner.
2. Characterizing the produced materials and its attributes (by e.g., BET, XPS, FTIR, Raman, TEM, BET).
3. Preliminary performance testing of the synthesized materials on T-cell batteries (e.g., capacity measurements and cyclic voltammetry).

Requirements

- **The experimental part of this work will be conducted at the University Duisburg-Essen (Germany).** Thus, the student should consider commuting or living in Duisburg for most of the project period.
- The student should be motivated to learn and carry a hands-on project.
- No previous knowledge on flame synthesis, cathode materials, or batteries is required.
- No previous experimental experience is required.

Benefits

The student will be working in a fast-paced collaborative environment and performing the experimental work on industry-standard laboratories. By the end of the project, the student will be:

- Capable to operate a spray-flame reactor equipped with a SpraySyn burner.
- Familiar to high-standards on safety regulations.
- Competent on nanomaterial characterization techniques and analysis of the data.
- Knowledgeable on the basics on battery electrochemistry and testing of electrochemical performance.

Supervisor	Giulia Finotello
2nd supervisor	Dennis Thuy
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

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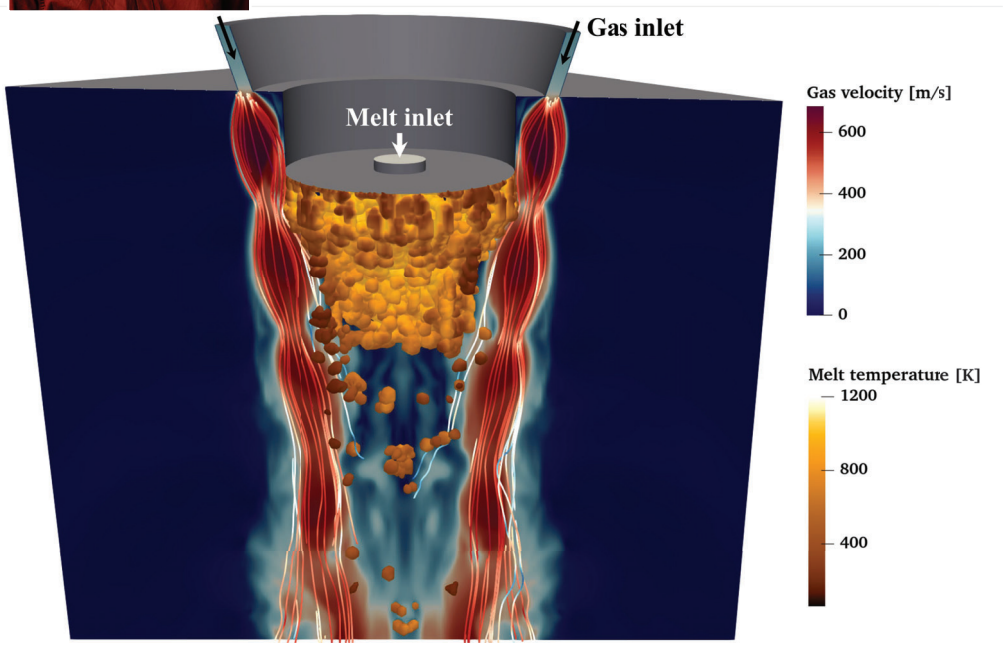
Simulation of breakup and solidification of liquid metal droplets in gas atomization

Dennis Thuy*, Giulia Finotello, Joris Remmers, Niels Deen

*E-mail: d.p.l.thuy@tue.nl



Scan the QR for a video impression!

Figure 1: Simulation in OpenFOAM of the breakup of liquid metal in a gas atomizer

INTRODUCTION

Metal 3D printers can be part of a completely circular production environment where scrap metals can be used as the raw material to produce powder for the printers. While metal 3D printers are already in an advanced state, the small-scale production of metal powder is still in need of development.

In a gas atomizer, metal powder is produced by breakup of a liquid metal jet under the influence of high-pressure gas flow, as shown in figure 1. While the metal droplets are breaking up, they also cool down rapidly and solidify in-flight.

After solidification, the metal particles can no longer break up. Therefore, the solidification determines the final properties of the powder. It needs to be accurately modeled in simulations of liquid metal atomization.

TASKS

The project revolves around CFD simulations in which the breakup and solidification of the liquid metal droplets are modelled.

You will test several breakup models to see which one is most suitable for the liquid metals in the gas atomization process.

Besides, you will develop a solidification model for these metal droplets and implement it in the code. The goal is to predict the properties of the metal powder, so that the process can be optimized for metal 3D printers!

GOAL

The goal of the project is to develop a numerical model that can show the influence of solidification and breakup on the properties of gas atomized metal powder. This knowledge will be used to finetune powder properties to the requirements of metal 3D printers.

BENEFITS

- Freedom to shape the research to your interests
- Work with OpenFOAM, one of the most popular open-source CFD packages
- Learn to make cool visualizations of your simulations!

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

Available for ME

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

A RANS turbulence modeling framework for means and oscillating flow fields

Stein Stoter
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Keywords: *Turbulence modelling, RANS, Fourier representation*

INTRODUCTION

Turbulence modeling frameworks based on the Reynolds-averaged Navier-Stokes (RANS) equations are the main workhorse in CFD-industry turbulent flow solvers. Their popularity stems from computational efficiency and ease of use. Yet they lack in predictive capability, i.e., accuracy. This is due to the underlying models, which necessarily replace the unknown turbulence quantities with expressions based on mean quantities.

Project description

In this project, you will develop a new RANS framework, that not only aims to retrieve the mean quantities, but also the lower-order oscillations of the turbulent flow field. The expectation is that this fuller description of the complete physics alleviates the model deficiencies of classical RANS models.

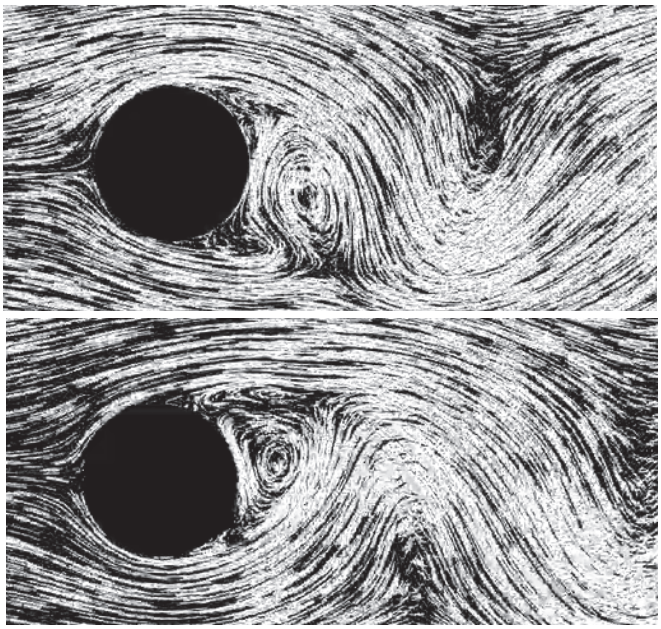

Fig 1: RANS simulation with clear low-frequency oscillation components.

RESEARCH TOPICS

- Perform a literature study to learn about the advanced RANS models.
- Develop a suitable model based on the RANS equations for the means and oscillations.
- Implement this model in an in-house turbulent flow solver, for turbulent channel flow (see below).
- Analyze the accuracy of the obtained solutions in comparison to a typical eddy-viscosity RANS model.

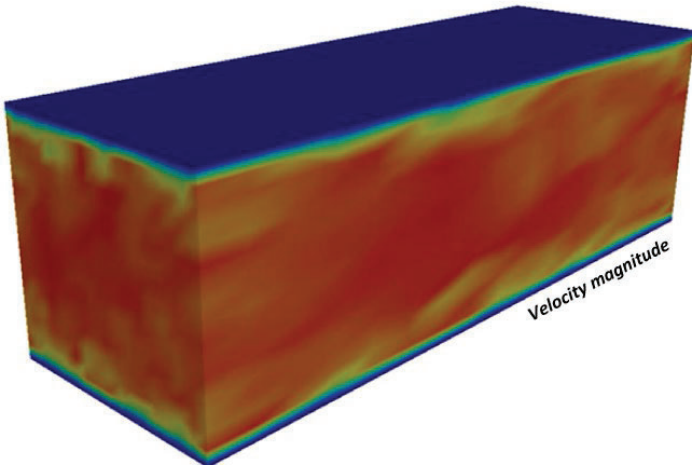

Fig 2: Main testcase: turbulent channel flow

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] Pope, S.B. (2000). *Turbulent flows*

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

Available for ME

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

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 (see Fig 1.). The quality of this scale interaction model dictates the quality of the coarse-scale approximation, as seen in the figure below. The ultimate application area of this research lies in the multiscale modeling of turbulent flow (Fig 2.)

