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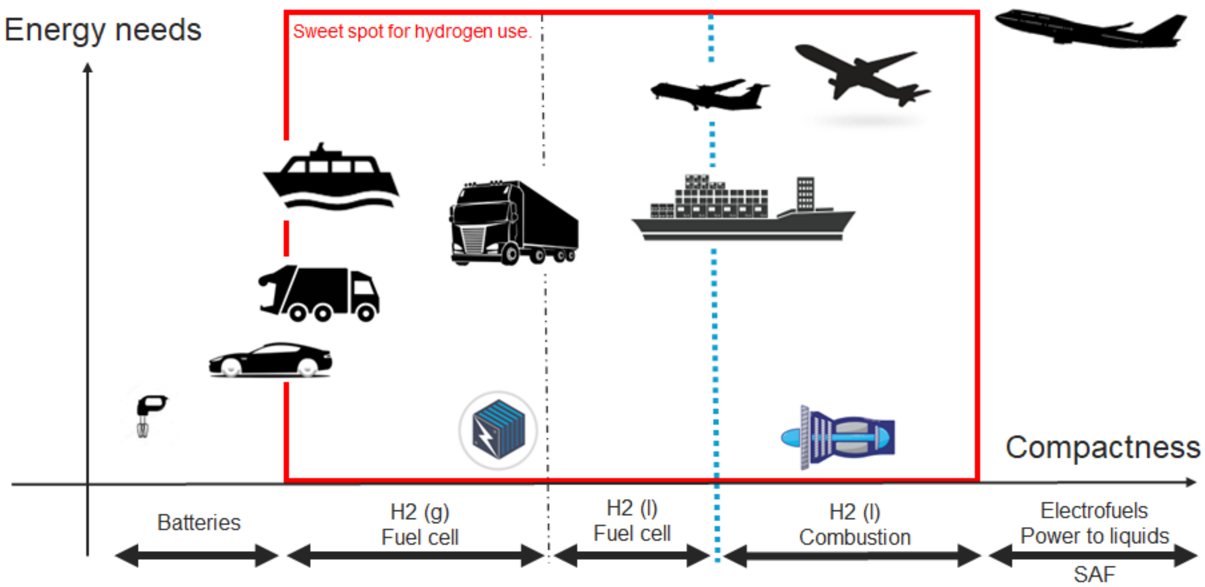
Annual report 2022: Technologies and innovations for a future sustainable hydrogen economy (TechForH2)



TechForH2 is a new competence center for multidisciplinary hydrogen research with the overall aim of developing new technology for greening heavy transport.

Revision history
2023-02-23 circulated to board for review
2023-03-09 accepted on-board meeting

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Abstract

Transports generate about 25% of the global CO_2-emssions and represent about a third of the Swedish national emissions. To meet the Paris agreement targets, Sweden is aiming for net zero emissions by 2045. Although lighter transports are suitable for battery electric propulsion, there is today many arguments for expanding the hydrogen use in the heavier transport areas. A large potential for synergies across transport modes and for new innovations exist for new hydrogen propulsion solutions. For this reason, the TechForH2 excellence center was proposed and later funded for start in 2022. TechForH2 is led by Chalmers University of Technology in collaboration with RISE and partnering with the member companies Volvo, Scania, Siemens Energy, GKN Aerospace, PowerCell, Oxeon, Stena Rederi, Johnson Matthey and Insplorion.

The TechForH2 center concentrates its work around five multidisciplinary research arenas, (1) lightweight composite storage solutions for cryogenic hydrogen, (2) additive manufacturing for hydrogen fuel supply systems, (3) nanoplasmonic hydrogen sensor maturation, (4) fuel cell development and integration, (5) the future of hydrogen – societal challenges. All five arenas are now well up and running and eight Ph.D. research positions have been opened and launched. Although the core research activities revolve around the Ph.D. projects, Chalmers university is boosting the launch of TechForH2 by initiating seven post doc projects in the area of transport with a hydrogen focus.

