Master Thesis Project Proposals
Q3 2023-2024

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 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	**Prof. David Smeulders**
2nd supervisor	**Yukai Liu**
Daily supervisor	**Yukai Liu**
Company	**N.A**
Starting date	**Any time**
Exp./Num./Design	**Primarily experimental**

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Experimental study of low frequency acoustic transducers

David Smeulders and Yukai Liu
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INTRODUCTION

The subsurface of the Earth can be used for hydrogen and CO2 storage, but also to extract geothermal energy (hot water). To accurately predict the potential of the subsurface for such applications, permeability assessment of the formation is essential. Borehole acoustic waves can be used to obtain this information. To perform laboratory measurements on borehole waves, acoustic transducers need be designed and constructed. The project is aimed to design, manufacture and test a low-frequency transducer from combined piezoelectric ceramic plate layers.

Fig. 1. Geothermal energy production in Iceland

TASKS

Task1: Build piezoelectric transducer from available ceramic plates.
Task2: Use existing software to predict transducer properties and resonant frequencies
Task3: Perform borehole wave measurements using the new and existing transducers.

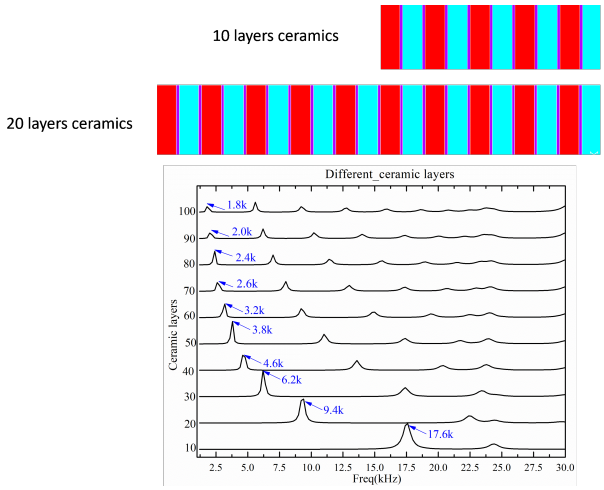

Fig. 2. Schematic of piezoelectric ceramics with 10 and 20 layers and modelling results.

RESEARCH GOALS

1. Determine how the number of piezoelectric ceramic layers affects the resonance frequency.
2. Compare experiment and theory .
3. Measure the waves of the newly constructed transducers in an existing borehole sample.

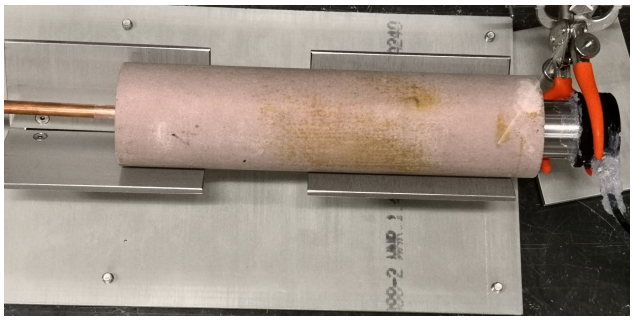

Fig. 3. Photo of borehole wave measurement setup

STUDENT PROFILE

- Interested in experimental studies, especially acoustic or electromagnetic experiments.
- Pro-active attitude.

Supervisor	**Dr. Azahara Luna-Triguero**
2nd supervisor	**Dr. Maja Rucker**
Daily supervisor	**Mohammad Hossein Khoeini**
Company	**Internal**
Starting date	**Anytime**
Exp./Num./Design	**Numerical and experimental**

ETFD

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Advancing analytics for subsurface hydrogen storage: 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

Hydrogen is taking increasingly important role in the energy transition as it has the potential to replace fossil fuels. Hydrogen has higher energy per mass but lower energy per volume than natural gas. Therefore, to meet the energy demand of the industry and society, bulk energy storage systems are required to store produced hydrogen from renewable sources. In this context, underground geological structures, e.g. depleted gas fields, are being considered as a potential option due to their natural large capacity and lower costs. However, underground hydrogen storage (UHS) is still at low level of technological maturity, and there are still several key components of hydrogen storage processes that needs to be fully understood.

One of these poorly understood processes is that during the injection and retraction of hydrogen in the subsurface porous media, hydrogen displaces the existing fluid, e.g., brine, which leads to the complex multiphase fluid flow (figure 1). Two main parameters governing the multiphase flow are surface area and surface energy of the porous rock. These two inherent physiochemical properties determine the extend and strength of the fluids' interactions with porous media and are key to computational models aiming to predict the behaviour of hydrogen in the porous reservoir. In this project, you will advance numerical and experimental methodologies based on iGC to obtain the relevant information needed for future models determining the safety and optimal performance of underground hydrogen reservoirs.

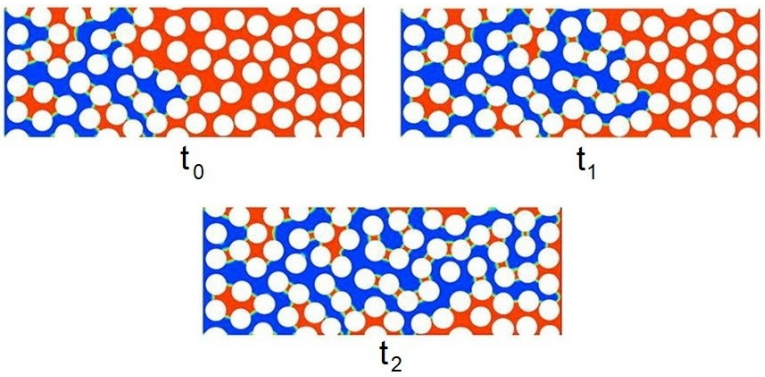

Fig. 1. Schematic representation of existing fluid displacement with hydrogen in porous media (adapted from [2])

Problem statement & Goal

From the theoretical perspective, the surface of a solid is often not composed of interacting sites with a unique energy, but of sites with a range of energy of interaction (figure 2) [2]. In rocks, this is for example due to varying mineral compositions. On the contrary, the surface energy we infer from iGC reflects only the average energy of all interacting sites.

In this study, you will develop an inverse method to obtain the distribution of interacting sites from the average surface energy measured by IGC. Aligned with other projects in our group your work will support steering future decisions on research and implemetation of UHS in NL.

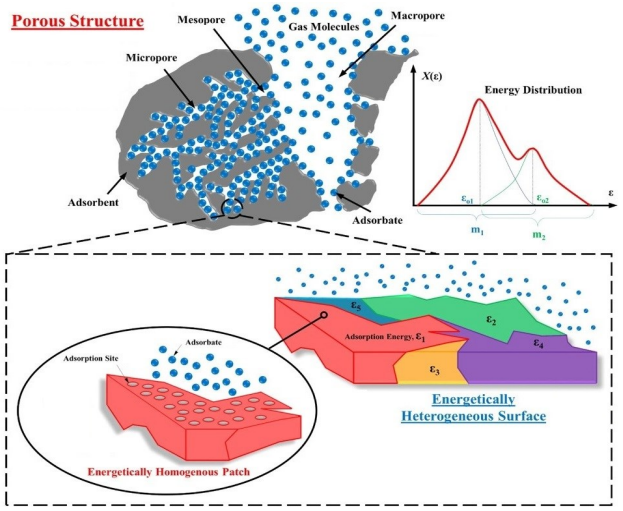

Fig. 2. Adsorption on a surface with different energy sites [3].

TASKS & STUDENT PROFILE

We are looking for the high-motivation student who has creative, solution-oriented, and interest in performing experiments and/or 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 numerical method and/or model the method in MATLAB
- Assessing the validity of the developed inverse method by comparing with measured experimental data.

REFERENCES

[1] Aniket S. A., et al. 'Pore-resolved two-phase flow in a pseudo-3D porous medium: Measurements and volume-of-fluid simulations', Chemical Engineering Science, 2021, 230, 116128.

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

[3] 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).

Supervisor	**Prof. Harald van Brummelen**
2nd supervisor	**Dr. Stein Stoter**
Mentor	**Tom van Sluijs**
Company	**N.A.**
Internal / External	**Internal**
Starting date	**Anytime**
Exp./Num./Design	**Experimental and numerical**

Available for ME

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Project number:

Theoretical and numerical investigation of outflow conditions in a multiphase model

Tom van Sluijs*, Stein Stoter, Harald van Brummelen

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INTRODUCTION

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 multiphase problems. See the figure down below or this video for a typical result.

The outflow conditions for pure species are well understood. However, outflow of the mixed phase that contains a phase transition region is more complex. Advanced outflow conditions need to be developed to model the mixed phase outflow and prevented the unphysical phenomena that occur using the general outflow conditions, see Figure 1.

This goal of this project is to develop and implement the mathematical description of appropriate boundary conditions for an outflowing mixed species.

TASKS

In this project, you are expected to do:

- Literature review, focused on multiphase flow, capillarity, the NSCH model and outflow boundaries
- Program a numerical implementation in our existing framework
- Qualitative and quantitative assessment of the numerical results
- Conclusion and advise on both modelling and the numerical implementation

STUDENT PROFILE

We are looking for a motivated MSc student who:

- is curious about the mathematical modeling of fluid dynamics, in particular multiphase flow, interface phenomena and boundary conditions.
- is interested in theoretical modelling, numerical methods, and programming.
- is looking to develop his/her personal skillset: physical modelling, numerical methods, literature study, programming, and data analysis.

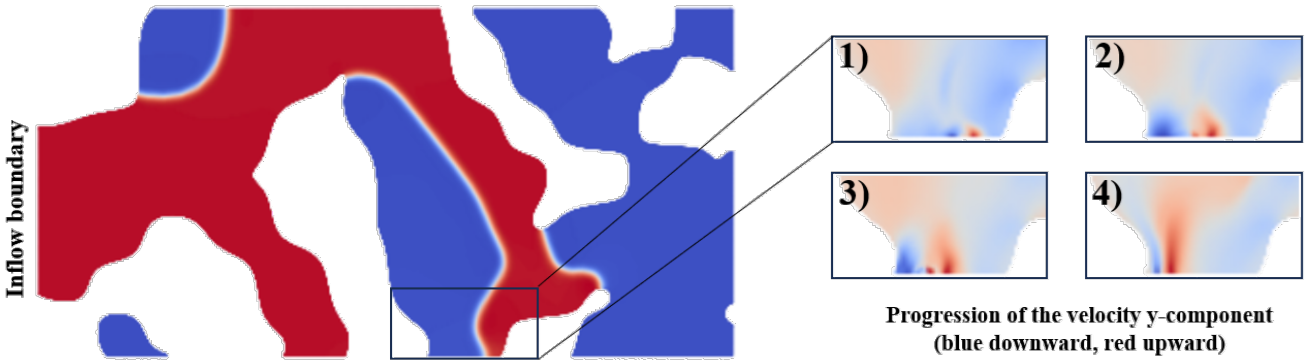

Fig 1.: Multi-phase flow through porous medium. Left: phasefield of two constituents at the time that an outflow boundary is reached. Right: evolution of the velocity field at what should be the outflow boundary. Showing erroneous and unstable velocity inflow (backflow) spikes.

REFERENCES

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

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

Keywords: Physical modelling, *Numerical methods, Finite Elements, Navier-Stokes, Cahn-Hilliard*

Stein K.F. Stoter, Tom B. van Sluijs, Tristan H.B. Demont, E. Harald van Brummelen, Clemens V. Verhoosel (2023) Stabilized immersed isogeometric analysis for the Navier–Stokes–Cahn–Hilliard equations, with applications to binary-fluid flow through porous media, Computer Methods in Applied Mechanics and Engineering, 2023, 116483, ISSN 0045-7825, https://doi.org/10.1016/j.cma.2023.116483.

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

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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.

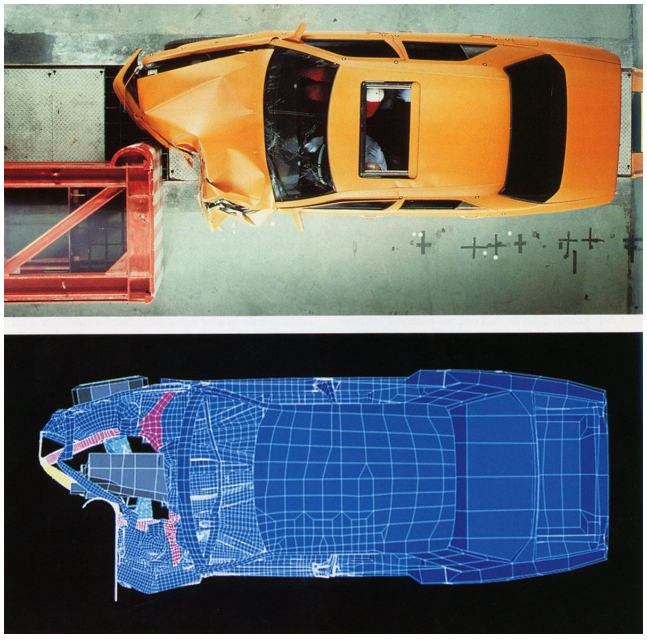

Fig 1: Crash-test simulation. Credit: Cray Research Inc.

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

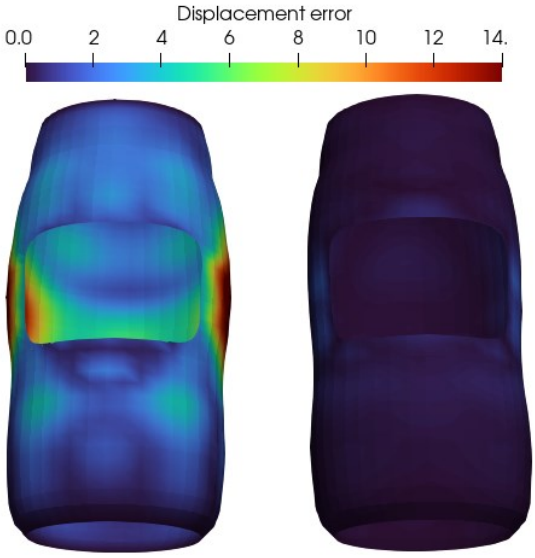

Fig 2: Error in the predicted displacement for the *linear* Kirchhoff-Love shell model, without and with the proposed solution method.

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

ETFD

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ASSESSING METAL-EXCHANGED MATERIALS FOR HYDROGEN STORAGE

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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].

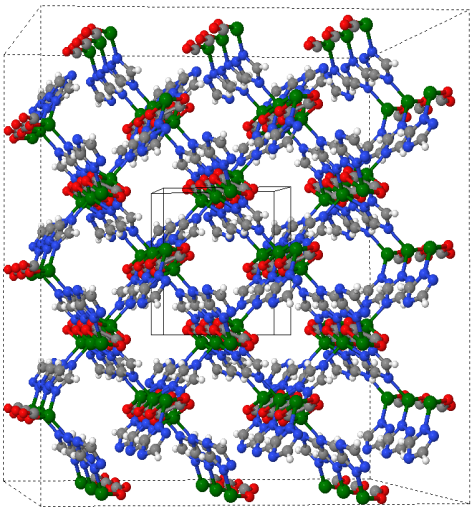
GOAL

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.