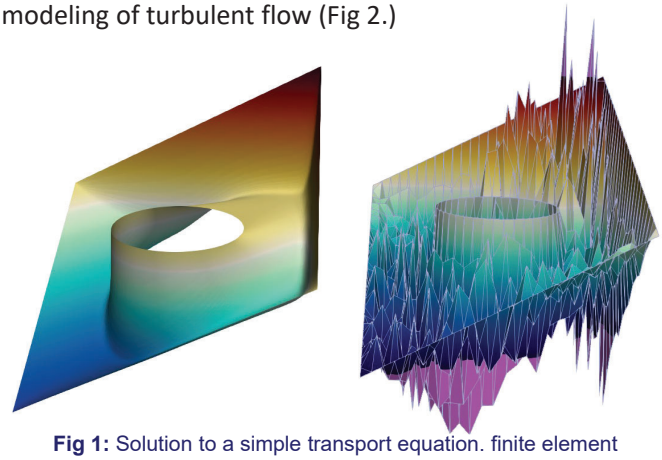

Fig 1: Solution to a simple transport equation. finite element approximation with (**left**) and without (**right**) scale interaction.

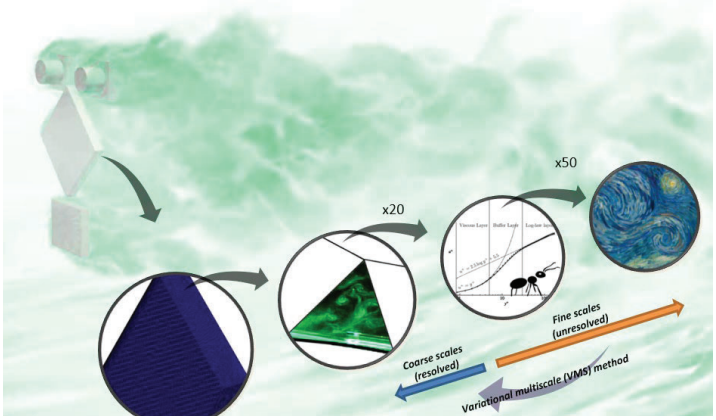

Fig 2: Scale interaction for turbulent flow.

PROBLEM STATEMENT

The scale interaction can be computed exactly (Fig 3.), 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.

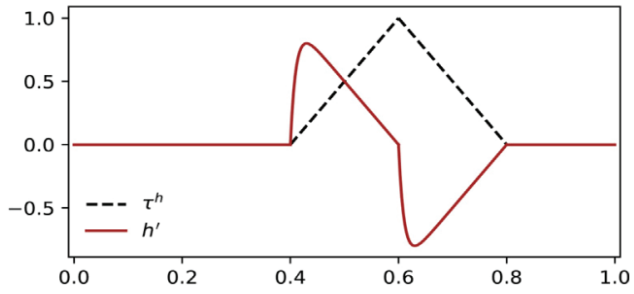

Fig 3: Scale-interaction function for a one-dimensional advective transport equation. For this particular case, the interaction function h' localizes to a single element.

RESEARCH TOPICS

- Perform a literature study to learn about the state-of-the-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 Fig 2.).
- Develop a machine learning code that can predict these functions.
- Study the effectiveness of the machine-learned model of the scale interaction.

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] 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	Boyan Xu
2nd supervisor	R.J.M.Bastiaans
Daily supervisor	Boyan Xu
Company	N.A.
Starting date	Anytime
Exp./Num./Design	Numerical

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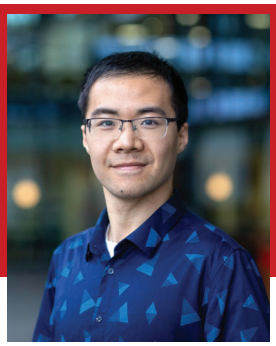


The Effect of Conjugate Heat Transfer on Near Lean Blow-off Bluff-body Stabilized Flame

Boyan Xu
b.xu1@tue.nl

INTRODUCTION

Ammonia, as a carbon-free fuel with transport and production advantages, has great potential to be utilized in gas turbine combustors. However, low reactivity, low laminar flame speed, and narrow flammability of pure NH_3 restrict its utilization. The pre-cracking of ammonia, which generates the $NH_3/H_2/N_2$ mixture, has been regarded as a strategy to overcome these drawbacks.

To reduce the emission of combustion, very lean condition is used for combustion. However, flame extinction, i.e., lean blow-off, should be prevented with this condition.

Current results based on bluff body stabilized $NH_3/H_2/N_2$ flame show that lean blow-off is very sensitive to the thermal boundary condition of bluff body. The conjugate heat transfer of the bluff body needs to be considered for predicting accurate extinction.

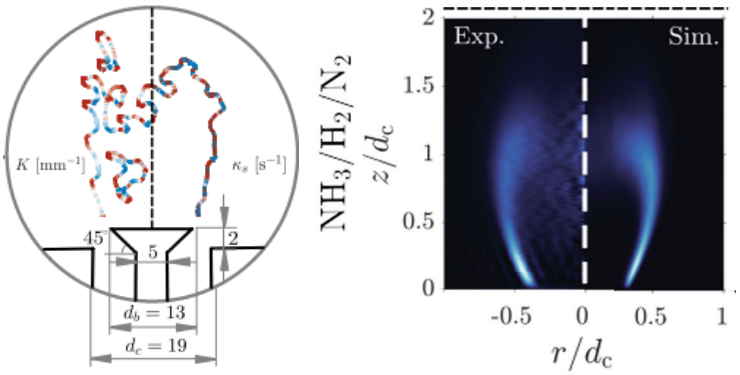


Figure1. a) Schematic of the bluff-body burner with transient flame surface; b) The comparison between experimental measurement and current simulation result(time averaged)

GOALS

Revise the current 3-D simulation model with including CHT and explore whether CHT plays an important role on the near lean blow-off $NH_3/H_2/N_2$ flame.

TASKS

- *Literature study on lean blow-off flame about the process and principle of extinction.*
- *Learn the using of CONVERGE CFD software and its setting about Conjugate Heat Transfer(CHT). Apply it on current simulation case.*
- *Analyze the heat transfer on bluff body surface.*
- *Process the simulation data and export them to picture or movie with MATLAB.*
- *Compare the flame characteristics and predict lean blow-off with CHT & without CHT.*

REQUIREMENT

- *Basic knowledge of fluid mechanics, heat transfer and combustion.*
- *Fundamental MATLAB skills.*

BENEFITS

- *Freedom for further researches to you interest*
- *Potential to participate in scientific paper writing*

REFERENCES

[1] Su, T., Xu, B., Bastiaans, R. J. M., and Worth, N. A. "Lean Blow-Off Behaviour of Premixed Bluff-Body Stabilized Hydrocarbon-Air Flames and Ammonia/Hydrogen/Nitrogen-Air Flames." ASME. J. Eng. Gas Turbines Power. November 2024; 146(11): 111011.

[2] G. Generini et.al. COMBUSTION MODELLING OF THE T100 MICRO-GAS TURBINE BURNER INCLUDING THE INFLUENCE OF THE STRETCH AND HEAT LOSS/GAIN EFFECTS ON THE FLAME, Proceedings of ASME Turbo Expo 2024.

Supervisor	Xander Seykens (TNO, TU/e)
2nd supervisor	Bart Somers (TU/e)
Company	TNO
Internal / External	External
Starting date	1/9/2024
Exp./Num./Design	Numerical

Available for ME-SET-AT

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Development and validation of a phenomenological H2-HPDI Combustion Model

XANDER SEYKENS
EMAIL: X.L.J.SEYKENS@TUE.NL

INTRODUCTION

Hydrogen is considered as an important (future) fuel for heavy duty combustion engines for mobility and power generation. The hydrogen-diesel High Pressure Direct Injection (HPDI) combustion concept is considered as a feasible combustion concept with high performance potential (power output, load response). This combustion concept is driven by the direct injection of hydrogen which is ignited using a small pilot fuel (e.g. diesel) injection. For engine optimization, fast-computing models with predictive capabilities ("phenomenological model") simulating the HPDI combustion process are desired. These models allow performing iterative engine simulations for systematic optimization, engine concept and controls/diagnostics development. Main focus is on simulating in-cylinder pressure, heat flows and NO emissions.
Currently, a base H2-HPDI fuel injector and a H2-HPDI in-cylinder combustion model, built in the Matlab® environment, are available. These models will serve as the starting point of this assignment.

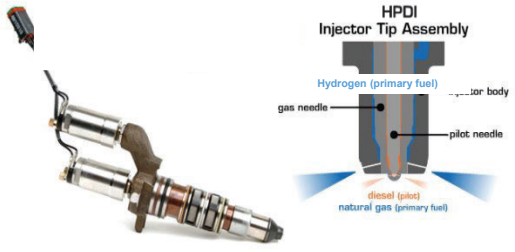


Figure 1: High Pressure Direct Injection of hydrogen is a promising hydrogen engine concept. .

OBJECTIVES

- Development and validation of a phenomenological Hydrogen High Pressure Direct Injection Injector and combustion model. Extension of the model with NOx emission formation.

APPROACH

- Literature study on HPDI (hydrogen) injection and combustion[1]
- Get acquainted with the available H2-HPDI injector and combustion model
- Linking HPDI injector model to the HPDI combustion model and validate simulation results against measurements
- Identify possible model improvements and design, implement and validate solutions
- Extend validated H2-HPDI model with NO formation model
- Validate H2-HPDI model for NOx emissions using available measurement data
- HPDI combustion model sensitivity study towards optimizing efficiency and emissions
- Writing report and presenting results

REQUIREMENTS

- Affinity with combustion engines and numerical work
- Good Matlab modellig skills

LOCATION AND SUPERVISION

The master thesis work will be executed at TNO Powertrains Department located on the Automotive Campus in Helmond. You will be assigned a TNO and TU/e supervisor.