Sammanfattning

Transporter genererar cirka 25% av de globala CO_2-utsläppen och står för ungefär en tredjedel av de svenska nationella utsläppen. För att klara Parisavtalets mål siktar Sverige på nettonollutsläpp till 2045. Även om lättare transporter lämpar sig för batterielektrisk framdrivning finns det idag många argument för att utöka vätgasanvändningen i de tyngre transportområdena. Det finns en stor potential för synergier mellan transportmoder och för nya innovationer inom vätgasområdet. Av denna anledning föreslogs kompetenscentret TechForH2 och erhöll därefter finansiering för start under 2022. TechForH2 leds av Chalmers tekniska högskola i samarbete med RISE och samarbetar med medlemsföretagen Volvo, Scania, Siemens Energy, GKN Aerospace, PowerCell, Oxeon, Stena Rederi, Johnson Matthey och Insplorion.

TechForH2-centrat koncentrerar sitt arbete kring fem tvärvetenskapliga forskningsarenor, (1) lätta kompositlagringslösningar för kryogent väte, (2) additiv tillverkning för vätgasbränslesystem, (3) nanoplasmoniska vätegassensorer, (4) bränslecellsutveckling och integration, (5) vätgasens framtid - samhällsutmaningar. Alla fem arenorna är nu väl igång och åtta doktorandtjänster har öppnats och lanserats. Även om kärnverksamheten i centrat kretsar kring doktorandprojekten, så har Chalmers kick-startat lanseringen av TechForH2 genom att initiera och finansiera sju post doc-projekt inom transportområdet med vätgasfokus.

TECHFORH2 ORGANIZATION

TechForH2 is today comprised of eleven partners, Chalmers as the coordinating body, and with Rise as an additional funding recipient. In addition, nine industrial partners contribute, ranging from large multinational companies to SMEs. The current complete partner listing is:

- Chalmers University of Technology
- RISE Research Institutes of Sweden
- Volvo Technology
- Scania
- Siemens Energy
- GKN Aerospace
- PowerCell
- Oxeon
- Stena Rederi
- Johnson Matthey
- Insplorion

The TechForH2 board

Upon submitting this report, the TechForH2 board has had four meetings (2022-04-29, 2022-05-23, 2022-12-01 and 2023-03-09). Since the number of partners in TechForH2 is relatively moderate it is feasible to maintain two members per partner in the board, where one of the members has the representing vote and the other member is having the substitute vote. This allows for continuity and company internal dialogue. The current listing is:

Name / organization	Organization
Tomas Grönstedt, Director	Chalmers
Maria Grahn, Co-director	Chalmers
Selma Brynolf	Chalmers
Sinisa Krajnovic, Rector's Delegate	Chalmers
Anders Lundbladh	GKN Aerospace
Pauline Leonárd	GKN Aerospace
Per Hanarp, Chairman of Board	Volvo
Monica Johansson	Volvo
Karl-Johan Nogenmyr	Siemens Energy
Annika Lindholm	Siemens Energy
Per Stålhammar	Scania
Ingergerd Annergren	Scania
David Mattsson	RISE
Karin Arrhenius	RISE
David Nilebo	Insplorion
Elin Langhammer	Insplorion
Åsa Bye	PowerCell
Andreas Bodén	PowerCell
Mikael Larsson	Johnson Matthey
Mikaela Wallin	Johnson Matthey
Elisabet Liljeblad	Stena Rederi
Andreas Martsman	Oxeon
Florence Morerau	Oxeon
Emma Westsson	Energimyndigheten

Table 1: Members of the TechForH2 board

The research disciplines

To ensure academic excellence, industrial relevance and autonomy TechForH2 is organized around research disciplines, in total seven, led by a research leader/leaders. Several of the research leaders both have a strong scientific background and have worked in industry developing technology. All seven disciplines had substantial funded on-going research, prior the launch of TechForH2. The difference for the research projects run in TechForH2 is that they are frequently of a more multi-disciplinary nature and are typically also run with a larger number of industry partners. The seven different disciplines are:

1. **Materials technology** with research leaders full professor Leif Asp (lightweight composite materials and structures) and professor Martin Fagerström (computational fracture mechanics)
2. **Manufacturing technology** with research leaders Emmy Yu Cao (professor in materials technology) and Lars Nyborg (full professor in surface engineering)
3. **Cryogenics & heat management** with research leader Tomas Grönstedt (full professor turbomachinery)
4. **Vehicle level understanding** with research leaders Lucien Koopmans (full professor in combustion engineering) and David Sedarsky (associate professor in experimental fluid dynamics)
5. **Transport & society** with research leaders Maria Grahn (associate professor in energy systems) and Selma Brynolf (researcher in energy and environmental analysis)
6. **Safety & sensors** with research leader Christoph Langhammer (full professor in chemical physics)
7. **Fuel cell technology** with research leader Anna Martinelli (professor in surface chemistry)

These seven research areas were defined in dialogue with industry during the application process of TechForH2. Critical research disciplines were singled out by industry. Areas where also a strong research competence existed was then prioritized, to establish the seven areas listed above.

The multidisciplinary research areas

TechForH2 was established, and may also be modified, by allowing the seven research disciplines introduced above to form new multidisciplinary research areas. The basic process is illustrated in Figure 1 below.

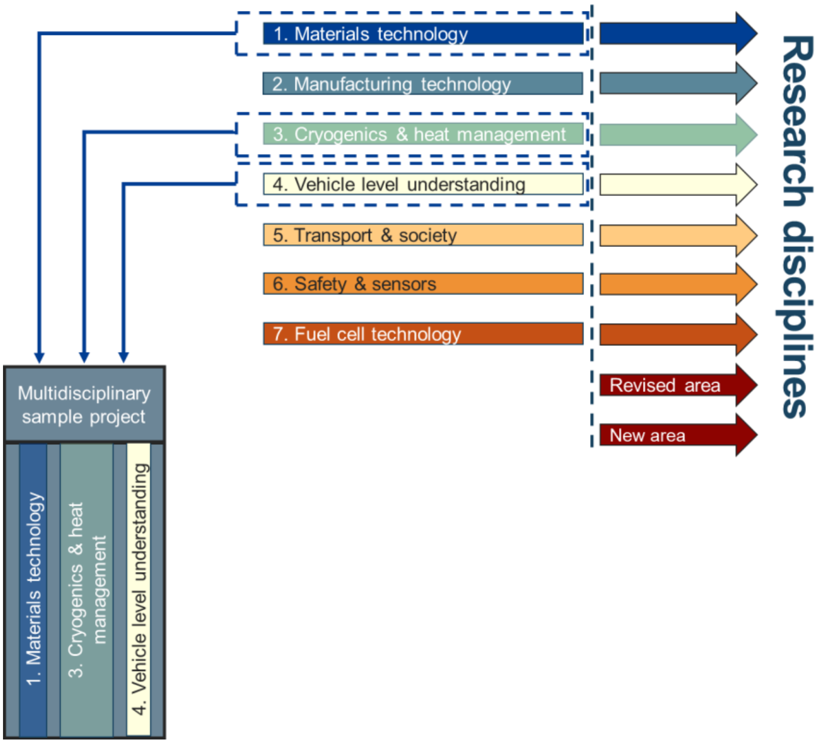

Figure 1: TechForH2 process for establishing new multidisciplinary research areas.

This center design logic allows TechForH2 to be dynamic against changes in the applied hydrogen area and enables some steering capability as the hydrogen economy evolves. In a potential extension, that is after the first five years, some of the areas above may be deleted, re-prioritized and/or new areas may simply be added to the center activities. This center design also allows clustering new partners around a few new projects and managing a number of IP-critical aspects without a too large administrative burden.