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

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CHILLING WITH NANOFLUIDS: Atomistic Insights

A. Luna-Triguero, M. E. A. Zakhari
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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	**Henk Ouwerkerk**
2nd supervisor	**Rick de Lange**
Daily supervisor	**NA**
Company	**TU/e & Heat Power**
Starting date	**TBD**
Exp./Num./Design	**Experimental**

ETFD

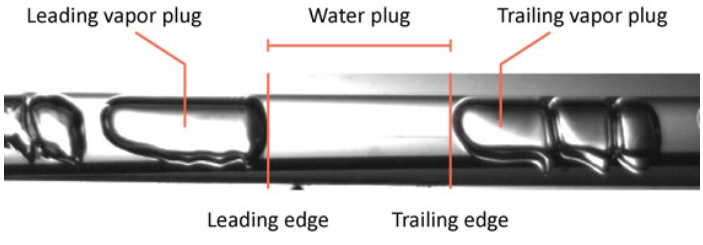
TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Study of steam generation phenomena in the once through boiling visualization set-up

Henk Ouwerkerk & Rick de Lange
H.Ouwerkerk@tue.nl & H.C.d.Lange@tue.nl

INTRODUCTION

Heat Power and TU/e together developed the sub critical once through boiler: a fast responding steam generator that can start from cold within minutes. Also, the once through boiler is of modular design and can be easily adapted for different applications. Heat Power has already successfully realized several real-size once through steam boilers (OTB's) in the range 80-2000kW thermal power. The principleworks, however the boiling process can still be unstable. To study and visualize the once through boiling process, an experimental set-up with a quartz boiler tube and high speed cameras was realized, see pictures below.



TASKS & GOALS

- Perform experiments with the setup with- and without the boiling nucleation system (a bubble generator)
- Study the occurring boiling nucleation phenomena and find the reproducibility.
- Study literature for similar experiments or simulations and check both similarities and novelties that might be eligible for publication in a journal

STUDENT PROFILE

- Hands on mentality
- Eager to gain experimental experience
- General Matlab skills
- General scientific writing skills

REFERENCES

Contact
Henk Ouwerkerk: H.Ouwerkerk@tue.nl
and
Rick de Lange: H.C.d.Lange@tue.nl

Supervisor	**Henk Ouwerkerk**
2nd supervisor	**Rick de Lange**
Daily supervisor	**NA**
Company	**TU/e & Heat Power**
Starting date	**TBD**
Exp./Num./Design	**Experimental**

ETFD

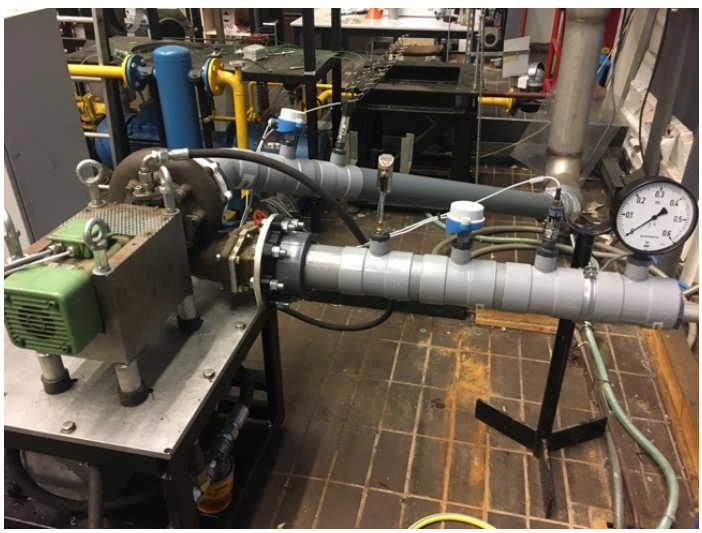
TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

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

Henk Ouwerkerk & Rick de Lange
H.Ouwerkerk@tue.nl & H.C.d.Lange@tue.nl

INTRODUCTION

Heat Power & TU/e developed a compact, fast responding and Steam and gas turbine: the Rankine Compression gas turbine (RCG). 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.



TASKS & 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.
- 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.

STUDENT PROFILE

- Hands on mentality
- Eager to gain experimental experience

REFERENCES

Henk Ouwerkerk: H.Ouwerkerk@tue.nl
and
Rick de Lange: H.C.d.Lange@tue.nl

Supervisor	Dr. Yousef Damianidis Al Chasanti
2nd supervisor	Dr. Camilo Rindt
Mentor	
Company	
Starting date	January 2024
Exp./Num./Design	Num

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Hydraulic and Thermal Analysis of District Heating Networks

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Yousef Damianidis Al Chasanti
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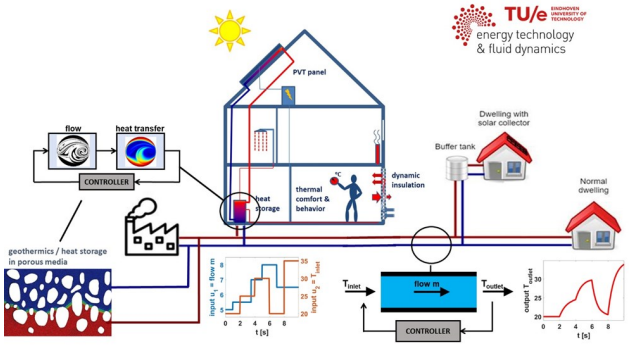
INTRODUCTION

Due to the serious effects of climate change and increasing global temperatures, many countries are actively working to decarbonize their economies. Heating and cooling activities in modern economies account for 50% of global energy consumption and 45% of carbon emissions [1]. District heating networks transport hot fluids, usually water, from the energy source to individual buildings. The centralized heat production in district heating networks is more energy-efficient than individual building heat generation. Our group has developed a numerical model tailored for district heating networks, predicting heat loss and temperature distribution. This model :t.



TASKS

- Develop mathematical formulations that govern the flow in hydraulic piping networks for district heating. These equations will encompass the flow rates for each node and the head losses in each segment of the network. The mathematical formulations must be flexible enough to accommodate any arbitrary number of sources and demand nodes.
- Write a computer code to solve the piping network equations using the Hardy Cross iterative method [2].
- Combine the hydraulic pipe network model with the existing unsteady-state thermal model that calculates the temperature distribution along the pipe segment [3].
- Conduct an analysis using the combined thermo-hydraulic model and test it in real-world scenarios related to district heating networks.

GOALS

- Assess the feasibility of using pipe network analysis for modelling district heating networks.
- Examine how the configuration of the piping network impacts the performance of district heating networks.
- Estimate the head loss and compare it to the thermal losses.

STUDENT PROFILE

- Experience in thermo-fluid engineering with a passion for sustainable energy projects.
- Knowledge of basic programming principles.
- Experience in numerical analysis methods, including finite difference and iterative solvers.
- Experience in pipe flow analysis is preferred but not required.

REFERENCES

1. Mckinsey &Company (2021). Net-zero heat long-duration energy storage to accelerate energy system decarbonization, Technical Report
2. Bhave, P. R. (1991). Analysis of flow in water distribution networks. Technomic Publishing Co., Inc., Lancaster, PA., Book
3. Jiang, M., Speetjens, M. F. M., Rindt, C. C. M., & Smeulders, D. M. J. (2023). A data-based reduced-order model for dynamic simulation and control of district-heating networks. Applied Energy, 340, Article

Supervisor	**Camilo Rindt**
Company supervisor	**Ruben van Gaalen**
Mentor	
Company	**Philips**
Starting date	**Any**
Exp./Num./Design	**Numerical**

ETFD

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Optimal cooling topology for MRI gradient coils

Camilo Rindt, Ruben van Gaalen
c.c.m.rindt@tue.nl, ruben.van.gaalen@philips.com

INTRODUCTION

MRI scanners are a crucial tool for diagnosing a wide range of afflictions, most prominently cancer. By magnetizing hydrogen atoms in a body, it becomes possible to visualize the different kinds of tissues that are present.

One important type of electromagnet in a MRI system is the so-called gradient coil. These coils supply a linearly sloped, time varying magnetic field in the three Cartesian degrees of freedom (i.e. x, y, z) by means of a carefully designed electric current pattern. By inducing these gradients on the magnetic field, it becomes possible to distinguish scanned regions from each other.

At Philips, several methods are employed for optimization of the electromagnetic design of gradient coils [1]. However, the resulting conductor patterns also require cooling by means of water flowing through tubes. For the positioning of these tubes, there is still demand for a more rigorous optimization method than those currently in use.

TASKS

Create an axisymmetric thermal model of a gradient coil. By keeping this model as simple as possible it can be used to perform fast optimizations for the positioning of cooling tubes.

Figure 1: Gradient coil

GOALS

- Create an axisymmetric thermal finite element model.
- Use linear/quadratic programming optimization techniques to find optimal positions of cooling tubes.
- Possibly, extend the model with nonlinearities that can be optimized with iterative methods.

STUDENT PROFILE

- Proficiency with MATLAB or similar scripting languages (e.g. Python).
- Knowledge about heat transport and the underlying equations.
- Knowledge about linear algebra.
- Proficiency with numerical methods.
- Knowledge about electromagnetics and/or fluid dynamics is a plus.

REFERENCES

[1] Peeren, G.N. (2003) Stream Function Approach for Determining Optimal Surface Currents. PhD thesis. Eindhoven University of Technology.

Supervisor	**Dr. Michael Abdelmalik**
2nd supervisor	**Dr. Michel Speetjens**
Mentors	**Joost Prins and Hugo Melchers**
Company	**N.A.**
Internal / External	**Internal**
Starting date	**Any time**
Exp./Num./Design	**Num./Exp.**

ETFD

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

NEURAL OPERATORS FOR OPTIMAL CONTROL OF HEAT TRANSFER

Michael Abdelmalik*, Michel Speetjens, Joost Prins and Hugo Melchers

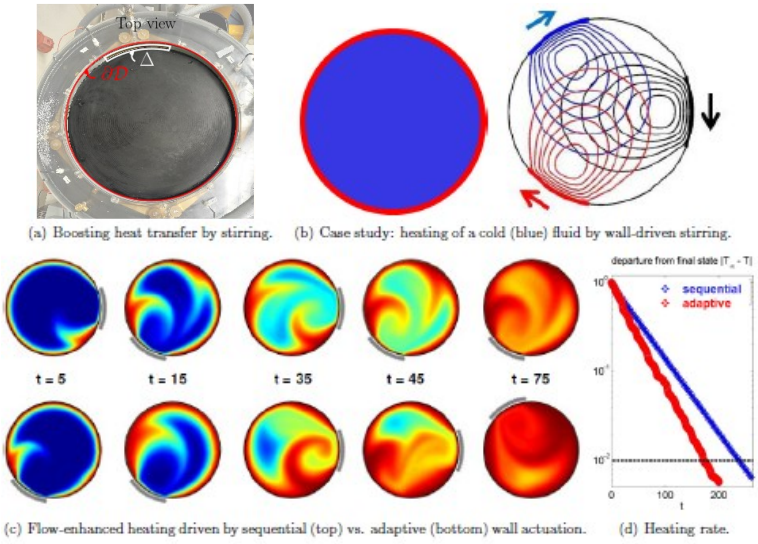
***E-mail: m.abdel.malik@tue.nl**

INTRODUCTION

Simulation of complex physical phenomena has been the primary focus of computational sciences, where methods are developed to solve PDEs. However, conflicting constraints of accuracy and tractability have hindered the application of many of such methods, and their reduced order counterparts, to control problems. In this project we are concerned with controlling the transfer of heat during stirring.

ROTATING ARC MIXER

We consider the heat transfer within a fluid in an industrial Rotating Arc Mixer (Fig 1a) [1]. While fluid is initially at room temperature, it is heated via the mixer walls (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). We ask the question**: what is the optimal stirring sequence for distributing the heat within the fluid?**



(a) Boosting heat transfer by stirring. (b) Case study: heating of a cold (blue) fluid by wall-driven stirring.

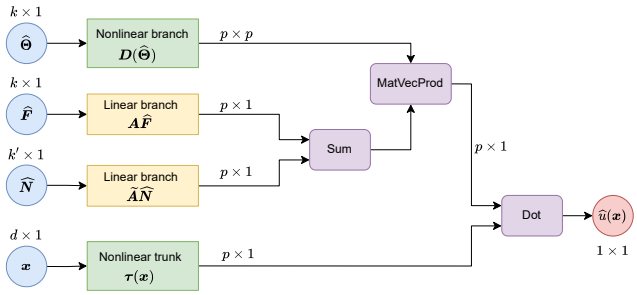
(c) Flow-enhanced heating driven by sequential (top) vs. adaptive (bottom) wall actuation. (d) Heating rate.

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

While counterintuitive, sequential actuation of the sliding walls is suboptimal (Fig. 1c) for distributing heat within the fluid [1]. To develop an optimal/adaptive stirring strategy we would like to design a controller that optimizes the actuation of the sliding walls for optimal heat distribution (eg Fig. 1c, bottom) [1].

NEURAL OPERATORS FOR HEAT TRANSFER

A physics-based heat transfer model predicts the effects of the possible actions of the controller, and the controller bases its decision on these predictions. Although a heat transfer model based on partial differential equations is at our disposal, solving these equations takes too long to be effective when used in hybrid with a controller in an experimental setting. In this project, we want to explore the potential of fast and variationally-based surrogate neural operators, e.g. as shown in Fig. 2 [2], when used in hybrid with a controller.



RESEARCH TOPICS

- The design and training of a neural surrogate [2] for heat transfer testing it in hybrid with a controller in numerical (and possibly laboratory) experiments.
- Refinement of the control strategy in [1] for achieving maximum heat transfer.
- Validation of the heat transfer controller against experiments.

REFERENCES

[1] R. Lensvelt, M.F.M. Speetjens, H.Nijmeijer, Fast fluid heating by adaptive flow reorientation, Int. J. Therm. Sci. **180**, 107720 (2022).

[2] Patel, D., Ray, D., Abdelmalik, M. R., Hughes, T. J., & Oberai, A. A. (2022). Variationally mimetic operator networks. *arXiv preprint arXiv:2209.12871*.

Supervisor	Ir. Ronald Lamers
2nd supervisor	Dr. Michel Speetjens
Mentor	
Company	Thermo Fisher Scientific
Internal / External	External
Starting date	Any time
Exp./Num./Design	Num./Exp.