REFERENCES

1. *Literature on high pressure direct injection combustion, E.g. consult the SAE Mobilus database*

Supervisor	Xander Seykens
2nd supervisor	Bart Somers
Company	TNO
Internal / External	External
Starting date	01/09/2024
Exp./Num./Design	Numerical, Experimental

Available for ME-SET-AT

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Aftertreatment for hydrogen internal combustion engine

XANDER SEYKENS
EMAIL: X.L.J.SEYKENS@TUE.NL

INTRODUCTION

Hydrogen is considered as an important (future) fuel for heavy duty combustion engines for mobility and power generation. Hydrogen internal combustion engines (H2-ICE) have high potential for ultra-low engine-out NOx emissions. However, for certain applications, aftertreatment technology is anticipated to be used for first generation of hydrogen engines. The impact of hydrogen on the performance of available aftertreatment technology is not fully clear. At TNO measurements on hydrogen combustion engines with and without aftertreatment have been performed. The goal of this assignment is twofold: On the basis of this data, the impact of hydrogen can be quantified. Next to this, the aftertreatment models used as part of current aftertreatment controls needs to be updated based on these findings.

OBJECTIVES

- Updating available aftertreatment component models and controls to capture main impact of the use of hydrogen as fuel in a heavy duty internal combustion engine

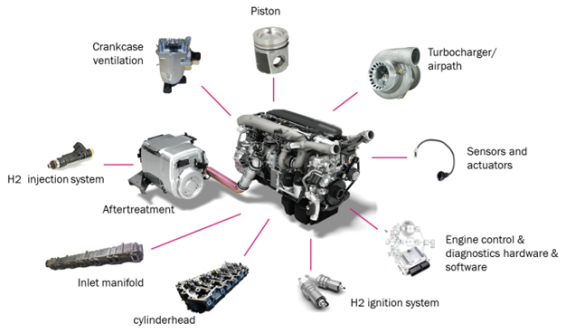


Figure 1: Hydrogen internal combustion engine and use of aftertreatment.

APPROACH

- Literature study on hydrogen as fuel for combustion engines and aftertreatment technology [1]
- Review of available aftertreatment component models
- Evaluation of available measurement data on aftertreatment components used on an heavy duty H2-ICE
- Updating available aftertreatment component models to capture main impact of hydrogen fuel
- Model validation on basis of available measurement data
- Assessment of impact use of hydrogen on aftertreatment controls with use of updated aftertreatment component models
- Verification of available the performance of aftertreatment controls using updated aftertreatment component models
- Writing report and presenting results

REQUIREMENTS

- Affinity with combustion engines and aftertreatment technology
- Interest in numerical work and hands-on experience with Matlab-Simulink®

LOCATION AND SUPERVISION

The master thesis work will be executed at TNO Powertrains department at the Automotive Campus in Helmond. You will be assigned a TU/e and TNO supervisor.

REFERENCES

1. *Literature on high pressure fuel injection systems and measurements of fuel injection rate, mass and momentum. E.g. consult the SAE Mobilus database*

Supervisor	Dr. Ir. Yunus Tansu Aksoy
2nd supervisor	Tess Homan
Company	
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Experimental

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Gentle collection of virus-laden droplets:

Droplet impact on oblique surfaces suppressing splashing

Yunus Tansu Aksoy
e-mail: y.t.aksoy@tue.nl

INTRODUCTION

Quantification of infectious viruses in air and assessing their transmission potential via small or large respiratory droplets is crucial for risk assessments of pandemic outbreaks which is notoriously difficult to perform. Whether the air contains infectious virus in sufficient amounts to infect new hosts, and whether this virus is present in small or large droplets that stay dispersed in air for long versus short time periods respectively, is almost impossible to demonstrate (Coleman, 2021). Environmental factors such as temperature and humidity may change droplet dynamics, droplet sizes and number density (through evaporation or condensation) (Bourouiba, 2021) and virus infectivity very rapidly (Herfst, 2017). We want to collect those virus-laden droplets without changing their infectivity as gentle as possible. The collection process requires droplet impact on a solid substrate without harming the droplet. It is already known that the droplet impact dynamics significantly change when nanometer-sized particles are present in the fluid (Aksoy 2022). In this project, the student will study droplet impact on a solid substrate for droplet collection for virus quantification purposes.

REQUIREMENTS

Interest in

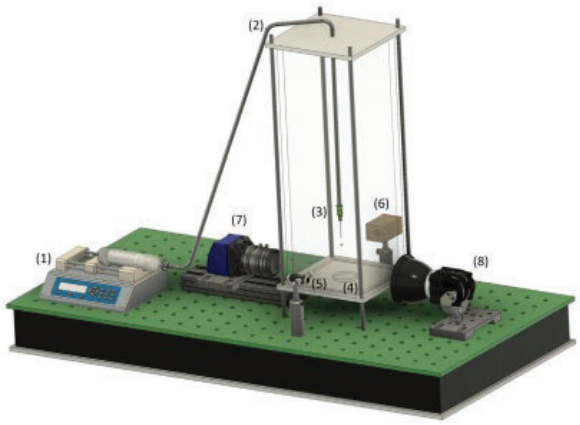
- Experimental work
- Fluid mechanics
- Motivation to carry on hands-on project

OBJECTIVE

The main objective of this thesis is to identify the droplet impact conditions allowing users to gently collect the deposited droplets without harming the viruses inside.

PROJECT DESCRIPTION & APPROACH

This experimental project starts with a literature study. Based on the motivation and literature knowledge, the student will build an experimental setup for characterizing post-impact droplet dynamics via high-speed camera. The impact conditions will include several droplet release heights ,i.e., Weber numbers, different surface conditions, e.g., hydrophobic/hydrophilic, and different droplet sizes. Initially, milimeter-size droplets are foreseen, yet smaller droplets can be preferred to match real conditions in the final stages of the project. No real virus will be used during the experiments due to safety reasons!



Typical experimental setup (Aksoy, 2022)

REFERENCES

Aksoy (2022) *Journal of Colloid and Interface Sciences* 606 pp 434-443
Bourouiba (2021) *Annual Review of Fluid Mechanics* 53:1 pp 473-508
Coleman et al. (2022) *Clinical Infectious Diseases* 74:10 pp 1722-1728
Herfst et al. (2017) *Current Opinion in Virology* 22 pp 22-29

Supervisor	Xander Seykens (TNO)
2nd supervisor	Bart Somers (TUe)
Company	TNO
Internal / External	External
Starting date	01/09/2024
Exp./Num./Design	Experimental, numerical

Available for ME-SET-AT

TNO innovation for life

Modeling of exhaust water recovery model for H2-ICE

XANDER SEYKENS
EMAIL: X.L.J.SEYKENS@TUE.NL

INTRODUCTION

The Hydrogen internal combustion engine is expected to play an important role in realizing sustainable heavy duty transport and meeting 2050 climate goals. At TNO, located on the Automotive Campus in Helmond, research and development on hydrogen internal combustion engines is on-going. For lean burn Spark-Ignited hydrogen engines the use of port water injection, in which water is injected into the intake ports of the engine, is an attractive solution to mitigate NOx emissions and maintain combustion stability during dynamic engine operation. The high exhaust water content of hydrogen engines offers the possibility to realize a self-sustaining system, using water recovered from the exhaust gases for the port water injection. This assignment targets the further development of a phenomenological model of the exhaust water recovery system that allows sizing of such system and development of dedicated water recovery/injection strategies. As a starting point you will use a base model built in the Matlab® simulation environment. Initial focus will be on the further development of a water condenser model including modeling of two-phase flow and liquid water extraction/collection.

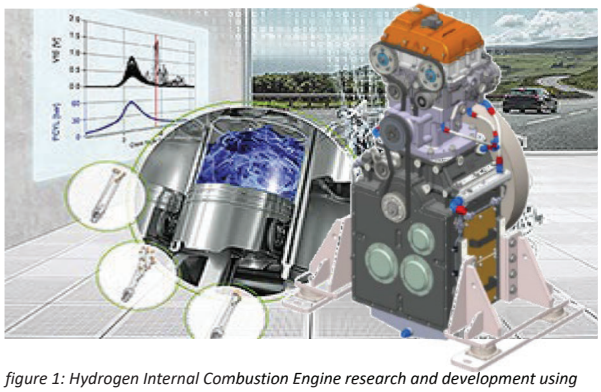


figure 1: Hydrogen Internal Combustion Engine research and development using single-cylinder research engine at TNO [1].

OBJECTIVES

- Further development of a phenomenological exhaust water recovery system model enabling system sizing and water injection strategy development.

APPROACH

- Short literature study on hydrogen combustion engines, water injection and water recovery
- Review of available model and identification of required model extensions.
- Develop and implement model extensions
- Functional demonstration of extended model capabilities on a selected use-case and demonstration of main sensitivities
- Writing report and presenting results

REQUIREMENTS

- Affinity with combustion engines
- Good understanding of thermodynamics
- Experience with Matlab®

PERIOD

Start possible from September 2024. This Master thesis assignment can be converted into 14 week internship.

LOCATION

The project will be executed at TNO Powertrains department at the Automotive Campus in Helmond. You will be assigned a TU/e and TNO supervisor.