As the center was planned and applied for, it became evident that a focusing of the effort was needed. For instance, the national German research commitments only in the area of hydrogen technology (e.g. H2Giga, H2Mare, TransHyDe) are more than **an order of magnitude** larger than **all** the energy agency competence centers together. Hence, a national Swedish initiative may easily spread too thin, if it is attempting to cover the entire chain of development (production, use and large-scale storage). TechForH2s initial focus therefore concentrates on **hydrogen use** with an emphasis on vehicle integrated solutions.

The five multidisciplinary research areas where TechForH2 is active are:

1. **Lightweight composite storage solutions for cryogenic hydrogen** (combining the research disciplines materials technology, vehicle understanding and cryogenic & heat management)
2. **Additive manufacturing for hydrogen fuel supply systems** (combining manufacturing technology and cryogenic & heat management)
3. **Nanoplasmonic hydrogen sensor maturation** (safety & sensors as well as transport & society)
4. **Fuel cell development and integration** (fuel cell technology, cryogenics and heat management, vehicle level understanding and transport & society)
5. **The future of hydrogen – societal challenges** (transport & society with inputs from potentially all disciplines)

The international research network

TechForH2 faces several challenges to rapidly establish itself as a leading research center in the hydrogen area. One of TechForH2's strategies is to tackle this by limiting the research scope to certain aspects of hydrogen use, by establishing an application close research focus liaising with globally positioned Swedish industry and by pro-actively setting up a research network with hydrogen relevant internationally leading researchers. This was done during the application process isolating key collaborative partners in critical areas by signing bilateral letters of intent between the TechForH2 research leaders and each of the relevant researcher at the foreign university. The structure of the network is illustrated in Figure 2 below.

Figure 2: TechForH2 research collaboration network. TechForH2 has written individual LoIs with key hydrogen technology relevant researchers in Europe, to kickstart activities and make TechForH2 an internationally well-known research center.

The research leaders and their relation to the collaborative network is specified in Table 2 below.

Research leaders	Scientific network contacts
Leif Asp	Senior Lecturer, Soraia Pimenta, Imperial College London.
Fiona Schulz/Yu Cao	Full professor, Mariangela Lombardi, Politecnico di Torino.
Tomas Grönstedt	Associate professor Vishal Sethi (ENABLEH2 coordinator), Cranfield University, Arvind Rao, Delft university.
Anna Martinelli	Full professor, Luis M. Varela, USC Santiago.
Lucien Koopmans	Professor of Technology, David Blekhman, Cal. State Univ, Los Angeles.
Maria Grahn, Selma Brynolf	Associate Professor, Iva Ridjan Skov, Ålborg University. Senior Research Ass. Dr Nishtabbas Rehmatulla, Bartlett Energy Institute, UCL, London.
Christoph Langhammer	Prof. Bernard Dam, Delft University, Ass. Prof. Andrea Baldi, Vrije Universiteit, Amsterdam

Table 2: Research leaders' relation to the collaborative network (separate LoIs have been put in place)

Year 2022 highlights

The center was officially established at Chalmers on the 18th of March 2022 [1]. A key challenge to overcome during 2022 was the development and signing of the contract. Although the number of partners in TechForH2 is not overwhelming, the nature of the partners ranges from small relatively recently started innovation companies to large multinational players. This creates different commercial types of interest and requires a contractual balancing. Eventually the contract was finalized with the last signature in place 2022-09-23.

Despite the contractual delays the home department (M2 – Mechanics and Maritime Sciences) decided to take a balanced risk and allow the start of 6 Ph.D. students already in June 2022 (Decision M2 2022-0162). This decision allowed a controlled launch of the center and has been a key milestone for the fact that the center is now well up and running. The center board has had three meetings in 2022 (2022-04-29, 2022-05-23 and 2022-12-01). The third meeting was also the official kick-off of the center in which the research areas and key researchers was in place as nicely illustrated in below. The event was picked up by Dagens Industri [2].