Available for ME-SET

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number:

MODEL-BASED THERMAL DRIFT COMPENSATION FOR ELECTRON MICROSCOPES

ThermoFisher SCIENTIFIC
The world leader in serving science

Ronald Lamers, Michel Speetjens*
***E-mail: m.f.m.speetjens@tue.nl**

INTRODUCTION

Thermo Fisher Scientific develops electron microscopes capable of visualizing individual atoms. A common problem for these devices is so-called “thermal drift”, i.e. positioning inaccuracies of O(nm/min) due to thermal expansion, which can already be caused by heat loads of O(mW). Thermal drift can often be mitigated by a microscope design that is less sensitive to thermal deformation and/or by reducing the drift (heat) sources. However, if insufficient, then a further option is active adjustment of the position of the stage holding the sample to counteract the thermal drift. Essential for such methods for “thermal drift compensation” is to understand the thermo-mechanics behind the drift and translate this in predictive models for practical use.

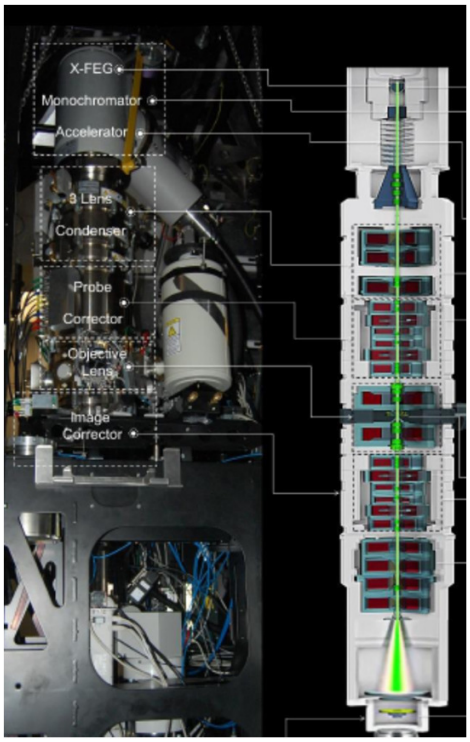


Fig. 1. Typical electron-microscope system.

MODELLING ISSUES

Modelling techniques for predicting thermal drift exist yet their application to realistic systems has proven challenging in previous studies done at Thermo Fisher Scientific. This stems primarily from fundamental assumptions in the early modelling stages. However, the impact of such assumptions on the prediction accuracy and how to improve current models while maintaining practical usability remains an open question.

PROJECT

The main project goal is the ***development of new models for thermal drift compensation*** in electron microscopes. This will be done via a modular test set-up at Thermo Fisher based on an actual microscope and involves the following steps and subgoals:

- Literature study on the impact of thermo-mechanical effects on positioning accuracies in complex industrial precision systems and ways to model and tackle this.
- Identify assumptions and factors causing mismatches between current models and test set-up such as e.g. convective/radiative boundary conditions, simplified geometries, contact resistances, uncertain material properties, impact of vacuum, measurement errors.
- Use insights from the above literature study and analysis of the test set-up versus current models to develop new models for thermal drift compensation.
- Develop an experimental strategy that enables systematic validation and testing of the new models using the test set-up and its instrumentation.
- Further develop and fine-tune the new models using insights gained from the experimental study.

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.

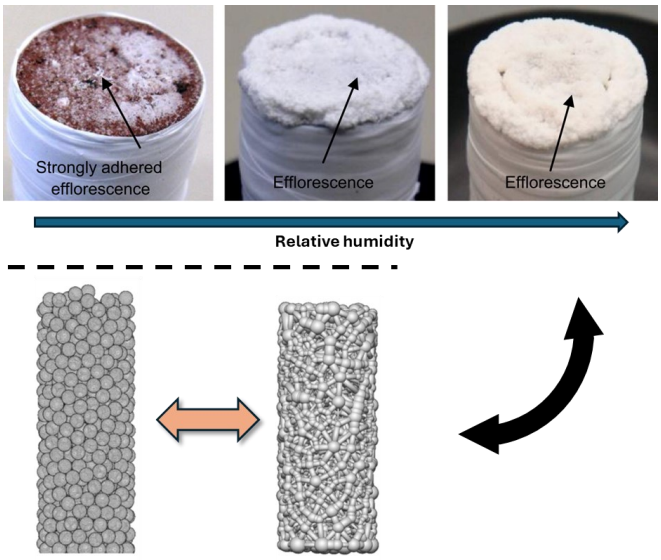
One of the still poorly understood aspects is the interplay between the change of the pore space and the progress of the drying, clearly visible in the form of efflorescence [1,2].

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

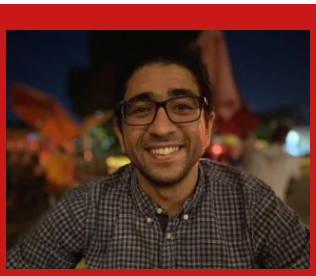
[3] Eghbalmanesh et al. *CFD-validated pore network modeling of packed beds of non-spherical particle* doi:10.1016/j.ces.2023.119396

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

Available for ME

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number: 2022 Q4-01



Rarefied Heat Transfer for Space Exploration

Michael Abdelmalik*, Timo van Opstal

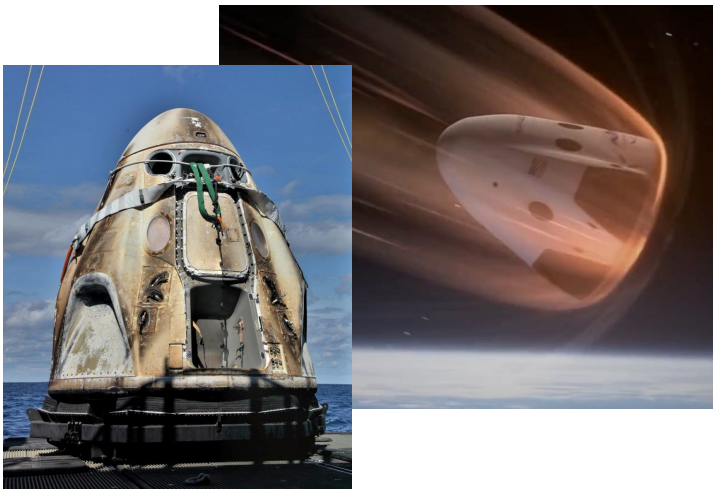
***E-mail:m.abdel.malik@tue.nl**

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

INTRODUCTION

Heat transfer in rarefied gases is a critical aspect in different applications. For instance, the design of reusable spacecraft such as the SpaceX Dragon, see figures below, relies on accurate simulations in the design of heat shields since experiments are very costly.

Continuum/equilibrium models, such as Navier-Stokes, fail to govern gas flow in such applications 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.



Scorched heat shields after successful reentry of the SpaceX Dragon (left) and artist's impression of reentry flight (right)

Stochastic methods, such as Direct Simulation Monte Carlo (DSMC) are the mainstay method for BE in the rarefied regime. However, the stochastic nature of DSMC precludes resolution of the continuum-to-rarefied transition regime.

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

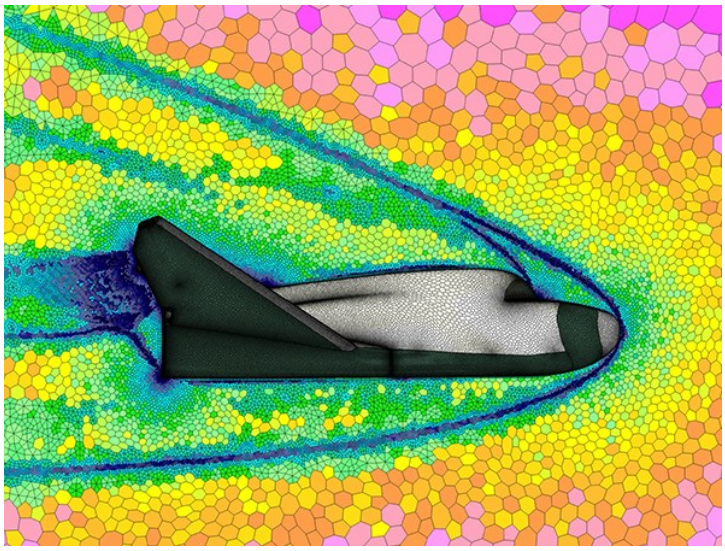
TASKS

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

STUDENT PROFILE

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

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



Supersonic re-entry simulation using continuum models

REFERENCES

[1] Levermore, "Moment closure hierarchies for kinetic theories." *Journal of statistical Physics* 83.5 (1996): 1021-1065.

[2] Abdelmalik, et.al.. "Moment Closure Approximations of the Boltzmann Equation Based on ϕ-Divergences." *Journal of Statistical Physics*164.1 (2016): 77-104.

Supervisor	**Dr 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.

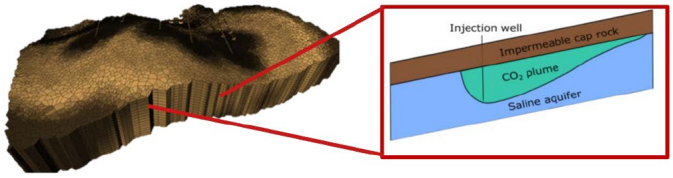


Figure 1: Subsurface CO_2 storage

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

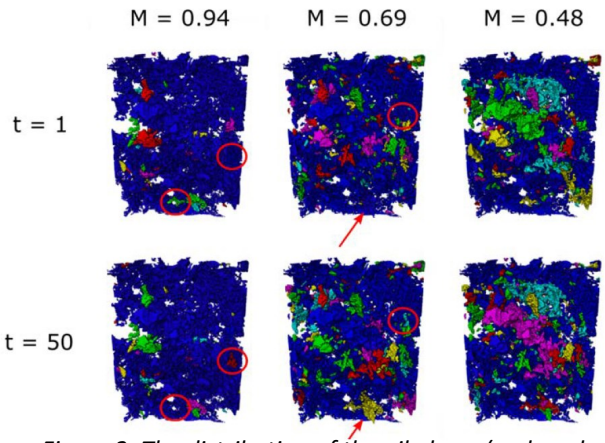


Figure 2: The distribution of the oil phase (rock and water transparent) for different viscosity ratios (M) at two different times t). Each connect region of oil has been assigned a different colour to show the connectivity.

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	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.

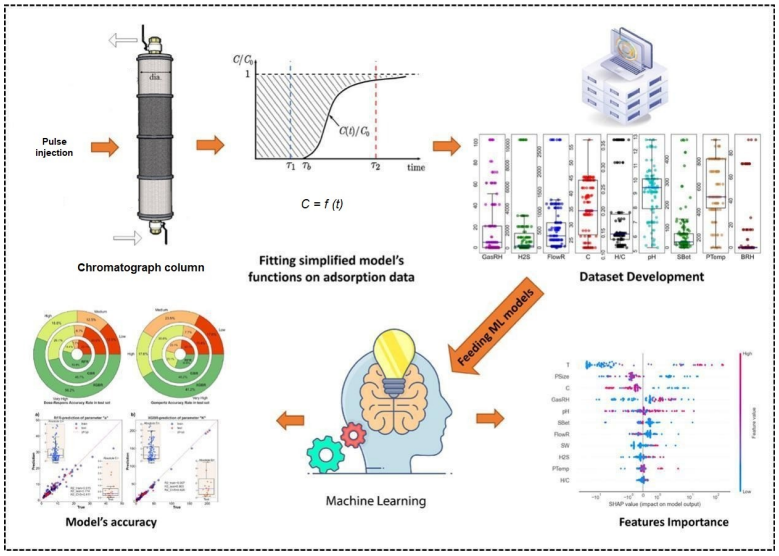


Fig. 1. Schematic representation of using ML approaches in gas chromatography column (adapted from [2])

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.

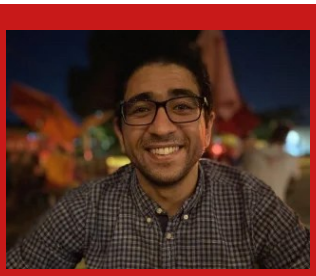
[2] F.Qaderi, et. Al , A novel machine learning framework for predicting biogas desulfurization breakthrough curves in a fixed bed adsorption column, Bioresource Technology Reports, 2024, 25, 101702.

Supervisor	Michael Abdelmalik
2nd supervisor	Wenjie Jin
Company	ASML
Internal / External	External (Paid)
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number: 2024 Q3



Physics-Encoded Neural Networks for Solving Non-linear Wafer Deformation

Michael Abdelmalik*, Wenjie Jin, Sander Gielen

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

Keywords: *Machine Learning, Neural Networks, Nonlinear Deformation, EUV lithography*

INTRODUCTION

In EUV lithography, wafer heating introduces overlay errors which need to be corrected during the exposure in a feedforward manner. Linear thermal expansion of the wafer is cheap to compute. However, non-linear deformation of the wafer due to the slip between wafer and its support stage requires time consuming iterations to find a solution, making it infeasible for online calculations. Recent studies showed that physics encoded neural networks (**PeNN**) can be used as a fast surrogate model without the need of expensive labeled training data.

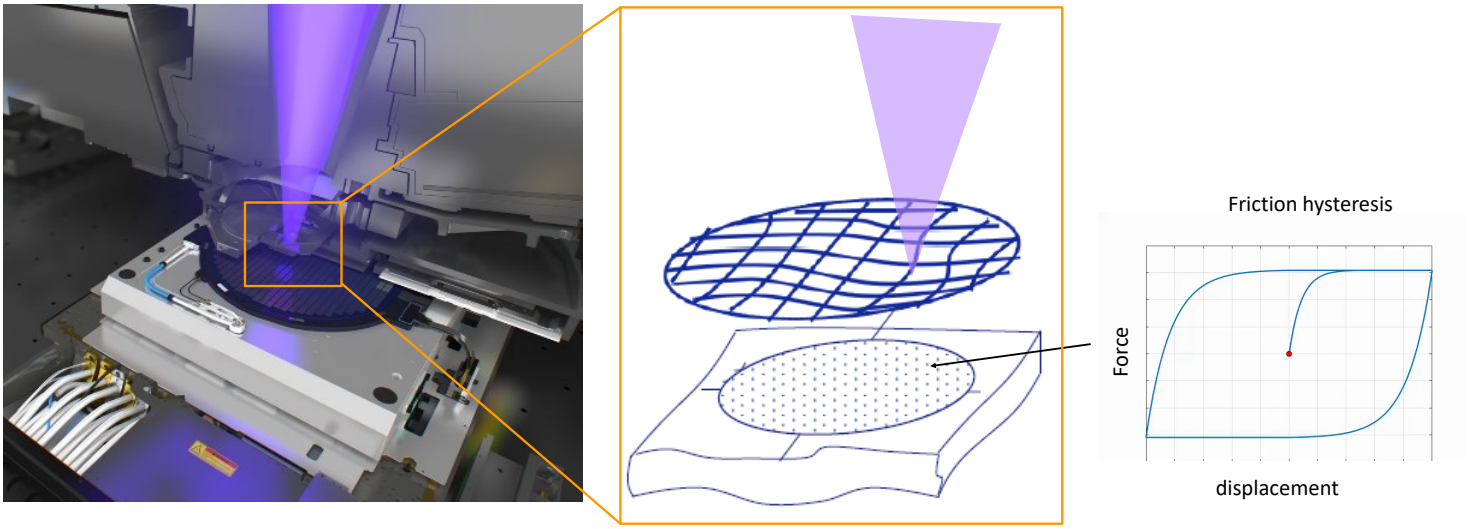
TASKS

- Formulate suitable objective/loss function(s)
- Generate training and validation datasets,
- Construct tailored **PeNN** architectures,
- Train and validate network

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.