REFERENCES

1. *TNO, https://www.tno.nl/en/focus-areas/traffic-transport/roadmaps/sustainable-traffic-and-transport/sustainable-vehicles/how-hydrogen-can-accelerate-energy-transition-in-the-transport-sector/*
2. *Literature on hydrogen combustion engines. E.g. consult the SAE Mobilus database*

Supervisor	Xander Seykens (TNO)
2nd supervisor	Bart Somers (TUe)
Company	TNO
Internal / External	External
Starting date	01/09/2024
Exp./Num./Design	Experimental, numerical

Available for ME-SET-AT

TNO innovation for life

Modeling lean burn SI H2-ICE with water injection for NOx reduction in H2-ICE

XANDER SEYKENS
EMAIL: X.L.J.SEYKENS@TUE.NL

INTRODUCTION

The Hydrogen internal combustion engine is expected to play an important role in realizing sustainable heavy duty transport and meeting 2050 climate goals. At TNO, located on the Automotive Campus in Helmond, research and development on hydrogen internal combustion engines is on-going. The spark-lean burn ignited hydrogen engine is characterized by extremely low engine-out NOx in steady state operation. Main NOx dominantly results from dynamic engine operation. Here, the use of port water injection is an attractive solution to reduce combustion temperatures and reduce NOx formation rates. Furthermore, reduction of in-cylinder temperature is a means to stabilize the combustion process avoiding uncontrolled combustion (knock, pre-ignitions). This internship targets to model the impact of the injected water on the combustion process and more specifically on the NOx formation rates and tendency towards unstable combustion. Starting point is a base phenomenological Spark Ignition (SI) Hydrogen combustion model simulating in-cylinder heat release. Matlab® will be used as the modelling environment. Measurement data is available to support model development.

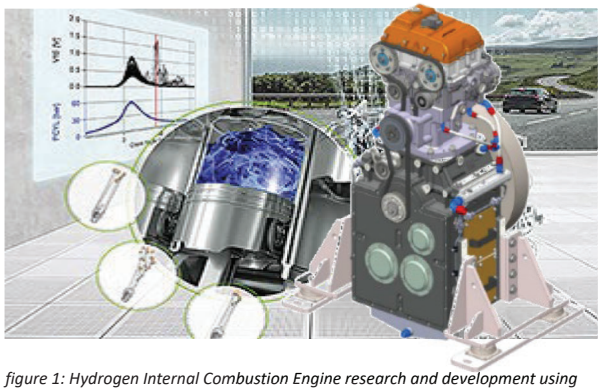


figure 1: Hydrogen Internal Combustion Engine research and development using single-cylinder research engine at TNO [1].

OBJECTIVES

- Extend the available PFI SI In-cylinder hydrogen combustion model to include the impact of water injection on NOx emission formation and to quantify the tendency towards unstable combustion.

APPROACH

- Short literature study on hydrogen combustion engines and water injection
- Analysis of available model and measurement data
- Develop and implement a model for the inclusion of the impact of water injection on NOx emissions and combustion stability.
- Functional demonstration of extended model capabilities and demonstration of main sensitivities
- Writing report and presenting results

REQUIREMENTS

- Affinity with combustion engines
- Good understanding of thermodynamics
- Experience with Matlab®

PERIOD

Start possible from September 2024. This Master thesis assignment can be converted into 14 week internship.

LOCATION

The project will be executed at TNO Powertrains department at the Automotive Campus in Helmond. You will be assigned a TU/e and TNO supervisor.

REFERENCES

1. *TNO, https://www.tno.nl/en/focus-areas/traffic-transport/roadmaps/sustainable-traffic-and-transport/sustainable-vehicles/how-hydrogen-can-accelerate-energy-transition-in-the-transport-sector/*
2. *Literature on hydrogen combustion engines. E.g. consult the SAE Mobilus database*

Supervisor	Michel Cuijpers
2nd supervisor	Noud Maes
Company	TU/e & Progression Industry
Internal / External	Internal/external
Starting date	TBD
Exp./Num./Design	Experimental

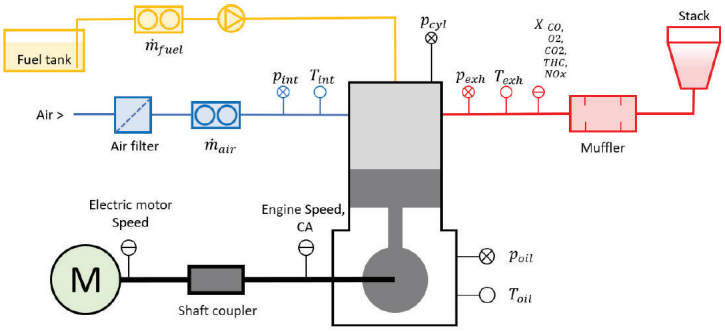
Available for ME

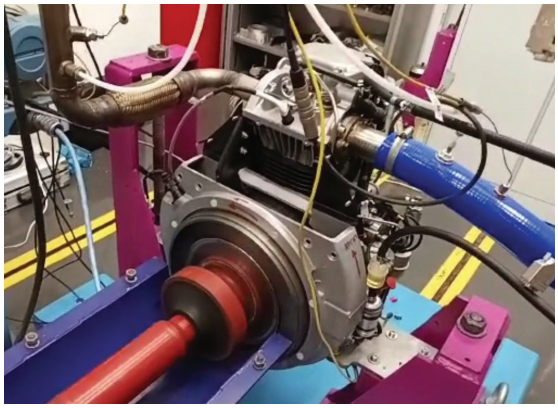
TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Progression-Industry
"GREEN" out of the box technologies

Investigating and programming injection strategy possibilities using an open ECU on a single-cylinder CI research engine

Michel Cuijpers, Noud Maes





Introduction

The energy transition from fossil- to E-fuels (renewable fuels produced by clean energy) and biobased fuels will not be an overnight transition. While a future energy surplus from sustainable sources is expected, the availability of E-fuels is still limited to small batches. This means that the world will have to wait for the availability of these fuels, but the engines need to be ready! In this work, particular focus will be given to a newly-commissioned single-cylinder CI research engine, equipped with a so-called open (programmable) ECU. This ECU will allow for modifying the injection strategy towards the fuels of interest.

Subject

The open ECU is used to investigate several fuels regarding combustion properties and emissions by optimizing injection strategy. The student will investigate functions of the Motec M142 open ECU, which is connected to a single cylinder CI engine.

Experimental apparatus

Newly commissioned Hatz 1D90E 4-stroke CI engine with an open ECU to control injection strategy.

Initial activities

- Literature study, familiarization with subject: what are important combustion properties?
- Assist regular experiments, learn to use the set-up (including safety aspects)
- Understanding ECU variables
- Determine data acquisition possibilities
- Initial test runs to check data-acquisition
- Get familiar with Design of Experiments (DoE) for creating an efficient measurement matrix
- Baseline and future fuels testing
- Data analysis

Where

TU/e, Mechanical Engineering, Power and Flow

Type

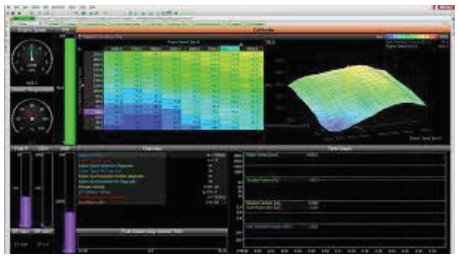
Experimental project

Keywords

Future fuels – Injection strategy – Combustion parameters – Open ECU

Contact

Michel Cuijpers, m.c.m.cuijpers@tue.nl



Supervisor	DAF supervisor
2nd supervisor	Xander Seykens (TU/e)
Company	DAF
Internal / External	External
Starting date	1/06/2024
Exp./Num./Design	Numerical

Available for ME-SET-AT

DAF
A PACCAR COMPANY

Diesel and Hydrogen ICE SCR deNOx NH3 virtual sensing embedded model for ultra-low NOx

XANDER SEYKENS
EMAIL: X.L.J.SEYKENS@TUE.NL

INTRODUCTION

The research it about development of robust SCR controls for Diesel and Hydrogen ICE exhaust gas aftertreatment systems that are capable of meeting EPA 2027 NOx and NH3 slip requirements. What improvements can be done to get more robust control design over 650 kmile emission life time?

Embedded models for the SCR deNOx system are using systems (virtual) sensors, e.g. temperature, exhaust flow and NOx sensors system in and out. Ultra low emission legislation EPA 2027 require NOx emission levels in tailipipe ranging 0-2 ppm, while the NOx sensor has an accuracy of +/- 5 ppm. Meeting these requirements is a challenge from model and control perspective and requires fundamental understanding of SCR catalyst dynamics flow and temperature, chemistry and ageing behaviour.

Since mid 2023 a proof of concept is running and first sensitivity studies are performed on the engine dynamometer. These test data can be used and applied in current SCR embedded model (S-function) simulation environment to assess the system capabilities and determine further model and control improvements to make the system more accurate on NOx and NH3 slip prediction and applying DEF (NOx reductant) compensations to correct for system biases.

OBJECTIVES

The main objective of this assignment is the development of robust SCR model for virtual sensing of NH3 storage and control objective to meet EPA 2027 35mg/bhph NOx emission requirements.

/ POWER AND FLOW

APPROACH

The complete assignment comprises 3 phases of which phase 1 is considered as part of the (extended) internship assignment.