Figure 3: TechForH2 kick-off at Volvo CampX.

Although the center only started recently, and all recruited researchers are very new, it is a pleasure to highlight an early research effort published in nature communications [3]. The work focuses on plasmonic sensors and has been co-authored by Christoph Langhammer, research leader in TechForH2, as well as Andrea Baldi (member of TechForH2 international collaborative network). Quoting from a Chalmers press release:

“The technology around hydrogen has taken a giant leap and therefore today's sensors need to be more accurate and tailored for different purposes. Sometimes a very fast sensor is needed, sometimes one is needed that works in a harsh chemical environment or at low temperatures. A single sensor design cannot meet all needs," says Christoph Langhammer, who is also one of the founders of a new competence centre: TechForH2”

Multidisciplinary research areas

Although the center was awarded to start early 2022, the final contract was drafted only 2022-08-09 and the last signature was received in 2022-09-23. In total 9 Ph.D. projects where initially planned for. Due to the long process of signing the contract, substantial financial risk was in place, and it was therefore decided to launch the recruitment filling 6 out of the 9 Ph.D. positions. The final three positions would be filled when the contract was completed. Hence the projects have been launched gradually during 2022. At the time of writing 8 Ph.D. students out of the planned 9 have now been recruited and are presented in the project area presentations below.

The multidisciplinary research areas are supported by seven post doc projects, funded by Chalmers University. These have been put in place to secure Chalmers own investment for the center. The projects are:

- Vehicle On-board storage integrating liquid and compressed hydrogen tanks – Project area 1
- Hydrogen in transport – Global, European, and Nordic perspectives – Project area 5
- Hydrogen diffusion combustion modeling – Project area 5
- Fossil-free ships: energy demand, production, storage, and consumption – Project area 5
- Systematic control of PEM fuel cells for vehicle applications – Project area 4
- Computational multi-scale platform for hydrogen utilization/storage/sensing – Project area 4
- Pathways for a sustainable introduction of hydrogen into the aviation sector – Project area 1

The total project commitment, for the first two years, is more than 19 MSEK to contribute to Chalmers' investment.

Recruited post docs and joint research activities are now presented below, summarizing the activities within the five multidisciplinary research areas.

Project area 1: Lightweight composite storage solutions for cryogenic hydrogen

Industry stakeholders
This multidisciplinary area is configured by collaborating across the disciplines of materials technology and cryogenics & heat management. Initially Chalmers, RISE, GKN Aerospace, Oxeon and Scania collaborated to define the content. As the work has progressed increased interest from Volvo has also been noted.

Basic disciplines
The **materials technology discipline** interfaces with a large number of hydrogen-driven research challenges, such as developing ultra-low weight polymer composites, exploiting benefits from 2D materials (e.g. graphene and ultra-thin carbon fibre tapes), creating barrier layers and coatings, developing material design methods to avoid liquid hydrogen leakage and tank failure, developing engineering guidelines for the design of linerless liquid hydrogen tanks, developing and exploiting metallic materials for mid-to-high temperature applications for hydrogen rich environments and studying the embrittlement of metallic materials subject to hydrogen.

The **cryogenics & heat management discipline** targets to develop models and methods to predict performance of cryogenic tanks, including thermal and fluid modelling, fluid sloshing, boil-off, influence of tank design parameters on mission performance, experimentally validated solutions, integration of turbomachinery in the fuel systems, heat management including optimal use of liquid/supercritical hydrogen as a heat sink, heat exchanger design, thermal performance of tank designs, modelling of vacuum and foam filled tanks, fluid aspects of composite tank design, dynamic cryo-tank modelling integrated into vehicles.

Joint projects and recruitment
During 2022 two Ph.D. projects have been defined and two Ph.D. students have now also been recruited. In addition, Chalmers has supported the project by defining and the funding two post doc project as stated earlier in this section.