Light induced deformation on a slip wafer

OBJECTIVE

The aim of this MSc project is to come up with an efficient **PeNN** model architecture, as well as a suitable training strategy, for solving the time dependent non-linear wafer deformation. We are seeking for a surrogate model which can provide generalized, accurate and fast solutions, suitable for real-time predictions.

REFERENCES

[1] Ren, P., Rao, C., Liu, Y., Wang, J.X. and Sun, H., 2022. PhyCRNet: Physics-informed convolutional-recurrent network for solving spatiotemporal PDEs. Computer Methods in Applied Mechanics and Engineering, 389, p.114399.

[2] Patel, D., Ray, D., Abdelmalik, M.R., Hughes, T.J. and Oberai, A.A., 2024. Variationally mimetic operator networks. Computer Methods in Applied Mechanics and Engineering, 419, p.116536.

Master Thesis project proposals

Q3 2024

Power and 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	**Marie-Aline Van Ende**
2nd supervisor	**Niels Deen**
Mentor	**Nishant Kumar**
Company	**-**
Starting date	**Anytime**
Exp./Num./Design	**Numerical**

Power &Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

CFD Simulation of the pressure drop across a packed bed furnace for the Direct Reduction of Iron

Nishant Kumar, Marie-Aline Van Ende*

***E-mail: m.a.p.p.van.ende@tue.nl**

INTRODUCTION

The direct reduction (DR) of iron oxide, usually followed by electric arc steelmaking, is an alternative route to the conventional blast furnace-basic oxygen route and aims to reduce CO_2 emissions in the iron and steel industry.

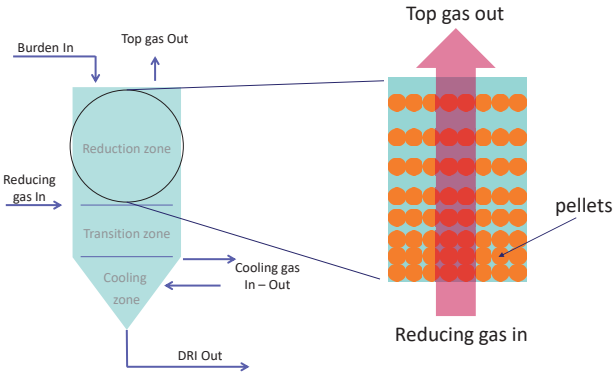


Fig. 1. Simple illustration of the reduction zone in the Midrex process.

The Midrex process is a shaft-type DR process where iron ore, charged atop and descending through a vertical shaft, is reduced to metallic iron by means of an ascending reducing gas (CO, H_2, CH_4). The reduction zone (Fig. 1), where most of the iron oxide reduction takes place, is located between the entry point of the reducing gases and the pellet charging point. The heating of pellets also takes place in this zone due to heat exchange with the hot reducing gas.

The reduction zone resembles a typical packed bed furnace, where hematite pellets are loaded and acts as a packing material. This packing material causes friction in the gas flow, generating friction losses.

Therefore, to ensure adequate pressure drop for the gas flowing through the column at a specified flow rate[1], the relation describing the pressure loss across the length of the packed bed due to the packing material must be determined.

Keywords: *Midrex, Direct Reduction of Iron, Packed column/bed*

OBJECTIVE

Develop a relation for the Pressure Drop across tube length in a packed bed furnace

PRE-REQUISITE

- Familiarity with any CFD software (such as ANSYS Fluent, Star-CCM+, OpenFoam, etc.)

TASK

- Create CFD simulation setup for the furnace
  - Realize geometry and the boundary conditions
  - Generate the flow path geometry
- Conduct parametric study to determine the influence of various input parameters (inlet gas temperature, inlet gas pressure, packing efficiency of bed, size of pellet, etc.)
- Develop the relation for the pressure drop based on those parameters
- Write master thesis report and present main findings

BENEFITS

- Experience working at the High Temperature Thermo-chemistry lab in Seoul National University, Korea
- Experience in design and analysis of numerical models

REFERENCES

[1] R. S. Subramanian. "Flow through Packed and Fluidized Beds." Department of Chemical and Biomolecular Engineering; Clarkson University: Potsdam, NY, USA (2002).

Seoul National University (SNU) campus is located at the feet of the Gwanaksan mountain, south of Seoul (SNU official Facebook page)

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

Power & Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

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

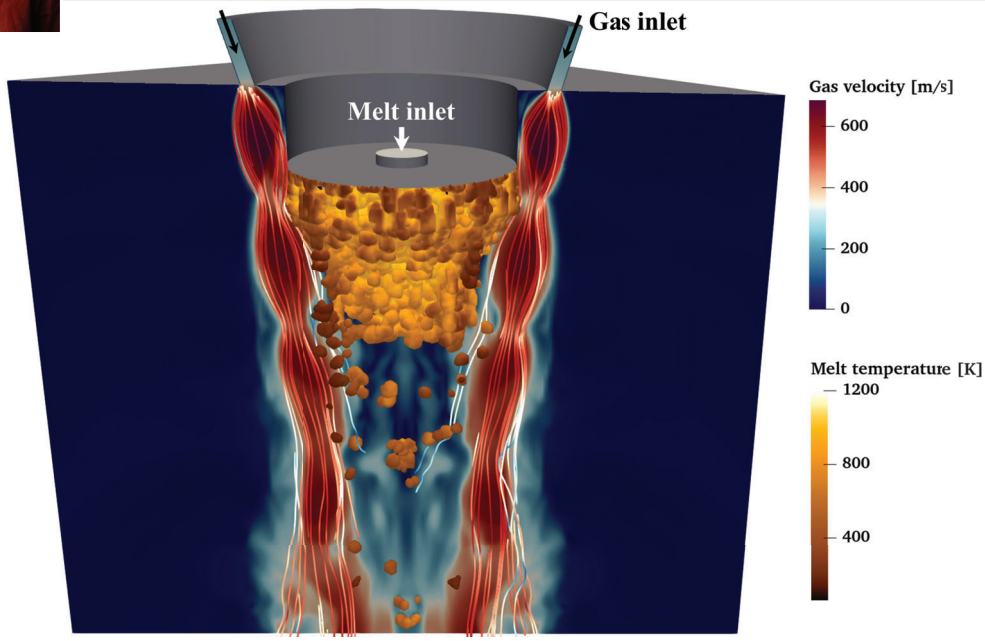


Figure 1: Simulation in OpenFOAM of the breakup of liquid metal in a gas atomizer

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 process is very important for 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.

The starting point is the work of a previous master student, who tested breakup models and implemented a simple solidification model in one of the Lagrangian solvers of the CFD software OpenFOAM.

Development of an efficient code that combines the breakup and solidification model for the droplets in the existing solver will be the focus of the project. Of course, it is possible to tune the project to your own interests!

GOAL & BENEFITS

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.

Besides actively contributing to the optimization of additive manufacturing feedstock, other benefits of this project include the freedom to shape the research to your interests, as well as getting to work with OpenFOAM, one of the most popular open-source CFD packages!

Supervisor	**Asst. Prof. Claudia-F. López Cámara**
2nd supervisor	**TBD**
Company supervisor	**Prof. Hartmut Wiggers**
Company	**EMPI, University Duisburg-Essen**
Starting date	**Anytime after February**
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
c.f.lopez.camara@tue.nl

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 methos 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.

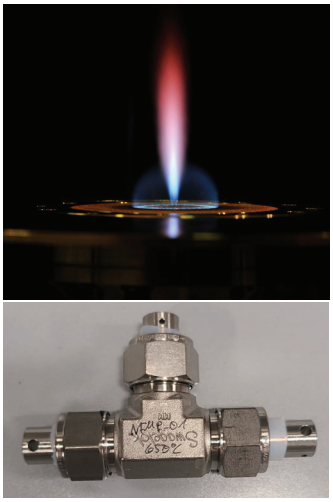


Figure 1. Top: Spray-flame from the University Duisburg-Essen. Bottom: T-battery for performance testing.

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	Dr. Xiaocheng Mi
2nd supervisor	
Daily supervisor	Shyam Hemamalini
Company	
Starting date	2024
Exp./Num./Design	Numerical

Power &Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Stabilising an iron flame in a coflow setting

Determination of flame speed, shape and characteristics

Xiaocheng Mi, Shyam Hemamalini
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INTRODUCTION

The iron power cycle is a novel alternative energy storage solution that is in active research and development the past few years. Iron powders burn in heterogeneous combustion mode that results in a unique discrete flame. **A deeper knowledge of the iron flame is indispensable in building the iron burners of tomorrow.**

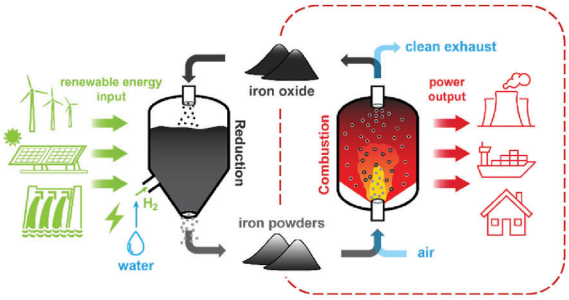

Fig. 1: The iron power cycle

This Master project involves **numerically simulating a stable iron flame in a coflow of air using the in-house code called NTMIX-CHEMKIN.** The code is a high-order DNS solver capable of simulating a Euler-Lagrange model of the iron flame with very high accuracy.

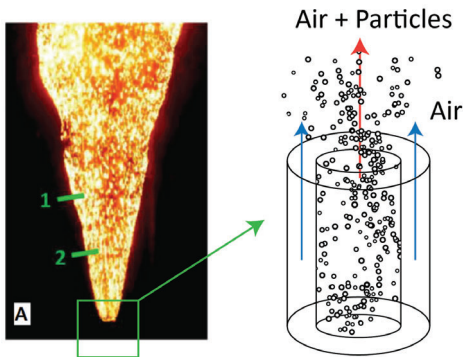

Fig. 2: Inverted Bunsen flame – coflow of air and iron particles

GOALS

1. A stable iron coflow flame simulated in NTMIX-CHEMKIN
2. Validation of flame speed measurements

MILESTONES

1. Literature review of iron powder combustion and iron coflow burners
2. Case setup of a coflow iron flame setting in NTMIX-CHEMKIN
3. Validation of the Euler-Lagrange model with experimental results
4. Extension of experimental results for diverse and practical use cases
5. Analysis and presentation of results

STUDENT PROFILE

A highly motivated Master student interested in energy transition, alternative fuels and numerical simulations is desired.

The following are potential benefits from this project:

1. Improvement of knowledge in combustion
2. Highly transferable skills in CFD and programming languages such as Fortran and Python.
3. Development of analytical and writing skills.
4. Opportunity to publish obtained results.

REFERENCES

1. Shoshyn, Yuri L., et al. "Experimental Research On Iron Combustion At Eindhoven University Of Technology." *Experimental Research On Iron Combustion At Eindhoven University Of Technology*. 2023.

Supervisor	Prof. Jeroen van Oijen
2nd supervisor	Gabriela Sanchez
Mentor	
Company	N.A.
Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Numerical

Available for ME-SET

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number: 01

Preferential diffusion effects and NOx formation in premixed hydrogen blends (H2/CH4)

Gabriela Sanchez*, Jeroen van Oijen

*E-mail: g.e.sanchez.bahoque@tue.nl

INTRODUCTION

During the last decades, the need to limit the combustion of traditional fossil fuels has increased considerably. Hydrogen plays an interesting role in this topic, since they generate less or no carbon-based emissions.

Despite the simple chemical kinetics of hydrogen oxidation, its combustion characteristics are different than those of hydrocarbon fuels. For example, hydrogen has a higher diffusivity (Le < 1), which leads to preferential diffusion effects and significantly different flame dynamics. It also results in locally richer regions with enhanced burning rate and higher temperatures (Fig. 1), having a negative impact in thermal NOx formation.

The goal of this project is to study the behavior of lean premixed hydrogen flames, and investigate how preferential diffusion, strain and curvature influence NOx formation rates.

TASK

In this project, you are expected to do:

- Literature review, focusing on hydrogen combustion.
- Simulations of 1D and 3D premixed lean hydrogen flames in the in-house codes (Chem1d and Disco).

OBJECTIVES

- Study the effect of preferential diffusion, stretch and curvature on NOx formation in 1D flamelets and in turbulent flow (3D).
- Investigate how we can model NOx chemistry with flamelet manifolds.

APPROACH

- Identify a proper chemical mechanism for hydrogen combustion, which includes NOx-chemistry.
- 1D flames will be solved with the in-house 1D code (Chem1d).
- 3D simulations will be performed with the in-house DNS code (Disco).
- Post-processing with Matlab or Python.

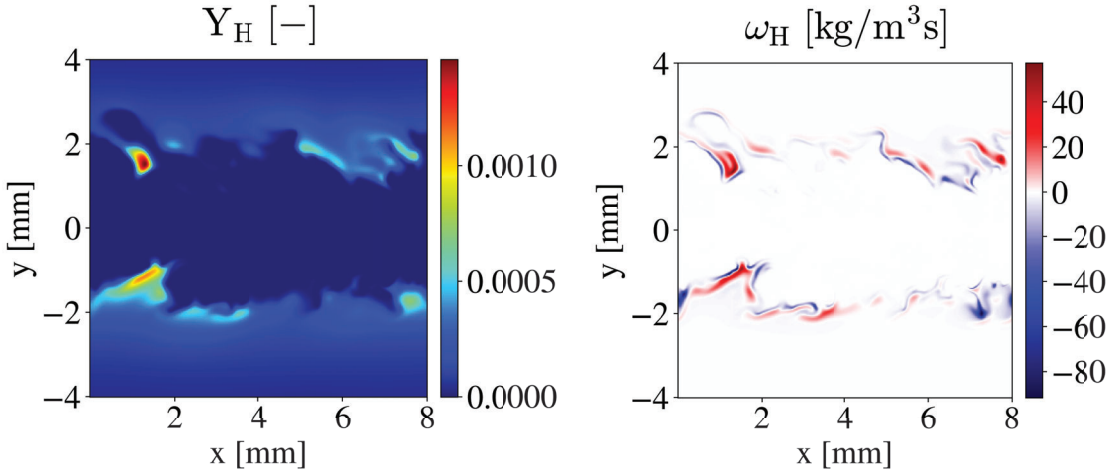

Fig. 1. Mass fraction of H and reaction rate of H in a pure hydrogen flame

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

Project number: 2023 Q2-01

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.