Phase 1 (internship or master thesis):

- Literature study on deNOx aftertreatment technology, modelling (virtual sensing) for diesel and hydrogen combustion engines
- Literature/IP study on control algorithm and sensor architecture for SCR deNOx aftertreatment
- Propose improved model and control design
- Provide preliminary simulation results to fund the proposed control design

Phase 2 + 3 (master thesis):

- Design Rapid Prototyping SCR model and Controls in Matlab-Simulink®
- Vehicle demonstrator

REQUIREMENTS

- Affinity with combustion engines and aftertreatment technology
- Interest in numerical work and hands-on experience with Matlab-Simulink®

LOCATION AND SUPERVISION

The master thesis work will be executed at DAF Trucks in Eindhoven. You will be assigned a TU/e and DAF supervisor.

Further information

- Marc van Aken – Principal Engineer Aftertreatment Systems – Paccar Global Engines
- E-mail: Marc.van.Aken@Paccar.com
- Phone: +31 (0)40 – 214 3964

REFERENCES

1. *Literature on Selective Catalytic Reduction (SCR) deNOx Catalysts, SCR dosing controls, model-based control E.g. consult the SAE Mobilus database*

Supervisor	Rob Bastiaans
2nd supervisor	N.A
Company	N.A.
Internal / External	Internal
Starting date	02/09/2024
Exp./Num./Design	Numerical

Available for ME-SET-AT-AIES

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number: 2024 Q1-01

Micro Gas Turbine combustion fueled by ammonia/hydrogen mixtures

Rob Bastiaans, r.j.m.bastiaans@tue.nl

INTRODUCTION

In the European FLEXnCONFU project we study the application of ammonia (NH_3) combustion for a gas turbine application. The reason is that, like hydrogen, ammonia is carbon free but has a much higher energy content under non-restricting temperature and pressure conditions. The disadvantage of NH_3 is that it has combustion properties that are worse. However, this can be solved by using mixtures of NH_3 and H_2, also because of the easy (partial) conversion of NH_3 to H_2.

The task of TU/e is to derive an accurate but efficient CFD model to make fast parameter variations possible in relevant applied geometries. In general, we use the Flamelet Generated Manifold (FGM) method for this to reduce the associated very stiff kinetics. Furthermore, we use efficient models to describe small scale turbulence flame interactions.

Your supervisor performs very expensive detailed high resolution Direct Numerical Simulations (DNS) on a supercomputer for validation of these modeling strategies.

The task of the BSc student is to setup equivalent combustion cases with the use of ANSYS Fluent using LES (Large Eddy Simulation) The student will study the model performance of FGM and small-scale interactions from these simulations. Now we obtained a case file for a gas turbine treated by the so called thickened flame model (TFM). It is your task to change it to FGM for the chemistry with H_2O as first controlling variable and possibly local flame curvature as a second.

TASKS

Your first is to reproduce the TFM results.Secondly you will construct an FGM table for use in Fluent after which we make a comparison. To investigate the fundamentals, inaccuracies and potential of FGM we might want to investigate its behavior for very simple laminar flames. In the end It is of interest, in particular, how results depend on the applied Karlovitz number, being the ratio between the smallest turbulent scales and the flame thickness:

$$Ka = \frac{\delta_L^2}{\eta^2}$$

Especially what happens when Ka passes the criti

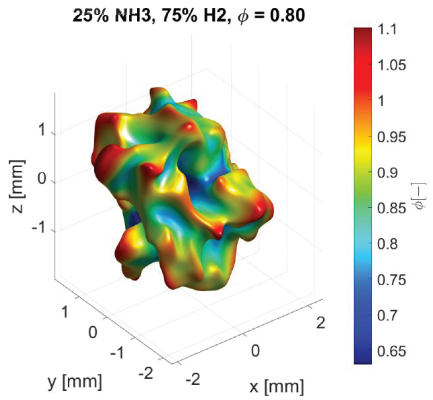


Figure 1: Flame isosurface colored with local equivalence ratio, Ka=10 [1].

REFERENCES

[1] Mukundakumar, N., & Bastiaans, R. J. M. (2022). DNS Study of Spherically Expanding Premixed Turbulent Ammonia-Hydrogen Flame Kernels, Effect of Equivalence Ratio and Hydrogen Content. Energies, 15(13), Article 4749. https://doi.org/10.3390/en15134749

Master Thesis Project Proposals
Q1 2024-2025

Energy Technology & Fluid Dynamics

Department of Mechanical Engineering

Eindhoven University of Technology

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Preface

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

Please select 2-3 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).

Daily supervisor	Dr. David Rieder
Supervisor	Dr. Maike Baltussen
Supervisor	Dr. Maja Rücker
Starting date	asap
Exp./Num./Design	Experimental & Numerical

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Collaborative Hide and Seek with droplets

Imbibition dynamics with 4D μCT imaging and multiphase CFD

D.R. Rieder*, M.W. Baltussen, M. Rücker

*d.r.rieder@tue.nl

INTRODUCTION

Multiphase flows traditionally belong to the most relevant phenomena for the energy-relevant industry, i.e. hydrogen-formation in electrolyzers, brine-displacement during CCS or synthesis of liquid fuels. However, those flows also belong to the least understood phenomena, due to the complex material interaction at the interfaces.

Additionally, gaining insights into those phenomena via multiphase CFD is often limited by unsatisfying overlap with experiments. There, the material and system properties are often not included in the models or simply not known, e.g. wettability and contact angle [1].

In this collaborative project between ME & CEC, we aim to improve our understanding of multiphase flow using simultaneously advanced multiphase CFD in combination with 4D (3D + time) μCT-imaging. Here, the droplet spreading inside a regular, idealized porous media will be studied and the experimental results compared with complementary simulations.

GOALS

You will design an idealized porous structure, conduct μCT experiments, compare those results with high-fidelity multiphase CFD, schematically shown in fig. 1. Finally, you will critically analyze the results and evaluate the quality of the current state of the art of multiphase models.

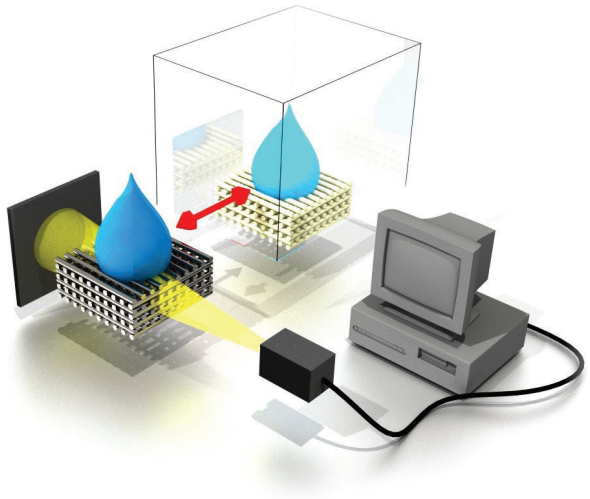


Figure 1: Schematic Imaging setup and comparison with simulation data for the imbibition of a droplet in an idealized porous media

BENEFITS

Within this project you will:

- Acquire in-depth knowledge of advanced experimental techniques and numerical methods
- Work in an international team addressing the current challenges for the energy-transition
- Advance our understanding of multiphase fluid dynamics
- Contribute to solving fundamental challenges for the transition to a sustainable energy sector

REFERENCES

[1] Rücker et. al The Origin of Non-thermal Fluctuations in Multiphase Flow in Porous Media doi: 10.3389/frwa.2021.671399

Supervisor	**Paul Grassia**
2nd supervisor	**Paul Grassia**
Starting date	**Flexible**
Exp./Num./Design	**Modelling/Numerical**

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Bubble Trains Flowing in a Channel

Paul Grassia*
p.s.grassia@tue.nl,

INTRODUCTION

There are many scenarios in which trains of bubbles flow along narrow channels (e.g. foam-based gas storage, foam-based soil remediation). As throughput is increased in such processes, there is a risk that viscous drag forces will break the train of bubbles apart. However it is also possible that the structure can stay together provided foam films between bubbles flatten out [1]. This project will explore the geometry of such flat film states.

GOALS

The goal is to develop models establishing limits on bubble sizes that can stack into a flat film state as a function of the number of bubbles within a train. This will in turn identify the domain of bubble sizes that admit rapid throughput within a channel or porous medium.

BENEFITS

You will be studying a system which admits a rich physical behaviour, but which simultaneously can be used in engineering practice. You will also be studying an unconventional class of models in which dynamics is largely replaced by geometry.

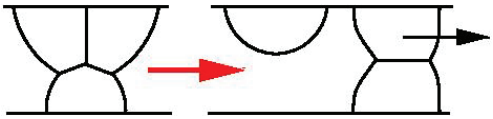


Figure 1: A bubble train that breaks up

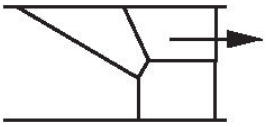


Figure 2. A flat film state that does not break

PROFILE

The project requires a student with an interest in foams and an understanding of and liking for geometry. Programming experience is also an advantage.

REFERENCES

[1] C. Torres-Ulloa and P. Grassia. Viscous froth model applied to the motion and topological transformations of two-dimensional bubbles in a channel: Three-bubble case. Proc. Roy. Soc. London Ser. A, 478:20210642, 2022 doi: 10.1098/rspa.2021.0642.