The two Ph.D. projects funded by the center are:

- PhD1: Composite technology for lightweight solutions of cryogenic/pressurized hydrogen tanks
- PhD2: Integration of lightweight solutions in complete aircraft and system evaluations

The PhD1 project was appointed in 2023-02-01 with Luis Fernando Gulfo Hernandez, a student with strong composite materials competence. In 2022-09-01, the PhD2 project was launched with Christian Svensson as PhD student. Christian is a former Chalmers student and has a background also in the Chalmers automotive formula student project.

In addition, the center funds efforts at RISE surveying and exploring a number of critical tank features for primarily road vehicle applications.

The research topics
Efficiency improvements and use of SAF promise to green the heavy transport sector. This is however generally not believed to be sufficient but other fuels and electrification is needed as a complement to SAF. Hydrogen is an attractive fuel, being enabled by the trend of ever decreasing production cost of green electricity observed over the last few decades. Back of the envelope calculations also show that the resulting energy density of the whole fuel system is substantially higher than battery-based concepts. This makes it a potential source of energy for heavy transport, for which battery based electrification may not be sufficient. Additionally, it may also prove to be substantially more energy efficient than going all the way to the use of electrofuels. This is particularly true if a substantial amount of energy is needed to capture CO_2 from the atmosphere.

To allow efficient use in vehicles compact and cost-effective storage is key. Several aspects related to enabling these aspects are explored in this multidisciplinary research area. The PhD1 project is targeting the development of efficient computation methods for thin-walled structures made from thin-ply composites.

Given the dimensions of the tanks (meters) and the wall thickness (millimeters) and thin-ply CFRP tape thickness (micrometers) multiscale methods are required. The work will build on conceptual studies at Chalmers performed in the project LH2-Tanks (Energy Agency 52439-1, 2021). Furthermore, the research will be conducted collaboratively, with a postdoc via the AoA Transport project "Vehicle On-board storage integrating liquid and compressed hydrogen tanks".

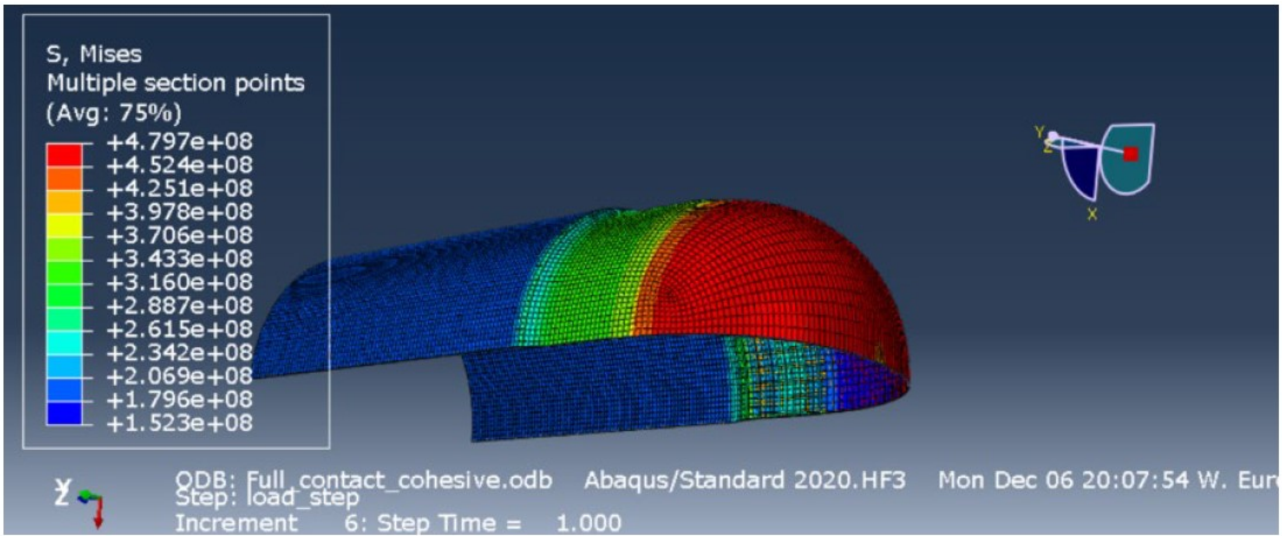

Figure 4: Stress analysis of a liner-less CFRP tank for liquid hydrogen storage, stresses in the overwrap. Results produced by Chalmers in the project LH2-Tanks.