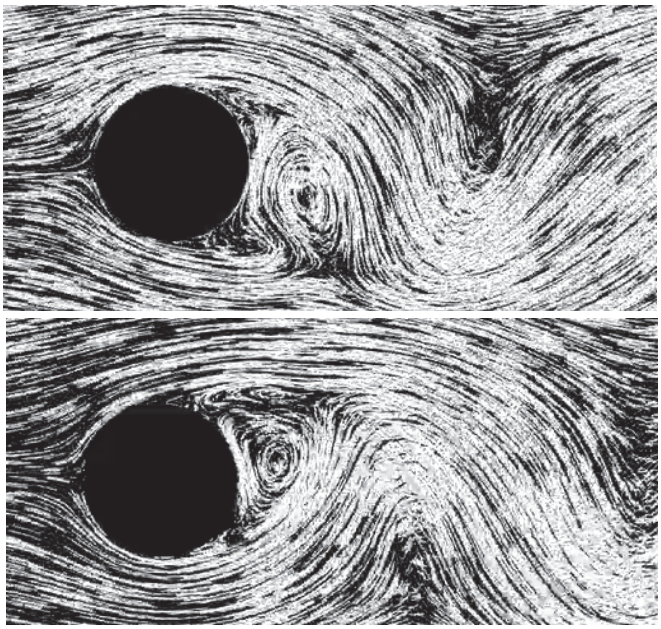

Fig 1: RANS simulation with clear low-frequency oscillation components.

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.

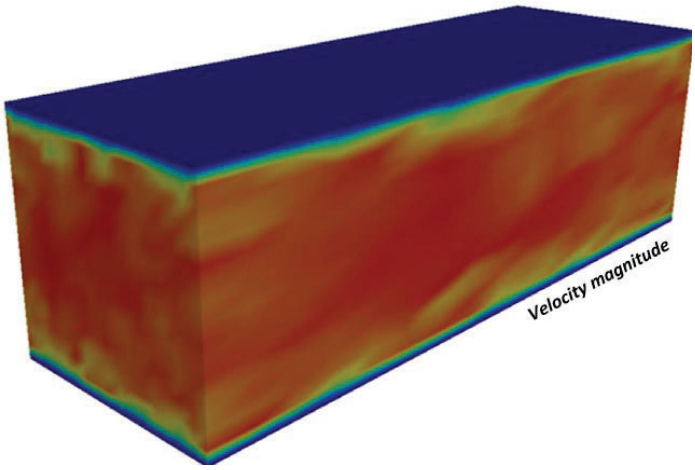

Fig 2: Main testcase: turbulent channel flow

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	**Asst. Prof. Claudia-F. López Cámara**
2nd supervisor	**TBD**
Company supervisor	**Prof. Hartmut Wiggers**
Company	**EMPI, University Duisburg-Essen**
Starting date	**Anytime before the end of June**
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.

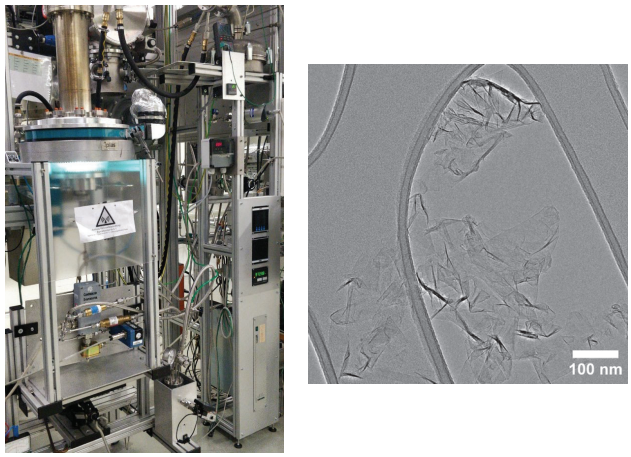

Figure 1. Left: Reactive zone of the microwave plasma reactor at the University Duisburg-Essen. Right: Few-layer graphene as seen under the transmission electron microscopy.

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)

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number: 2022 Q2

Numerical modelling of the acoustic-flame coupling in a porous burner

Hamed F. Ganji*, Jeroen van Oijen, Viktor Kornilov

*E-mail: h.faghanpourganji@tue.nl

Introduction

Thermoacoustic instability is resulted from an closed loop feedback between unsteady combustion and acoustic modes of the complete system. The appearance of thermoacoustic instability in combustion systems depends on thermoacoustic property (e.g., Transfer Function (TF)) of used burner/flame. Therefore, an attractive approach to cope with the instability is the purposeful design of the burner thermo-acoustics.

Tasks

In this project, you are expected to do:

- Literature review, focuses on thermo-acoustics theory
- Help to complete the CFD model of a porous burner made of ceramic fibers in Ansys Fluent.
- Using CHEM1D code to solve 1D flames to generate tables for FGM approach.

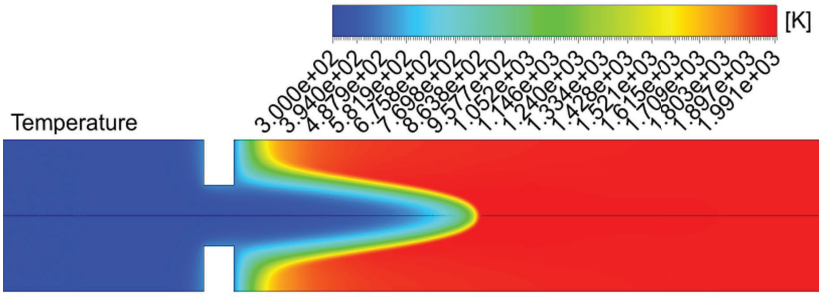

Fig2. Temperature contour.

Objectives & Approach

In this project we are going to develop a CFD model of the special porous burner made of Ceramic fibres produced by Orkli in Spain (Fig 1.) . This will help us to improve our understanding the acoustic quality of the stabilized flame on this burner deck. In the next phase, this model will be used along with other numerical and experimental tools in flame stabilization process in domestic boilers.

Requirements

- High motivation to research in numerical combustion and acoustics.
- Experience in Fluent, Matlab and Latex.
- Ideally experience in CFD .

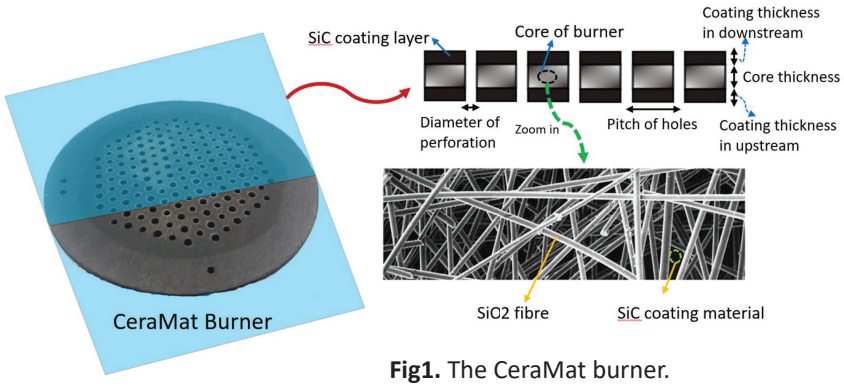

Fig1. The CeraMat burner.

REFERENCES

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2. J. van Oijen, L. de Goey (2002), Modelling of premixed counterflow flames using the flamelet generated manifold method, Combust. Theor. Model., 6 (3) (2002), pp. 463-478

Supervisor 1st	Dr. Yali Tang
Mentor	Ge Ding
Internal / External	Internal
Starting date	2024 Q3
Exp./Num./Design	Experimental and Design

Power & Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Electroreduction of iron oxide suspension in alkaline solution

*Contact: d.ge@tue.nl or y.tang2@tue.nl

BACKGROUND:

- Iron powders can act as a major CO_2-free energy carrier for the long term, via cyclic combustion and reduction processes (Fig. 1) . Regeneration of iron powder from combustion product is the key to close the cycle.

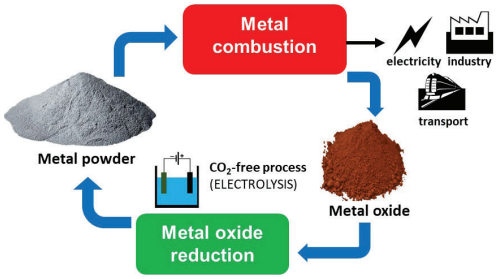


Fig. 1. Recyclable metal fuels cycle

- Applying electrolysis for reduction from iron oxides to metallic iron offers advantages such as no CO_2 or particle emissions, low energy consumption, direct usage of (renewable) electricity, and no intermediate step of producing a 'green' reducing agent (e.g., hydrogen). A proof-of-concept has been achieved (Fig. 2).

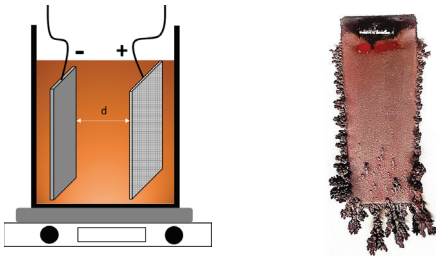


Fig. 2. Electroreduction reactor and iron dendrite

- In the routes (Fig.3) of electrochemical reduction of iron oxide, a part of the iron oxide first reacts to form ions and then is reduced to iron. To explore this route, the solid particles in the electrolyte need to be separated, keeping only the ionic solution.

RESEARCH QUESTIONS:

- How to achieve the flow circulation.
- How to separate the solid and liquid in electrolyte.
- How to maintain the electrolyte at a fixed temperature during cycling.

POSSIBLE ASSIGNMENTS:

- Build an electrochemical setup with:
  - Iron oxide electroreduction.
  - Solid-liquid separation of the electrolyte .
  - Ionic solution flow circulation system.
  - Temperature maintenance system.
- Perform electrochemical experiment.

REQUIREMENTS:

We are looking for a high-motivated student who has passion to do multi-disciplinary approaches. Some general requirements are expected:

- Familiar to perform chemical experiment.
- General knowledge in automation design.
- General knowledge in (electro)chemistry is beneficial.
- Creative, independent, and high curiosity.

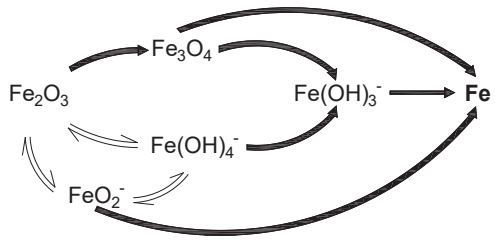


Fig. 3. Iron oxide electroreduction map

REFERENCES

[1] Majid, A.I, et al. (2022), Systems and Methods for Continuous Electrolytic Production of Metallic Iron, US Provisional Patent, 63/363,627

[2] Debiagi, P. , Rocha, R. C. , Scholtissek, A. , Janicka, J. , & Hasse, C. . (2022). Iron as a sustainable chemical carrier of renewable energy: analysis of opportunities and challenges for retrofitting coal-fired power plants. Renewable and Sustainable Energy Reviews, 165.

Supervisor	Tahsin Berk Kiymaz
2nd supervisor	Dr. ir. Nijso Beishuizen, Prof. Dr. Jeroen van Oijen
Company	BOSCH Thermotechniek
Starting date	Anytime
Exp./Num./Design	Numerical

Power &Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Numerical Investigation on Hydrogen Flame Flashback and Quenching Behavior

Tahsin Berk Kiymaz, Nijso Beishuizen, Jeroen van Oijen

E-mail: t.b.kiymaz@tue.nl

INTRODUCTION

With the aim of pursuing decarbonization, hydrogen is considered one of the leading energy vectors. There has been an increased interest in the research of hydrogen as a fuel in recent years since it is a promising alternative to fossil fuels. There are various fields of applications for hydrogen combustion from gas turbines to domestic boilers. However, this transition comes with its own challenges. The characteristics of hydrogen are significantly different than conventional fuels such as hydrocarbons. During this transition, the essential point is to make hydrogen combustion safe. Our aim is to investigate the hydrogen flame characteristics and understand the quenching and flashback behavior numerically. These findings will be used to develop fully hydrogen-fueled domestic boilers.

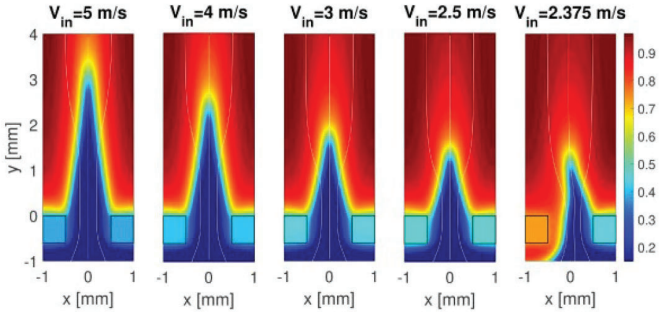


Figure 1: Visualization of flashback of a laminar premixed flame stabilized on a burner. Temperature contours are scaled with the adiabatic temperature. Flashback occurs at V=2.375 m/s. [1]

TASKS

-Literature study on laminar hydrogen flames and modeling hydrogen flames in near-wall conditions

- Modeling of reactive flows using computational fluid dynamic (CFD) approach

- Building a numerical setup for the modeling of flame flashback and quenching phenomenon for various hydrogen-air mixtures

-Postprocessing of the obtained results

GOALS

--Modelling of laminar hydrogen flames and understanding the flashback and quenching behavior.

-Understanding the key points of modeling flame wall interaction for hydrogen flame.

-Investigating the differences between detailed chemistry modeling and Flamelet Generated Manifold (FGM) method during quenching.