Supervisor	David Rieder
2nd supervisor	Revanth Sharma
Starting date	Asap
Exp./Num./Design	Numerical

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

High-fidelity upscaling of gas flow in porous media – Stepping from kinetic gas theory to Pore Network Models

David Rieder[+], Revant Sharma[*]
[+]d.r.rieder@tue.nl , [*]r.k.sharma@tue.nl,

INTRODUCTION

The performance of a variety of key technologies for the transition to a sustainable society is highly dependent on the flow in very narrow pore spaces, i.e. for carbon capture and storage, in electrodes of electrolyzers or application of supported catalyst. However, predicting gas flow in highly porous media is still riddled with uncertainties, besides decades of research [1].

Especially the influence of the contact of solid wall and gas molecules is considered to be the dominating effect in those small pores. Recently, highly performant state-of-the-art solvers allow for high-fidelity predictions of the gas flow under such regimes. This allows the study so called 'slip'-effects and their incorporation in application-scale pore network models.

A successful incorporation of those 'slip'-effects then allows rapid upscaling for predicting gas flows in real applications and lays the foundation for the modeling of complex multiphase flows.

GOALS

Study the gas flow in nano- and mesopores with state-of-the art kinetic gas solvers and employ pore network models to derive continuum scale properties.

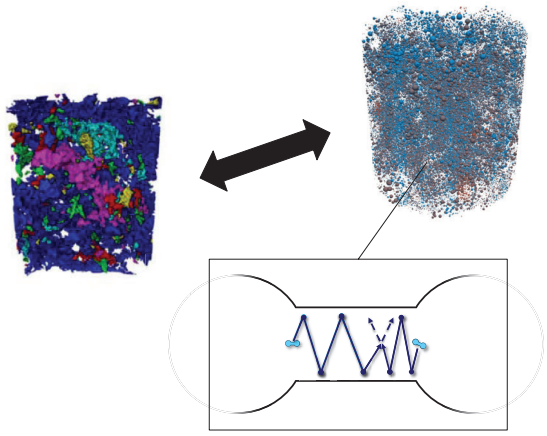


Figure 1 A porous material may be approximated by a network of pores and throats. Accurate predictions of flow in such porous media highly depends on the capturing the relevant transport phenomena, e.g. the wall contact.

BENEFITS

- You will be working with an international team of scientist on a highly challenging and relevant topic
- Gain insights into multiple models at different scales
- Contribute to the fundamental challenges of transitioning to a sustainable economy

PROFILE

We are looking for a highly motivated student who is not afraid to ask critical questions. Prior experience with modelling of porous media is a plus, but not a requirement. Do you feel up to such a challenge? Let's have a talk!

REFERENCES

[1] V. Pavan, L. Oxarango *A New Momentum Equation for Gas Flow in Porous Media: The Klinkenberg Effect Seen Through the Kinetic Theory* **2007** J. Stat. Phys. DOI:10.1007/s10955-006-9110-2

Supervisor	Dr. Azahara Luna-Triguero
2nd supervisor	Shima Rezaie
Mentor	N.A.
Company	Internal
Starting date	Any time
Exp./Num./Design	Numerical

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

ASSESSING METAL-EXCHANGED MATERIALS FOR HYDROGEN STORAGE

S. Rezaie, A. Luna-Triguero
E-mail: s.rezaie@tue.nl, a.luna.triguero@tue.nl

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].

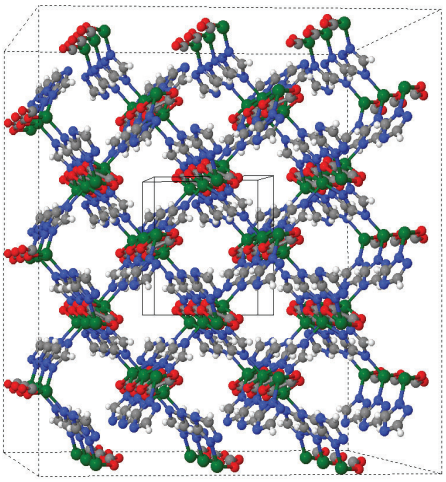
GOAL

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.



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.

Supervisor	Dr. Azahara Luna-Triguero
2nd supervisor	Dr. Monica E. A. Zakhari
Mentor	
Company	Internal
Starting date	Any time
Exp./Num./Design	Numerical

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

CHILLING WITH NANOFLUIDS: Atomistic Insights

A. Luna-Triguero, M. E. A. Zakhari
E-mail: a.luna.triguero@tue.nl, m.e.a.zakhari@tue.nl

INTRODUCTION

The pursuit of energy-efficient and environmentally friendly refrigeration and heat transfer technologies has become paramount due to the escalating demands for cooling in various industrial, residential, and commercial sectors. Conventional refrigerants, such as hydrofluorocarbons (HFCs) and hydrochlorofluorocarbons (HCFCs), have raised significant environmental concerns due to their high global warming potential (GWP) and ozone-depleting properties. As a result, there is an urgent need to explore alternative approaches that can enhance cooling and heat transfer performance and mitigate the environmental impact of refrigeration systems.

One promising alternative in the quest for innovative refrigeration and heat transfer solutions involves the use of nanofluids [1]. Nanofluids are engineered suspensions of nanoparticles in conventional heat transfer fluids, such as water or refrigerants. Incorporating nanoparticles, particularly Metal-Organic Frameworks (MOFs) and zeolites, into these fluids has garnered significant attention for their exceptional thermal properties and potential applications in advanced cooling systems. [2,3]

GOAL

Compute using molecular simulations and ML potentials relevant properties of nanofluids (Fig. 1) for cooling applications.

TASK

In this project, you are expected to:

- Review relevant literature on nanofluids MOFs@Rx pairs.
- Compute relevant properties of the species e.g. heat capacity and thermal conductivity.
- Assess the performance and efficiency of the systems.

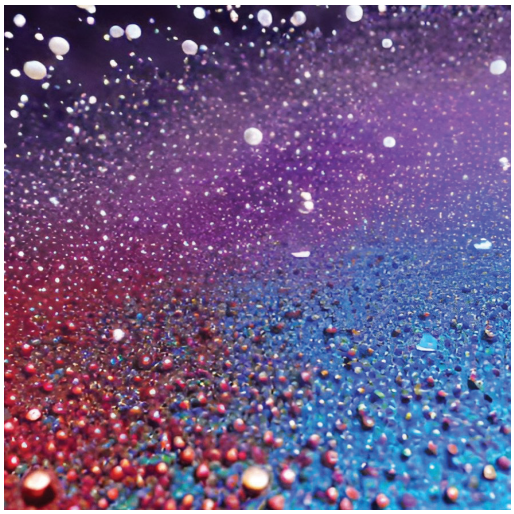


Fig. 1. Nanoparticle suspension in refrigerant. Schematic representation.

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] McGrail, B. P., Thallapally, P. K., Blanchard, J., Nune, S. K., Jenks, J. J., & Dang, L. X. (2013). Metal-organic heat carrier nanofluids. Nano Energy, 2(5), 845-855.
[2] Nandasiri, M. I., Liu, J., McGrail, B. P., Jenks, J., Schaef, H. T., Shutthanandan, V. (2016). Increased thermal conductivity in metal-organic heat carrier nanofluids. Scientific Reports, 6(1), 27805.
[3] Hu, J., Liu, C., Li, Q., & Shi, X. (2018). Molecular simulation of thermal energy storage of mixed CO2/IRMOF-1 nanoparticle nanofluid. International Journal of Heat and Mass Transfer, 125, 1345-1348.

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

Available for ME

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number: 2023 Q2-01

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

Clemens Verhoosel, 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 crash-test 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.

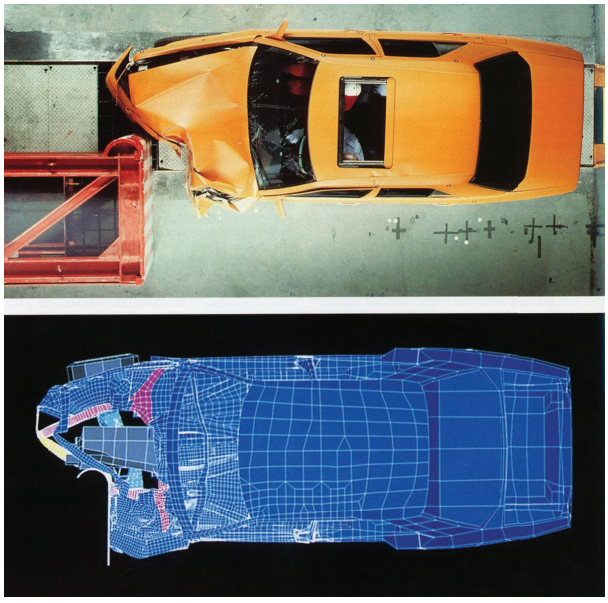


Fig 1: Crash-test simulation. Credit: Cray Research Inc.