The PhD1 project will develop mechanical design methods allowing conceptual designs studies planned in the PhD2 project. Linerless tanks show a great potential to become lighter than corresponding metal-lined concepts. Challenges are cost in large scale production, proving thermal cycling resilience, ways to avoid undetectable tank damage and proving that the tanks do not leak.

Several alternatives for on-board storage of hydrogen exist:

1. Pressurized hydrogen and fuel cell
2. Pressurized hydrogen and combustion
3. Cryogenic hydrogen and fuel cell
4. Cryogenic hydrogen and combustion

This project is focussing primarily on "4. Cryogenic hydrogen and combustion", but it will to some degree also evaluate option "1. Pressurized hydrogen and fuel cell" and "3. Cryogenic hydrogen and fuel cell". For the case "4. Cryogenic hydrogen and combustion" the focus will be placed on the conceptual design of the vehicle and the integration of the tank system / fuel system. For PhD2, the prime transport mode studied is aviation.

In addition to the four combinations above, the option of cryo-compressed tanks is a potential candidate. This concept allows increasing the power density further, but at the cost of a much higher weight than for the cryogenic option. This makes them a candidate for areas where the weight penalty is not too great but where the effect of increasing storage volume may increase profitability. Hence, primarily for heavy road transport but also for naval transport.

A conceptual design sketch of a previous study on cryogenic hydrogen for aviation is shown in Figure 5 [4].

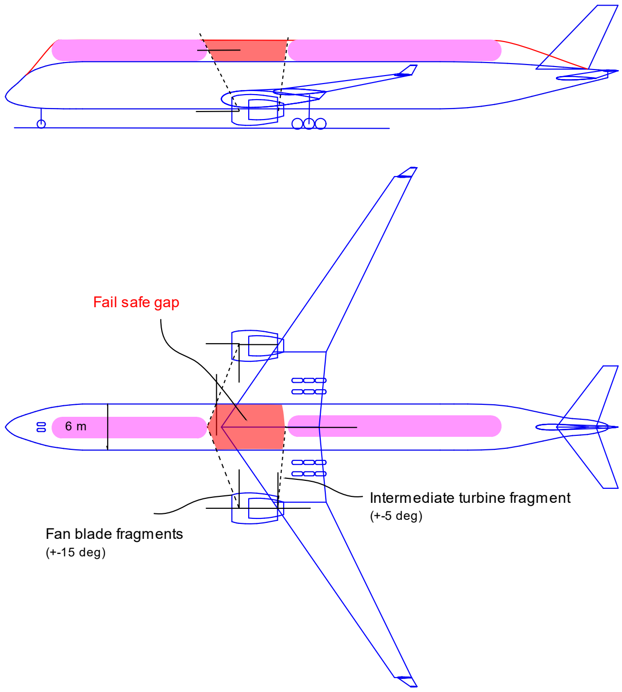

Figure 5: Conceptual design of hydrogen tank integration into tube-and-wing turbofan engine aircraft architecture [4]

An early step in the project has been to define which conceptual design tool to use for airframe tank integration. Initially it was planned to use the Pacelab software [5], but to increase flexibility and make sharing of models easier another software, SUAVE [6], has been chosen over Pacelab. This tool is open source and allows previous work on conceptual tank modelling to be integrated into the software. Aircraft models developed at Chalmers within the project NordicZero [7, 8] and EnableH2 [9] have been inherited.