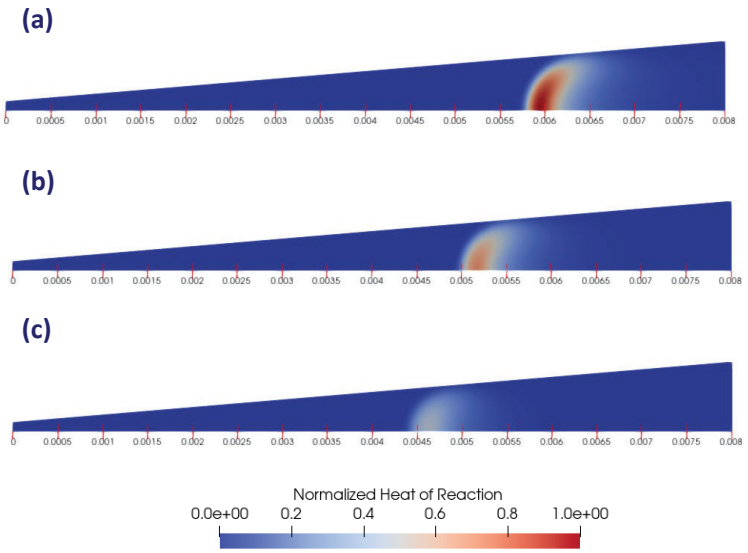


Figure 2: Quenching process of Hydrogen-Air premixed flame in a diverging duct, Φ=0.5 a) t=0, b) t=0.0012s, c) 0.0024s

BENEFITS

-Learn how to model reacting flows using CFD methods

-Get hands-on experienced on one of the most widely used CFD software in the industry (ANSYS Fluent)

-Be a part of the clean energy transition

-Get familiar with the fuel of the future

REFERENCES

[1] Vance, F. H., de Goey, L. P. H., & van Oijen, J. A. (2022). Development of a flashback correlation for burner-stabilized hydrogen-air premixed flames. Combustion and Flame, 243, 112045. https://doi.org/10.1016/j.combustflame.2022.112045

Supervisor	Diego Quan Reyes
2nd supervisor	Nijso Beishuizen
Company supervisor	
Company	
Starting date	2024
Exp./Num./Design	numerical

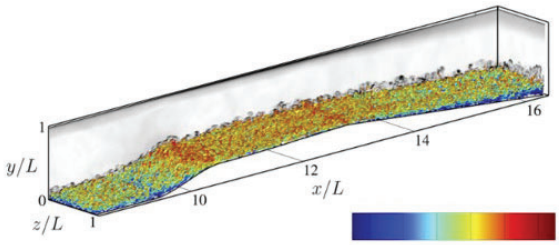
Power &Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

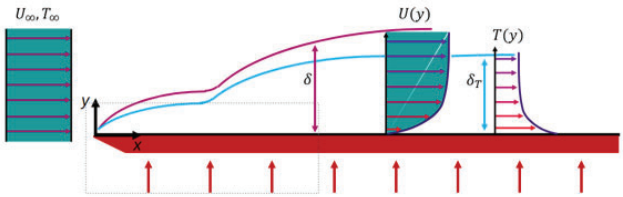
Turbulence modeling of heated walls

Diego Quan Reyes, Nijso Beishuizen, Jeroen van Oijen

INTRODUCTION



From: Vaquero et al, Phys. Fluids (2019)

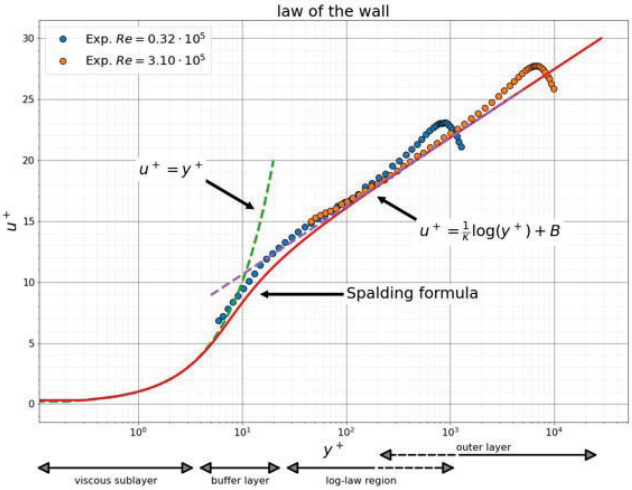


Even with today's computer power, the combined flow and heat transfer over heated or cooled surfaces is computationally very challenging due to the requirements on the mesh size necessary to resolve the large velocity and temperature gradients near the wall. Therefore, a lot of research has been done on turbulent wall models.

The basic idea for all wall models comes from the observation that all turbulent flow profiles close to walls are self-similar, meaning that they are the same when using scaled velocities and distances. This means that the large gradients close to the wall do not need to be resolved because they are known from this universal 'law of the wall'. This known profile can be imposed and used to accurately compute wall shear stresses and therefore friction, lift, drag and pressure drop.

The modeling of *heated* walls has been less well developed compared to adiabatic walls. It is known that temperature profiles are also self-similar, but in the case of real gases with temperature dependent properties, there is a lack of data.

GOALS & TASKS



- Literature study on thermal wall modelling.
- Derivation of (thermal) law of the wall for temperature dependent gas properties and implementation/visualization.
- Extract thermal law of the wall from Direct Numerical Simulations (DNS).
- Improve thermal law of the wall correlation for large temperature range.
- Implement thermal law of the wall in turbulence model and validate.

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REFERENCES

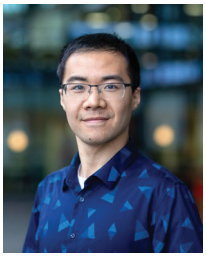
[1] H. Schlichting, *Boundary Layer Theory*
[2] Deissler and Eian, *NASA technical note 2629 (1952)*
[3] Irrenfried & Steiner, *2019* https://doi.org/10.1016/j.ijheatfluidflow.2019.108495

Bachelor/Master/Internship Project

Technische Universiteit Eindhoven University of Technology

Jet in cross flow with ConvergeCFD

Boyan Xu, Rob Bastiaans



Introduction

Jet in Crossflow(JICF) is used in the primary zone of gas turbine combustors as a means of controlling the air–fuel mixture ratio and the emissions of nitrogen oxides (NOx); Micro-Mix combustion technology using JICF has advantages on emissions & anti-flashback.

The NOx-emissions of gas turbine has attracted human's attention because of their harm to health and living environment. Reducing NOx-emissions can be achieved by enhancing the mixing process of reactants and by lowering the residence time of these reactants in the hot flame regions. The micro-mix technology can form miniaturized non-premixed combustion thus keeps the residence time of NOx forming reactants short and avoids the danger of flashbacks.

As shown in Fig.1, the air enters the Micro-mix burner structure, passes the air-guiding-panel (AGP) gate, and mixes with the fuel jet that is injected perpendicular into the air crossflow. The free air-jet that mixes with the fuel is separated from the inner recirculation zone by the inner vortex shear layer.

The using of multicomponent fuel□ NH3 /H2 mixture has many advantages. The wild using and safety character of NH3 and the high burning velocity of H2 are complementary to each other.

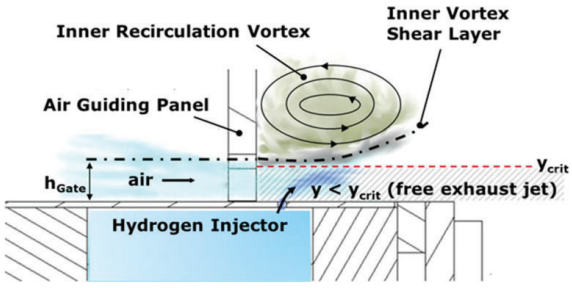


Fig 1: Micro-mix injection, drawn by Funke [1]

Project

The 1-D simulation of NH3/H2 diffusion flame has shown that the NH3/H2 ratio can affect the amount the NOx apparently. However, in 3D flow field, turbulence and the complex crossflow structure may couple with the flame behaviors. The emission level of JICF flame should be evaluated under different equivalence ratio and proportions of H2 addition in NH3.

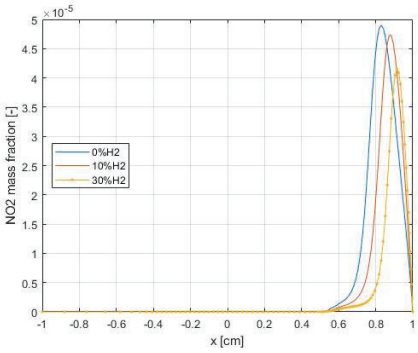


Fig 2: The NOx profile of 1-D NH3/H2 diffusion flame

CONVERGE is a wildly using Commercial CFD software which could be used to solve combustion-fluid relative problems. In this project, CONVERGE is planned to be use to simulate the 3D reacting flow field and calculate the generated pollutant.

Learning goals/Requirements/…

- The using of CONVERGE software(geometry drawing/case setting/post-processing/etc.).
- 1D- flamelet generation by Chem1d.
- Using FGM model in CONVERGE.
- The mechanism of forming NOx for NH3/H2 flame as well as its regulation.
- The potential research direction of NH3/H2 combustion.

Recommended literature

[1]H.H.-W. Funke, etc, Experimental and Numerical Study of the Micromix Combustion Principle Applied for Hydrogen and Hydrogen-Rich Syngas as Fuel with Increased Energy Density for Industrial Gas Turbine Applications, Energy Procedia, Volume 61, 2014, Pages 1736-1739,
[2]R.W. Grout, etc.,Direct numerical simulation of flame stabilization downstream of a transverse fuel jet in cross-flow, Proceedings of the Combustion Institute, Volume 33, Issue 1, 2011, Pages 1629-1637,

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Internal / External	Internal
Starting date	Any time
Exp./Num./Design	Experimental

Available for ME-AT

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Evaluating ultra-clean OME fuel combustion using optical diagnostic techniques

Noud Maes, Nico Dam, Zhongcheng Sun

Introduction

Environmental concerns and human health-being have emerged as critical challenges in the contemporary world. Heavy-duty engines continue to play a significant role in the transport section and cannot be replaced overnight. Consequently, its contamination is regarded as an inevitable urgent problem. E-fuels are considered as an effective solution to reduce the emissions to achieve sustainable transportation. Polyoxymethylene dimethyl ethers (OME_n), one of the most promising E-fuels, can be produced from CO_2 capture and electrolysis of water, exhibits huge potentials for reducing both soot and NO_x. Recently, tests of OME and diesel blends have been conducted on a heavy-duty MX13 engine. However, the elaborate combustion characteristics of different blends, including ignition and mixing-control combustion progress is not clear. In this work, particular emphasis is put on investigating the spray and combustion characteristics of pure OME_3, OME_x, and OME_x-diesel blends when compared to dodecane or diesel. Various optical technologies containing schlieren, OH* chemiluminescence, and DBI, will be considered to measure the spray penetration, ignition delay, lift-off length, soot mass, etc., in the case of a specific ECN Spray D injector with a heavy-duty sized hole.

Contact

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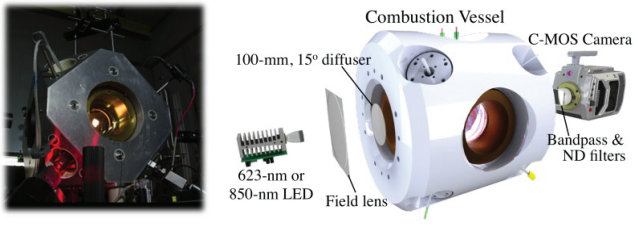

Figure 1. Photograph of EHPC & Schematic overview of DBI setup.

Project description

1. Establish a well-designed testing approach for OME fuels to determine relevant combustion caracteristics
2. Conduct advanced optical diagnostics on flames
3. Analyze effects of primary factors and interactions
4. Study and optimize the fuel blends on combustion process and soot formation

Experimental apparatus

This experiments are carried out on an optically-accessible, high-pressure, high-temperature combustion pre-burn vessel (Eindhoven High-Pressure Cell, in short EHPC), which is used to simulate the conditions at TDC for compression-ignition engines. The setup has optical access from multiple sides to host a magnitude of optical diagnostic techniques.

Tasks

- Literature study, getting familiar with the fuels, EHPC, combustion properties, and optical diagnostic techniques.
- Involvement with preparing the test matrix, the EHPC, and optics approaches
- EHPC calibration testing using dodecane
- Optical testing using different fuels
- Analysis of the data to finish a concise report

Requirements

- Affinity with experimental work & optical diagnostics
- Background knowledge on combustion and diagnostics
- Motivation and a hands-on mentality

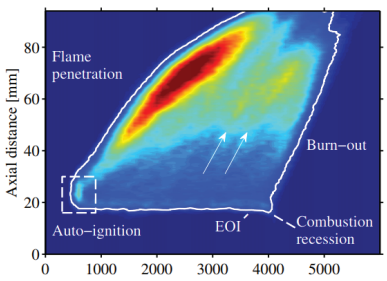

Figure 2. Radially integrated OH* intensity obtained in the EHPC as a function of axial distance and time, with a contour defined by the intensity at the location of the steady flame lift-off length.

Supervisor	Rob Bastiaans
2nd supervisor	
Company	N.A.
Internal / External	Internal
Starting date	Q2 2023
Exp./Num./Design	Theoretical and numerical

Available for ME-SET-AT-AIES

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number: 2023 24-01

`white holes' in premixed turbulent combustion kernels: analysis

Rob Bastiaans
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INTRODUCTION

Turbulent combustion is a very common large scale energy generation method, e.g. in gas turbines. Nowadays we concentrate on the combustion of carbon free fuels, here NH_3/H_2 mixtures. Design is very difficult as experiments are always small scale and expensive. Therefore, we try to simulate these events efficiently, though accurately.

Academically we perform direct numerical simulations (DNS) of canonical cases to establish a reference 'truth', by resolving everything.

The canonical case here is a turbulent flame kernel, see figure 1. It is very simple because it lives in a cubical domain with just 6 outflow BC's. For this case, your supervisor, last summer at a sabbatical leave at the Center for Turbulence Research (CTR) at Stanford University, found an interesting phenomenon occurring in these cases. He coined the term `white hole' for it , for combustion kernels, in contrast to `black hole' in cosmology.

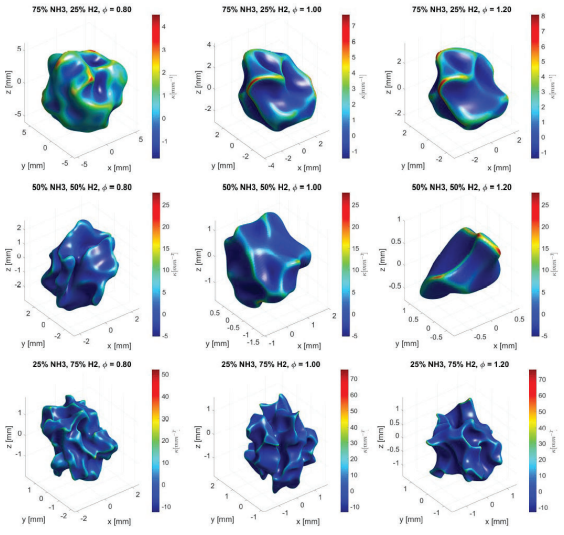

Figure 1: Turbulent premixed NH_3/H_2 combustion kernel.

The phenomenon occurs at gradually when time evolves**.** Gradually, the turbulence in the internal region and the largest fluctuations concentrate on the outer flame kernel edge. So, it was (speculatively, though) concluded that such a `white hole' emits information and avoid reentry of it.

OBJECTIVES

- Substantiating the `white hole' conjecture.
- Evaluation of entropy generation in the intern and extern of the kernel.
- Evolution of interscale kinetic energy transfer.

Candidate

- Has knowledge of combustion and CFD
- Has analytical skills
- Is interested in fundamental research of combustion physics

REFERENCES

[1] Mukundakumar, N. & Bastiaans, R., 2022, DNS Study of Spherically Expanding Premixed Turbulent Ammonia-Hydrogen Flame Kernels, Effect of Equivalence Ratio and Hydrogen Content, Energies, ***15*** *(13), 4749.*

[2] R. Bastiaans & X. Liu, 2023, Turbulent, premixed, spherical NH3/H2 combustion; Simulation optimization and existence of 'white holes', Annual Research Briefs, Center for Turbulence Research, Stanford University, pp. ?–? (to appear).