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

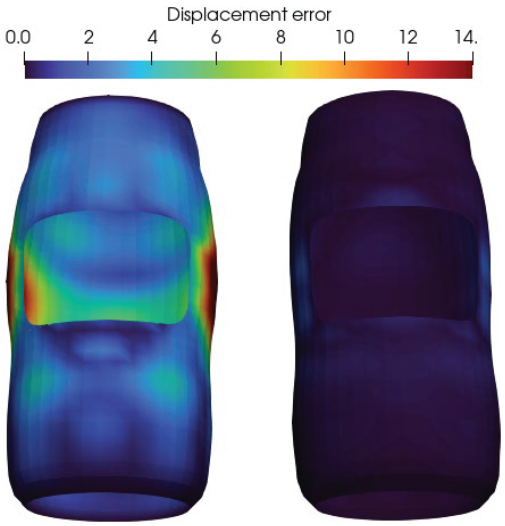


Fig 2: Error in the predicted displacement for the *linear* Kirchhoff-Love shell model, without and with the proposed solution method.

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

[1] 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 David Rieder**
2nd supervisor	**Dr Maja Rücker**
External Collaborator	**Dr Catherine Spurin (Stanford Univ.)**
Company	**Internal**
Starting date	**Any time**
Exp./Num./Design	**Analysis**

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Catching CO_2 entrapment and abrupt permeability changes in partially saturated porous rocks using CFD and 3D in-situ measurements from the Swiss Light Source

David Rieder*, Maja Rücker, Catherine Spurin

***d.r.rieder@tue.nl**

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.

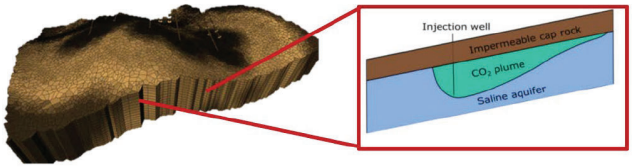


Figure 1: Subsurface CO_2 storage

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.

GOALS

Quantify the influence of the entrapments on the flow inside the rock by simulating the flow in OpenFOAM.

BENEFITS

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

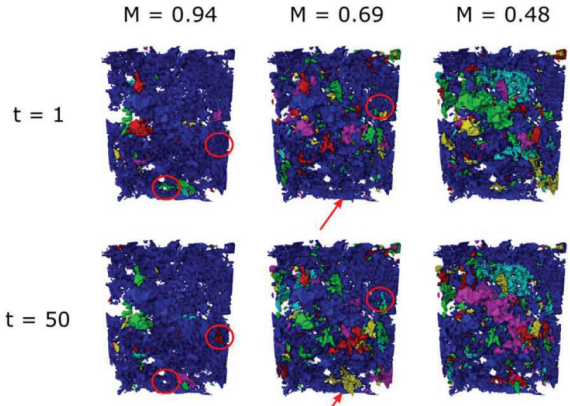


Figure 2: The distribution of the oil phase (rock and water transparent) for different viscosity ratios (M) at two different times t). Each connect region of oil has been assigned a different colour to show the connectivity.

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.

Supervisor	David Rieder
2nd supervisor	Maja Rücker
Daily supervisor	
Company	---
Starting date	asap
Exp./Num./Design	Numerical & Experimental

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Uncovering the perplexing effects of efflorescence on the drying processes of porous media

David Rieder, Maja Rücker
*Email: d.r.rieder@tue.nl

INTRODUCTION

Drying is a critical step in a variety of industrial processes, either due to its inherently high energy demand or its impact on the product quality. Especially during drying of porous objects with a non-volatile dissolved component, the dynamics of the deposition inside the pore space may be the performance limiting influence. As an example, the longevity of bricks strongly depends on the salt deposition during drying, the cost of supported catalysts is heavily influenced by the distribution of the catalytic component inside its pellet and pharmaceutical products may never reach application due to lacking control over the drying step.

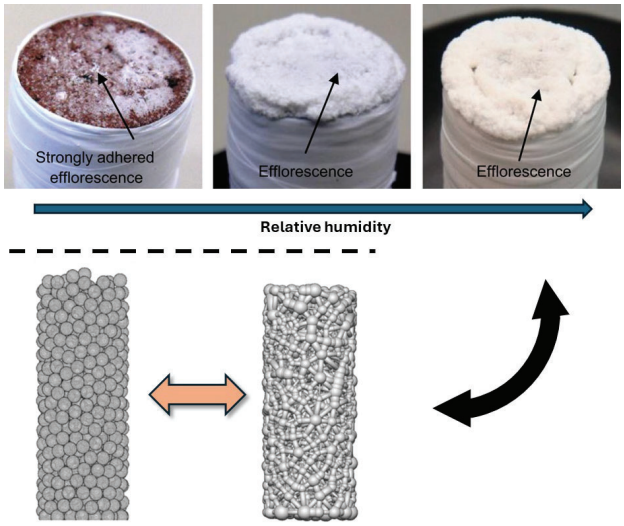
One of the still poorly understood aspects is the interplay between the change of the pore space and the progress of the drying, clearly visible in the form of efflorescence [1,2].

GOALS & TASKS

Your goal is to investigate the influence of mass-transport and precipitation during drying by use of a pore-network model. Further, you will evaluate your model by validation against complementary experimental data.

As part of this work you will:

- Develop a pore-network drying model
- Measure the change in pore space with state of the art 3D µCT machine



The quality of the salt deposition is heavily influenced by the drying condition. You will investigate this fascinating phenomena via pore network modeling and experimental tools. Images taken from [1] and [3]

STUDENT PROFILE

We are searching for a highly motivated student, who:

- wants to dive deeply into the challenging aspects of efflorescence
- is able to work independently
- has initial experience in formulating and solving transport models
- Has worked with Matlab, Python or C/C++ before

REFERENCES

[1] Gupta et al. *Paradoxical Drying of a fired-clay brick due to salt-crystallization* doi:10.1016/J.CES.2014.01.023

[2] Rieder et al. *Modeling the drying process of porous catalysts - impact of viscosity and surface tension* doi:10.1016/j.ces.2023.119261

[3] Eghbalmanesh et al. *CFD-validated pore network modeling of packed beds of non-spherical particle* doi:10.1016/j.ces.2023.119396

Supervisor	**Prof. David Smeulders**
2nd supervisor	**Dr. Bart Erich**
Daily supervisor	**Ruben D'Rose**
Starting date	**Asap**
Exp./Num./Design	**Numerical**

ETFD

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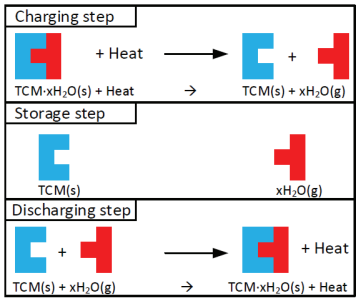
Optimization and validation of a TCM packed bed reactor

Ruben D'Rose*, Bart Erich, David Smeulders

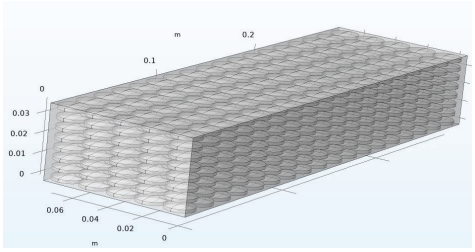
r.d.d.rose@tue.nl

INTRODUCTION

Long-term thermal energy storage is a key component in the framework of modern energy management. Thermo-chemical materials (TCMs) are a promising storage medium, since heat can be stored lossless and safely for prolonged periods. A common TCM reaction used in heat storage is the hydration of salt:



Usually, TCM powder is compacted into tablets of a certain shape and size and placed in the reactor in a more-or-less random packing. While an abundance of research has been carried out on the characterization of TCMs on the microscopic scale, studying TCM hydration on reactor level has not yet received as much attention. It has, for example, not been investigated whether complete hydration of the TCM mass in the reactor is efficient, or even possible, or if hydrating up to e.g. 70% is the better choice from an efficiency perspective. Other questions arise from the design (shape and size) of the used tablets and operating conditions of the system. For this matter, a 3D COMSOL model has been developed which includes the various transport mechanisms for water vapor and heat in both salt and air + the reaction kinetics of the TCM. This model will be used to study the effect of these parameters on the power output and storage capacity of the reactor.



TASKS

The task of this MSc project is to validate the existing model using experimental data AND standard numerical validation methods and to explore and optimize reactor performance by tuning the combinations of TCM tablet design, operating conditions and other parameters. An optional third task is to translate the COMSOL model to a continuous model using the Darcy equation, which will then be used to quickly iterate through numerous parametrized reactor designs.

GOALS

The main goals of this project are:

1. Validating the existing model and make improvements where necessary.
2. Use the validated model to explore and optimize the packed bed reactor.
3. (Optional) parametrize the tablet design and packing and translate the COMSOL model to a 3D continuous model using the Darcy equation.

STUDENT PROFILE

We are looking for a student who has affinity or is interested in developing affinity towards numerical methods. Having an interest in transport phenomena is a plus, as is experience with COMSOL and C++/Python.

REFERENCES

"Characterizing Changes in a Salt Hydrate Bed Using Micro X-Ray Computed Tomography", Arya et al.

"A thorough investigation of thermochemical heat storage system from particle to bed scale", Mahmoudi et al.

Supervisor	Dr. Maja Rucker
2nd supervisor	Dr. Azahara Luna-Triguero
Daily supervisor	Mohammad H. Khoeini, David Rieder
Company	Internal
Starting date	Anytime
Exp./Num./Design	Numerical & Experimental

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Machine Learning for high efficiency analysis of complex chromatographs

Mohammad Khoeini*, David Rieder, Azahara Luna-Triguero, Maja Rücker

*Email: m.h.khoeini@tue.nl

INTRODUCTION

Porous media are encountered almost everywhere to in science, industry and daily life, e.g. in batteries, chemical reactors, filters or concrete. Knowledge of their characteristic properties is crucial for a successful application design.

Gas chromatography allows the determination of a variety of the relevant properties [1]. However, classical evaluation of the chromatographs is often challenging, especially in the case of complex pore spaces with non-ideal surface properties. Either detailed modeling and subsequent fitting have to be conducted or empirical behavior determined from multiple chromatographs.

We are currently developing methods for expanding the standard evaluation routines and intend to utilize machine learning to maximize the knowledge gain per experiment and increase the fidelity of the derived parameters.

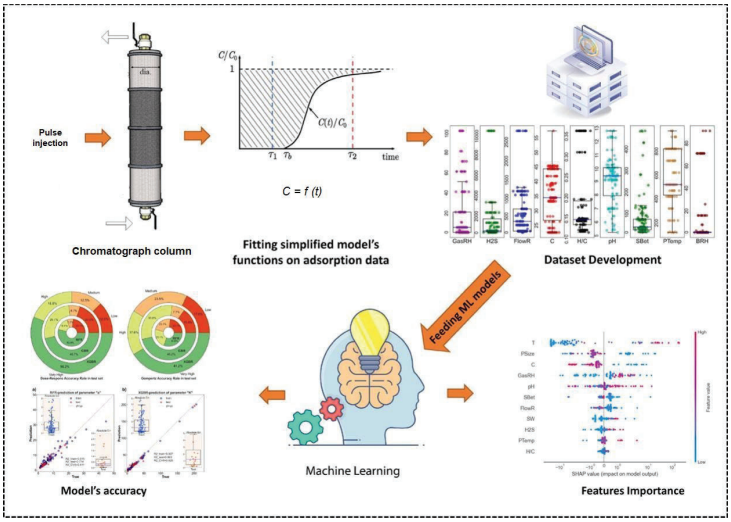


Fig. 1. Schematic representation of using ML approaches in gas chromatography column (adapted from [2])

TASKS

As part of this work you will:

- Train a neural network on an existing data-base of chromatographs
- Build a computational model to compute ideal chromatographs
- Conduct a sensitivity analysis on the machine learning model

GOALS

Develop a machine learning model, which is able to analyze a chromatograph and process parameters and determine otherwise difficult to estimate properties, i.e.

- Isotherms
- Tortuosity
- Surface energy distribution

STUDENT PROFILE

We are searching for a highly motivated student, who has:

- interest in possibilities of machine learning
- a hands-on mentality towards unexpected challenges
- Initial experience in formulating and solving transport models
- Experience with Matlab/Python is of advantage but not strictly necessary
- Analytical skills

REFERENCES

[1] H. Balard, Estimation of the Surface Energetic Heterogeneity of a Solid by Inverse Gas Chromatography, Langmuir 1997 13 (5), 1260-1269.

[2] F.Qaderi, et. Al , A novel machine learning framework for predicting biogas desulfurization breakthrough curves in a fixed bed adsorption column, Bioresource Technology Reports, 2024, 25, 101702.

Supervisors	**Max Beving, Arjan Frijns**
Company	**Cellcius**
Starting date	**asap**
Exp./Num./Design	**Exp/Num**

[cellcius]

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Materials for thermochemical heat storage

Max Beving, Arjan Frijns, Pim Donkers (Cellcius)
Contact emails: m.a.j.m.beving@tue.nl, a.j.h.Frijns@tue.nl

INTRODUCTION

A heat battery is developed within Cellcius (www.Cellcius.com). The core of the battery is a thermochemical material (TCM). This TCM can be charged and discharged using water. Such a battery can be used for space heating and to supply hot tap water in houses.

One of the main challenges is selecting the right material based on properties like: power output, working temperatures, cost and environmental impact.

TASKS

The student will mostly perform experimental work to characterize the TCM, which is selected by the student itself in collaboration with Cellcius.

Experimental: Material characterization will be performed on different levels:

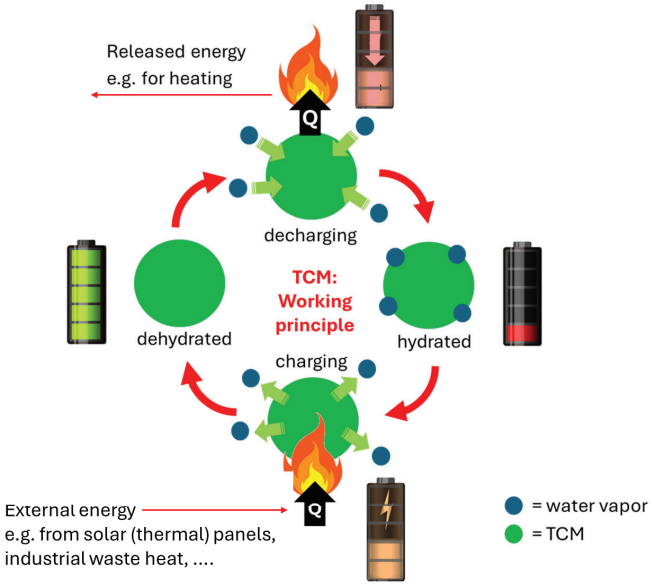
- TCM particles level: Using a TGA/DSC setup to measure capacity, charge-discharge times and power output of TCM particles.
- Particle-bed level: Self-made equipment at Cellcius to investigate system performance (temperature, power output, capacity charge & discharge times.

Modeling: Additionally, a 1D model will be developed to show the impact of the measured characteristics of the TCM.

GOALS

The ultimate goal is to find a material which can replace the material which is currently present in the Cellcius system.

To reach that, the first step is to select a TCM which will fit in a heating configuration whereby the TCM can be charged using a heat pump, commonly available in newly-built houses.



STUDENT PROFILE

- Interest in the energy transition.
- Familiar with concepts like a heat pump.
- Likes to work in the lab.
- Some basic programming skills in Matlab or Python.
- Drive to contribute to solving a present-day scientific challenge: the development of a household heat battery.

Supervisor	Michael Abdelmalik
2nd supervisor	Victorita Dolean (M&CS)
Company	N/A
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Neural Operators for Preconditioning Iterative Solvers

Michael Abdelmalik*, Victorita Dolean

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

Keywords: *Machine Learning, Neural Networks, Partial Differential Equations, Preconditioners*

INTRODUCTION

While partial differential equations (PDEs) play a fundamental role in the way we mathematically describe physical phenomena, the resolution of such equations is restricted by our capability of computing discrete solutions to the linearized system of equations. When the number of such equations becomes large, direct matrix inversion methods become prohibitively expensive, and the use of iterative methods becomes necessary. A key factor for effective use of iterative solvers is the availability of a *precondtioner* which approximates the action of the inverse.

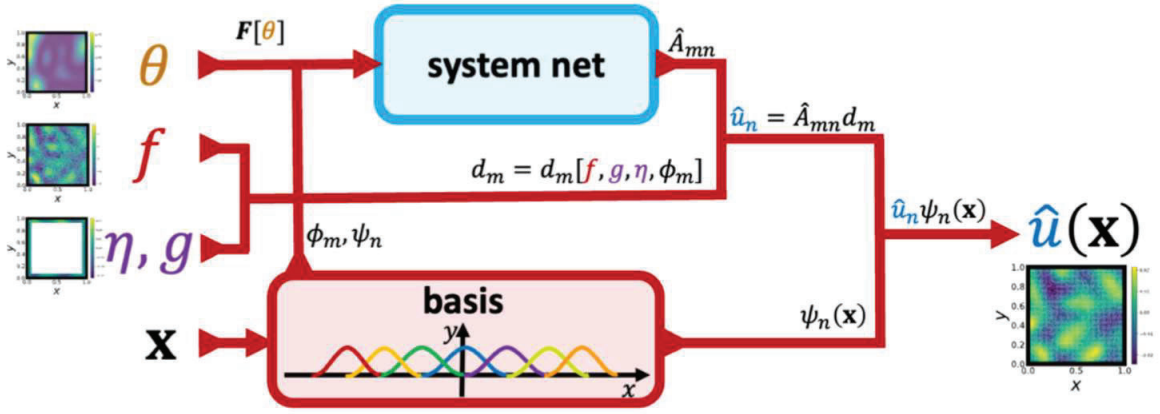
TASKS

- Formulate suitable objective/loss function(s)
- Generate training and validation datasets,
- Construct tailored Neural Operator architectures,
- Train and validate network
- Use neural operator to accelerate iterative solvers

STUDENT PROFILE

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

- machine learning and neural networks,
- mathematical modelling of physical phenomena,
- practical algorithms for mathematical models,
- programming (e.g., Python) and improving coding skills.



Neural Operator for Parametric PDEs

OBJECTIVE

The aim of this MSc project is to explore architectures for neural operators that can approximate the solution operator to a PDE. Moreover, we aim to use such an (approximate) solution operator to i) construct a reduced-order/surrogate model which can provide generalized, accurate and fast solutions; ii) to construct precondtioners to accelerate iterative solvers.

REFERENCES

[1] Neural Green's Operators for Parametric Partial Differential Equations (2024) . arXiv preprint arXiv:2406.01857.

[2] Variationally mimetic operator networks (2024). Computer Methods in Applied Mechanics and Engineering.