Supervisor	Boyan Xu
2nd supervisor	Rob Bastiaans
Company	N.A.
Internal / External	Internal
Starting date	Q2 2023
Exp./Num./Design	Theoretical and numerical

Available for ME-SET-AT-AIES

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number: 2023 24-01

`white holes' in premixed turbulent combustion kernels: acoustic forcing

Rob Bastiaans
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INTRODUCTION

Turbulent combustion is a very common large scale energy generation method, e.g. in gas turbines. Nowadays we concentrate on the combustion of carbon free fuels, here NH_3/H_2 mixtures. Design is very difficult as experiments are always small scale and expensive. Therefore, we try to simulate these events efficiently, though accurately.

Academically we perform direct numerical simulations (DNS) of canonical cases to establish a reference 'truth', by resolving everything [1].

The canonical case here is a turbulent flame kernel, see figure 1. It is very simple because it lives in a cubical domain with just 6 outflow BC's. For this case, your supervisor, last summer at a sabbatical leave at the Center for Turbulence Research (CTR) at Stanford University, found an interesting phenomenon occurring in these cases. He coined the term `white hole' for it , for combustion kernels, in contrast to `black hole' in cosmology.

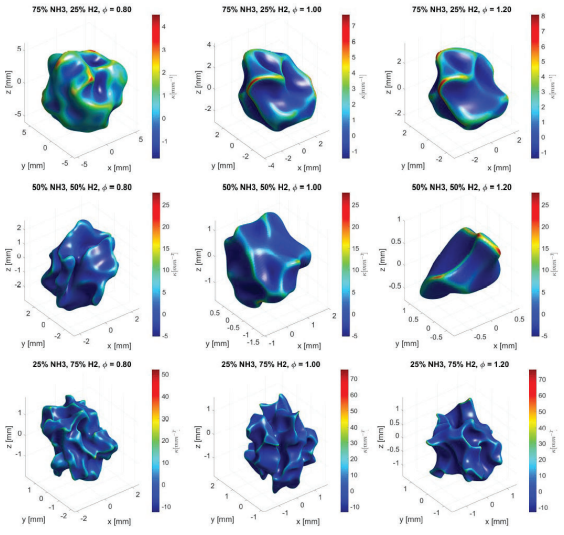

Figure 1: Turbulent premixed NH_3/H_2 combustion kernel.

The phenomenon [2] occurs at gradually when time evolves**.** Gradually, the turbulence in the internal region and the largest fluctuations concentrate on the outer flame kernel edge. So, it was (speculatively, though) concluded that such a `white hole' emits information and avoid reentry of it. Now I am looking to force local turbulence through acoustics emitted in 3 directions.

OBJECTIVES

- Substantiating the `white hole' conjecture.
- Introduce an acoustic field from 3 perpendicular sides.
- Evaluate its consequences when phases and amplitudes shift.

Candidate

- Has knowledge of combustion and CFD
- Has analytical skills
- Is interested in fundamental research of combustion physics

REFERENCES

*[1] Mukundakumar, N. & Bastiaans, R., 2022, DNS Study of Spherically Expanding Premixed Turbulent Ammonia-Hydrogen Flame Kernels, Effect of Equivalence Ratio and Hydrogen Content, Energies, **15** (13), 4749.*

[2] R. Bastiaans & X. Liu, 2023, Turbulent, premixed, spherical NH3/H2 combustion; Simulation optimization and existence of 'white holes', Annual Research Briefs, Center for Turbulence Research, Stanford University, pp. ?–? (to appear).

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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

Machine learning for scale interaction in advective transport equations

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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.)

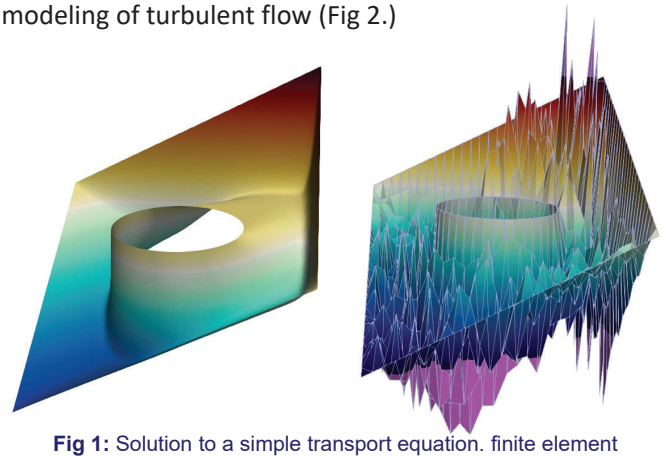

Fig 1: Solution to a simple transport equation. finite element approximation with (**left**) and without (**right**) scale interaction.

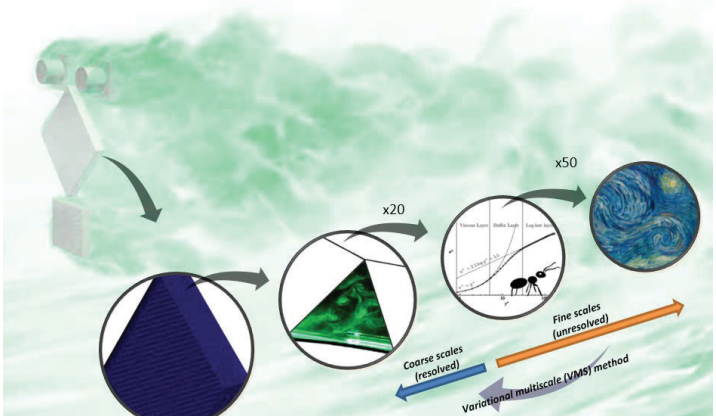

Fig 2: Scale interaction for turbulent flow.

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.

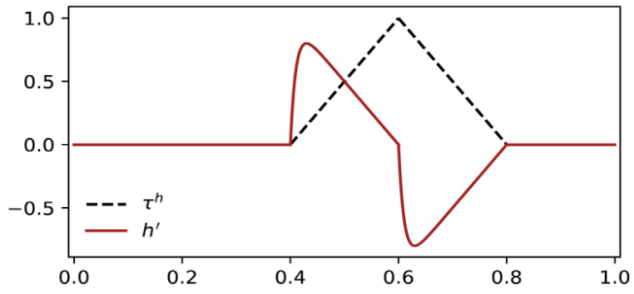

Fig 3: Scale-interaction function for a one-dimensional advective transport equation. For this particular case, the interaction function h' localizes to a single element.

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	Sina Tajfirooz
2nd supervisor	Hans Kuerten
Company supervisor	Sina Tajfirooz
Company	NRG
Starting date	Any time
Exp./Num./Design	Numerical

Power & Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Direct numerical simulation of turbulent stratified two-phase flow

S. Tajfirooz, J.G.M. Kuerten
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INTRODUCTION

*The **Nuclear Research and consultancy Group (NRG)** located in Petten, is one the major institutes responsible for nuclear research in the Netherlands. NRG is internationally recognized as the foremost provider of nuclear medicine, supporting over 30,000 patients annually. A significant focus of NRG's research is dedicated to enhancing nuclear reactor safety by utilizing Computational Fluid Dynamics (CFD) tools.*

*The modeling of **two-phase flows** holds significant importance in nuclear engineering applications. These applications include pressurized thermal shock, emergency core cooling, and boiling in a fuel rod bundle. In most instances, these applications involve turbulent multiphase flows. The characteristics of turbulent flow can vary considerably based on the type of two-phase flow regime present, such as dispersed, bubbly, slug, or stratified regimes.*

*This project focuses on the **stratified two-phase** regime. This regime, characterized by a large-scale interface between the gas and liquid phases, typically occurs in **reactor cooling systems**. The heat and mass transport across the interface is closely connected to the flow field and turbulence in both phases. Hence, accurate prediction of flow field and the coupled mass transfer is highly important for optimizing reactor cooling systems.*

*At NRG, in collaboration with national and international research partners (TU/e, ANL), we use **direct numerical simulation (DNS)** to capture the flow field in both phases in a **co-current turbulent stratified flow** (See Figure 3) .*

GOAL

*This proposal outlines a research direction focusing on the DNS of turbulent stratified two-phase flows using the **volume of fluid (VOF)** method. The open-source solver **Basilisk** will be used for this purpose.*

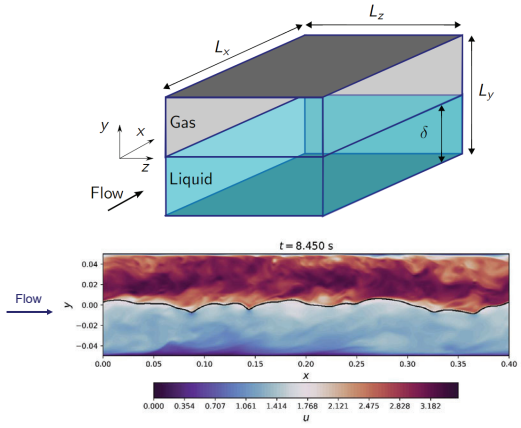

Figure 3: DNS of turbulent stratified flow. (a) schematic of the computational domain. (b) A snapshot of the interface and streamwise flow field at z=0.

*The goal is to set up a final **DNS case for generating benchmark data** that will be used for validation and improvement of lower-resolution models such as Reynolds- averaged Navier Stokes and large-eddy simulation.*

TASKS

- *Implement **averaging tools** to extract spatio-temporal statistics of the interface and flow field (e.g., time and space spectra, two-point correlation)*
- *Implement a **passive scalar transport** model in the current solver to investigate the combined effects of flow and heat/mass transfer.*
- *Perform **preliminary under-resolved simulations** to select appropriate computational settings for the final DNS simulation.*
- Post-process, analyze and report the results.

Prior knowledge of **C** and **python** is a plus.

BENEFITS

- Learn how to simulate two-phase flows using DNS
- Combination of programming and performing simulations for an industrially-relevant phenomenon
- Monthly allowance and compensation for housing and transportation for the period of your stay.

NRG

Supervisor	Victor Habiyaremye
2nd supervisor	Hans Kuerten
Company supervisor	Victor Habiyaremye
Company	NRG
Starting date	Any time
Exp./Num./Design	Numerical

Power &Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Investigation and validation of immersed boundary methods for two-phase direct numerical simulations

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INTRODUCTION

The Nuclear Research and Consultancy Group (NRG) is one of the main institutes involved in nuclear research in the Netherlands. In order to ensure nuclear reactor safety, NRG uses Computational Fluid Dynamics (CFD) for accurate predictions of the thermo-hydraulic behavior of the reactor.

Two-phase flow can occur in nuclear reactors, both in normal operation as well as in accident scenarios. It is therefore important to gain a better understanding of how such flows develop and evolve, and how they may affect nuclear reactor safety and performance. In order to achieve this goal, NRG is developing an in-house Direct Numerical Simulation (DNS) solver capable of efficiently simulating two-phase flows. This solver can make use of an Immersed Boundary Method (IBM) to simulate flows in complex geometries without complicating the numerical mesh.

GOALS

In this graduation project, the focus will be on further developing and validating the IBM in the in-house solver. First, this will be done in single-phase flow, and then, the interaction of two-phase flow with the IBM will be studied. The end goal is to have a robust and well-validated IBM implementation, as well as a first application of the IBM to a two-phase flow problem. The project's location is at the NRG site in Petten.

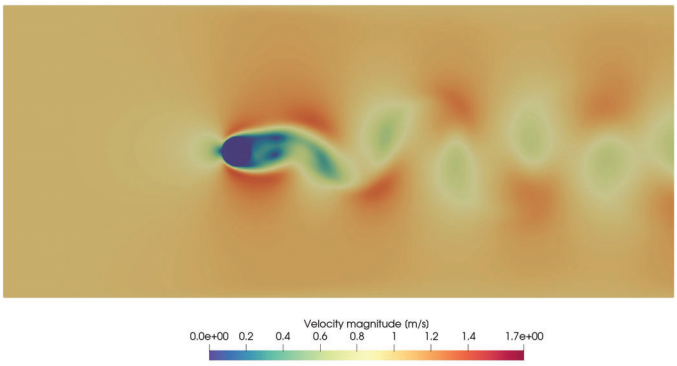

Figure 1. Vortex street behind a cylinder at Re=100, simulated using an IBM [1]

TASKS

- Review existing literature on IBMs to better understand the approach and identify validation cases
- Become familiar with the CFD code by running basic test cases
- Implement sampling and averaging tools for validation (for this, prior knowledge in C++ and/or OpenFOAM is a plus)
- Validate different IBM options in well-known flow configurations (e.g., see Figure 1).

BENEFITS

- Learn how to program in a CFD code
- Combination of writing code and running simulations
- Monthly allowance and housing/public transport compensation

NRG Nuclear. For life.

REFERENCES

[1] Fadlun, E. A., Verzicco, R., Orlandi, P., & Mohd-Yusof, J. (2000). Combined immersed-boundary finite-difference methods for three-dimensional complex flow simulations. *Journal of computational physics*, *161*(1), 35-60.

Supervisor	Tess Homan
2nd supervisor	Nico Dam, Hanneke Gelderblom
Company	N.A.
Internal / External	Internal
Starting date	Now available
Exp./Num./Design	Experimental and data analysis

Power & Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Virus-laden droplets: characterization

TESS HOMAN, Nico Dam, Hanneke Gelderblom
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Introduction

During the COVID-19 pandemic we all had to adhere to the 1.5 meter rule. But where does this advice come from?
For any type of virus it is important to know how it spreads. The big question about the coronavirus was: Does it spread through the air, i.e. is it airborne? You would think this is easy to measure, but still the proof is very limited. And if it is airborne, what type of measures should we take: masks, ventilation, keeping distance? This depends on the size and behaviour of the droplets that carry the virus. And when these droplets reach a new person, will the virus still be infectious?

In a collaboration with Erasmus Medical Center we aim to answer these questions. At the TU/e we will build a test setup to make and collect droplets containing virus-like particles. The entire process needs to be gentle in order to not disintegrate the virus.

Build a spray device

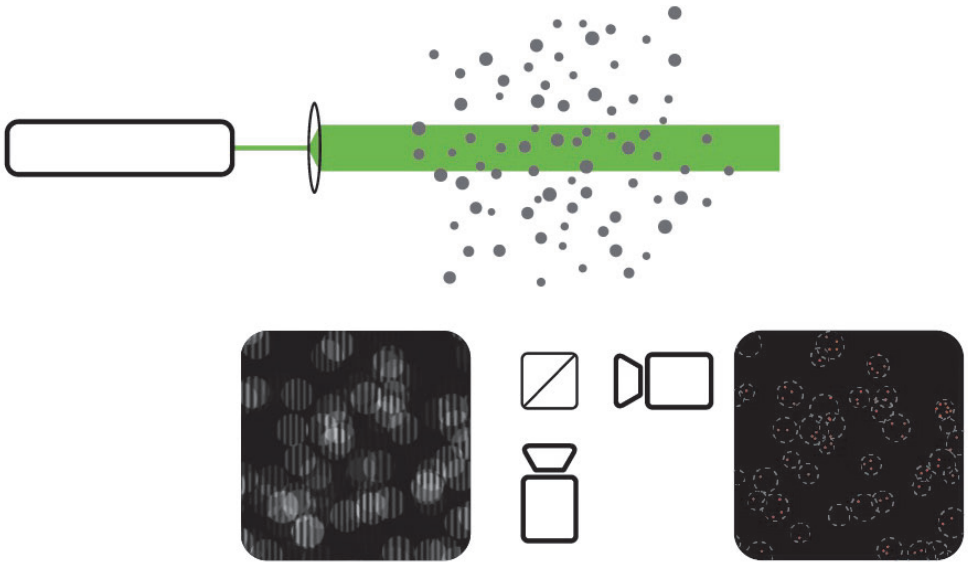
In this project you will build a device to create droplets in a gentle way. The resulting spray needs to be characterized: What is the droplet size distribution? How is the virus distributed over the droplets? Using optical techniques we will simultaneously measure the droplet sizes and the distribution of fluorescent virus-like particles.

Objectives

- Create a gentle spray of a visco-elastic (mucus-like) liquid
- Use IPI (Interferometric Particle Imaging) to measure the droplet sizes
- Use fluorescence to track the virus-like particles

You

- will be working in a lab
- will build a test setup
- will do experiments using optical techniques
- will use data analysis to interpret the data



To characterize the spray, we will use a thick laser sheet and a 2-camera setup that measures both the particle-size and the distribution of fluorescent nanoparticles. IPI image adapted from Evans *et al*. Rev. Sci. Instrum. **86**, 023709 (2015)

Supervisor	Yali Tang
2nd supervisor	Jan Hendrik Cloete (@SINTEF)
Company	SINTEF, Norway
Internal / External	External
Starting date	Any time
Exp./Num./Design	Numerical

Power and Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Wall-particle heat transfer modelling in Two-Fluid Simulations

YALI TANG, JAN HENDRIK CLOETE
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INTRODUCTION

Heat transfer between the particle bed and heat exchanger walls plays an important role in numerous fluidized bed reactor concepts that are proposed for more sustainable processes, such as adsorption-based CO_2 capture [1]. Somewhat surprisingly then, there are no suitable models to account for particle-wall heat transfer in the most commonly used computational fluid dynamics (CFD) method for simulating fluidized bed reactors [2], the two-fluid model (TFM). Based on a previous MSc work, this project therefore aims to further develop a recently proposed approach for including particle-wall heat transfer in TFM simulations [3].

Project

The first part of the project will require running TFM simulations in Ansys Fluent for a variety of experimental fluidized bed setups for which particle-wall heat transfer data exist in literature. Data generated from the simulations will then be used to optimize the parameters in a particle-wall heat transfer closure to achieve the best possible match with experimental data. An existing Matlab script will be upgraded and utilised for this purpose. The student will also be expected to improve the formulation of an existing particle-wall heat transfer closure based on physical arguments. This study will be performed in collaboration with researchers from SINTEF Industry, a non-profit research institute based in Norway, and the student will spend part of the project time in Trondheim, Norway. There are possible funding to support the staying of the student in Trondheim.

OBJECTIVES

- To further develop a recently proposed wall-particle heat transfer model
- To improve the model formulation based on physical arguments

APPROACH

- Perform TFM simulations using Ansys Fluent
- Optimize model parameters using Matlab
- Analyse and discuss the results

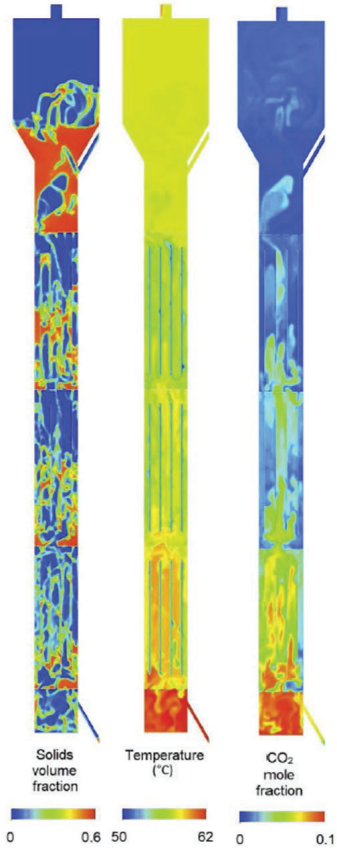

Figure 1: An example of a TFM simulation of a fluidized bed CO_2 adsorption reactor with particle-wall heat transfer included

REFERENCES

1. Dhoke C. et al. Review on Reactor Configurations for Adsorption-Based CO_2 Capture. Industrial & Engineering Chemistry Research. 2021
2. Alobaid F, et al. Progress in CFD Simulations of Fluidized Beds for Chemical and Energy Process Engineering. Progress in Energy and Combustion Science. 2021
3. Cloete J.H, et al. Developing a novel approach for modelling particle-wall heat transfer in fluidized bed reactors for CO_2 capture. In: 24th Fluidized Bed Conversion conference; 2022. Available from: bit.ly/3aaO4t7

Supervisor	Nico Dam
2nd supervisor	Tess Homan
Company supervisor	n.a.
Company	n.a.
Starting date	Any time
Exp./Num./Design	Exp. / Design

Power & Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

An acoustic bubble scraper

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Tess Homan (t.a.m.homan@tue.nl)

INTRODUCTION

Electrolysis, the splitting of liquid water into gaseous hydrogen and oxygen, is one of the ways to store surplus green electricity for later use. During electrolysis, gas bubbles form on a metal electrode surface, and this gives rise to an efficiency trade-off: the more gas is produced, the more electrodes are covered in bubbles, and the less free metal surface is available for more gas production.

Hydrogen bubble formation on a gold wire. As long as they are attached to the wire, they reduce its effective surface area. (Figure from Chen et al. (2018) JPC C122: 15421.)

Obviously, there is a need for an electrode cleaning procedure. In a previous master project (van den Brink, 2023) we have shown that bubbles can be manipulated by sound. In this project, want to employ sound to scrape bubbles of an electrode surface.

TASKS

- Study the literature on acoustic bubble formation
- Design a simple electrolysis setup combined with an acoustic field generator
- Perform experiments to optimize bubble scraping
- Analyze and present the results

GOALS

- Understand the interaction of sound with bubbles
- Construction of a simple electrolysis setup combined with an acoustic generator
- Assess feasibility of bubble scraping
- Assess prospects for upscaling

BENEFITS

Why choose this project?

- Interesting topic
- Relevant application
- Combination of experimental work, design and analysis
- Lots of room for your own input

Why not choose this project?

- *I hate research*
- *I hate to come up with ideas myself*
- *I hate enthusiastic supervisors*
- *I prefer numerical work*

REFERENCES

(A demonstration of acoustic particle manipulation. The movie concerns solid particles in air, but you will employ the method on gas bubbles in liquid.)

- van den Brink, Y. (2023). Design of an an acoustic bubble levitator (Report of the previous master project.)

Supervisors	Nicole Stevens
2nd supervisor	Giulia Finotello
Company	N.A.
Internal/External	Internal
Starting date	2nd quarter 2024
Exp./Num./Design	Experimental

Power & Flow

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Project number: 2024 Q2-3

Reduction of iron ore in a lab-scale fluidized bed

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Introduction

Iron powder is a good energy carrier which can be stored and transported in large amount. Energy is released by burning the powder resulting in solid iron oxides. These iron oxides particles can be recycled using green hydrogen via a reduction process. The products of this reduction process are solid iron and water vapor. The combination between these two steps, combustion and reduction, creates a carbon free cycle called the metal fuel cycle.

Initial experiments in a packed bed (thermogravimetric analysis) showed that full conversion to iron is possible using hydrogen, creating porous particles. However, the reaction rate was rather slow and sticking was found to occur. A lab-scale fluidized bed set-up has been designed and built to prevent this by allowing better mixing and heat transfer of the particles.

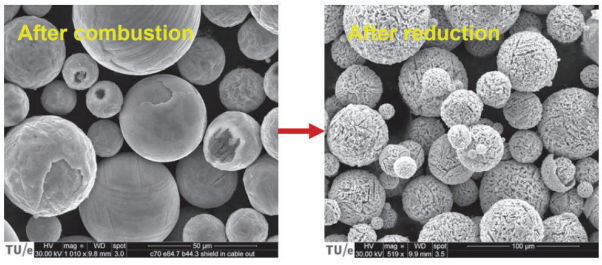

Figure 1: SEM images of combusted iron (left) and direct reduced iron (right) [1]

Project

Reduction experiments at elevated temperatures are executed in the fluidized bed using a hydrogen flow. The experiments can be conducted in two different regimes: bubbly regime and turbulent regime. Sticking behavior during reduction at different conditions can be studied. The particle size distribution of the powder can be analyzed before and after reduction experiments.

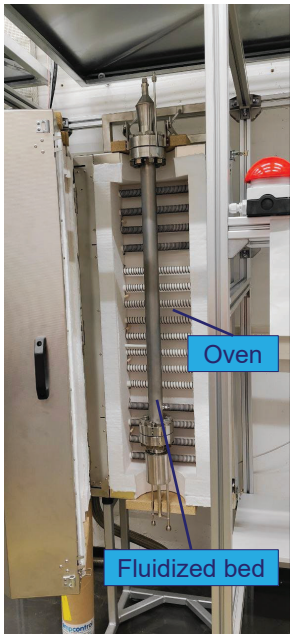

Figure 2: lab-scale fluidized bed

Goals

This project consists of two main goals:

1. Optimize the reduction process.
2. Investigate sticking behavior in both regimes

Tasks

- Study the theory on iron oxide reduction and sticking behavior.
- Investigate sticking behavior in two different regimes and possibly with different conditions (temperature, gas flow, H/D ratio) for reduction in the fluidized bed.
- Assess the powder in terms of size, morphology, porosity, composition and reduction degree.

/POWER AND FLOW

[1] Hessels C.J.M. et. al. 'Reduction kinetics of iron oxides fines, produced from iron combustion, using hydrogen' Powder Technology. 2021. (in process)

Supervisor	Prof Philip de Goey
2nd supervisor	Stijn van Aken
Company supervisor	
Company	Metalot
Starting date	Q3 2023-2024
Exp./Num./Design	Experimental

Power &Flow

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Large-scale cyclicity of iron powder as zero-carbon energy carrier

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INTRODUCTION

Metal fuels can be used to store and transport renewable energy (see fig. 1). By combusting iron powder, heat is released that can be utilized in industrial processes.

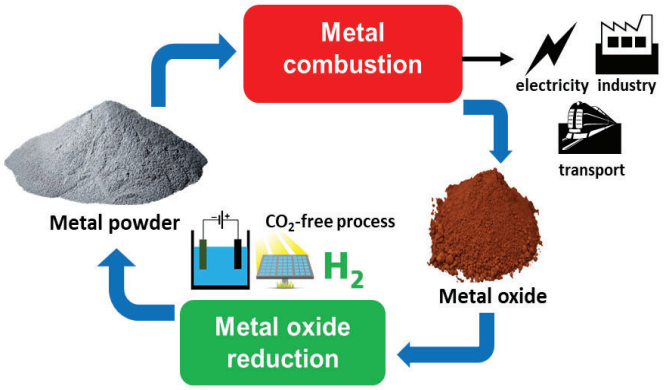

Fig. 1. A Recyclable metal fuels cycle

One of the key features of the metal fuels cycle, is the cyclicity of the iron powder. The cyclicity has been tested for a few cycles on small scale in a lab environment (grams). Currently, Metalot is working together with several partners to set up an experimental program to test the cyclicity of iron powder for many cycles and at large-scale (tons).

Keywords: *Iron Power, metal fuels, cyclicity, large-scale experiments*

TASKS

We are looking for a highly-motivated master graduation student who is interested in the energy transition, process engineering and metallurgy. In this project, you are expected to:

- Conduct experiments using the 500 kW iron powder combustion system (Fig. 2) and the 25 kW hydrogen based powder regeneration setup
- Analyse powder characteristics throughout repeated cyclicity testing

Fig. 2. 500 kW iron powder combustion system operated at Metalot

GOALS

- Determine the cyclicity of iron powder as zero-carbon energy carrier
- Determine the effect of repeated combustion and regeneration on iron powder characteristics

BENEFITS

- Experience to work in the company with experienced researchers on a completely new topic
- You will be working on multi-disciplinary approach (Mechanical Engineering & Chemical Engineering)
- Involved in the development phase of a promising method for green energy storage.

REFERENCES

- https://www.metalot.nl/projecten/
- https://ironfuel.nl/

Supervisor	Helen Prime & Jesse Hameete
2nd supervisor	Yuriy Shoshyn
Company	N/A
Internal / External	Internal
Starting date	Anytime
Exp./Num./Design	Experimental

Power & Flow

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Help develop carbon-free energy storage by exploring metal powder combustion

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INTRODUCTION

Global warming, driven by hydrocarbons, is a well-known problem. We need a carbon free, recyclable energy storage. Metal fuels are proposed as a solution, as they can be used to store energy and help with daily and seasonal energy fluctuations. We need to understand the combustion of metal powder to optimize the process and make the energy transition quicker and easier.

A Bunsen burner was built in McGill, Canada, specifically designed for metal powder combustion. This burner has been optimised for aluminium combustion, shown in Figure 1 for multiple mass flows. We wish to adapt this burner for iron combustion.

OUTLINE

The outline of this project will be the following:

- Set up, calibrate and test metal powder combustion using a Bunsen burner.
- Calibrate using aluminium powder and compare with results from Canada.
- Burn iron powder to measure various parameters and compare with other burners

You have a well-defined project plan, but there is a lot of freedom to make your own planning.

If this sounds like something you want to do for your graduation project, send me a message!

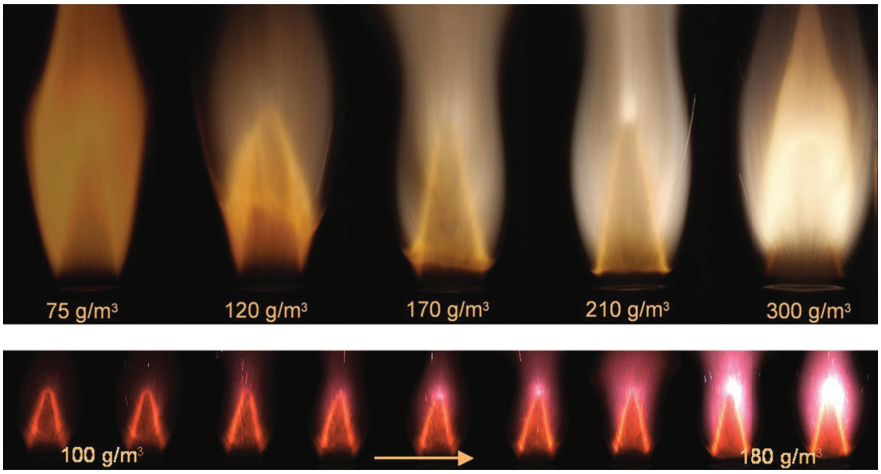

Image 1: Aluminum flame stabilized on a Bunsen burner for multiple mass flows.