Progress in relation to project goals

The projects aim to contribute to developing breakthrough ultra-low weight and low cost for hydrogen storage concepts. It is too early to quantify impact on cost and weight for pressurized and cryogenic concepts at this stage (R1a). The projects also aim to share design knowledge among Swedish industry partners (R1b), this task is also premature. At the end of the first five-year term the projects should also have contributed to make TechForH2 visible as an international hub for light weight research (R1c). In the medium term this is planned to be ramped up with the international research network activities. At the end of 2023 the aim is to achieve the milestone to have “design methods validated for pressurized and cryotanks” (Mile1).

To support innovation the project will deliver a better understanding of how the tanks are used in aviation service. This work is well underway with models currently able to predict time series of pressure and temperature development during use (as a function of tank design parameter assumptions). This should be the aim of a year 2023 publication (I1a). Evaluation of the TeXtreme composite technology for tank design is a little bit further down the road and may be delayed in relation to the delayed start of the different projects. It is still a key focus of the projects.

Current studies and publication plan

In 2022-08-15 Ioannis Katsivalis was recruited as post doc in the project “vehicle on-board storage integrating liquid and compressed hydrogen tanks”. So far work on two papers related to the performance of thin-ply composites is conducted. The first paper is entitled “Strength analysis and failure prediction of tow based thin discontinuous composites” and the second paper is entitled “Hydrogen diffusion for composite storage tanks”. The experimental work for the two papers is 80-90% completed and the writing is about 70% completed. The two papers are expected to be submitted in the next two months. There are also concrete plans to extend these studies which will lead to more publications.

In 2022-01-10 Alexandre Capitao Patrao was recruited as post doc in the project “Pathways for a sustainable introduction of hydrogen into the aviation sector”. Alexandre has a background in aerospace from Chalmers but was at the time of recruitment working as an engineer at GKN Aerospace. Alexandre is on leave of absence during the post doc. Here we plan to work on three publications during 2023, “The heat transfer potential of stator aero surfaces for a hydrogen fueled turbofan engines”, the “Aerodynamic optimization and system level impact of compact heat exchangers for intercooling and recuperation” and a “Techno-economic evaluation of hydrogen aircraft technologies”.

The PhD1 project was appointed in 2023-02-01 with Luis Fernando Gulfo Hernandez. In the first instance, the research will focus on developing more refined computational analysis methods for composite materials composed of ultra-thin discontinuous tapes. In 2022-09-01, the PhD2 project was launched with Christian Svensson as PhD student. Christian is a former Chalmers student and has a background also in the Chalmers automotive formula student project. We currently work on two publications, an analysis of a turboprop aircraft for the Nordic region and a paper on system evaluation of new tank liner concepts.

Project area 2: Additive manufacturing for hydrogen fuel supply systems

Industry stakeholders

This multidisciplinary area is configured by collaborating across manufacturing technology and cryogenics & heat management. Chalmers, Siemens energy, RISE and Volvo collaborated to define the content.

Basic disciplines

This research area focuses on the application of additive manufacturing to create tailored, optimized, and sustainable production solutions to implement hydrogen in energy, heat management, and transportation applications. Research challenges are to enable conversion of existing gas turbine solutions to hydrogen fuels, optimize post-AM (Additive Manufacturing) technologies to mitigate degradation by hydrogen, perform experimental validation and testing under realistic integrated conditions, incorporate additional aspects such as sensor technology into designs, develop models and treatments/methods to fight corrosion/oxidation and hydrogen embrittlement as well as electrical/thermal surface conductivity related problems. The long-term ambition is to develop and experimentally verify novel manufacturing and product solutions for hydrogen use, required for manufacturability in terms of materials, geometrical capabilities, and product performance.

Joint projects and recruitment

During 2022, two Ph.D. projects had been defined and two Ph.D. students were recruited. In addition, Chalmers has supported the project through Production AoA and Faculty funding. A postdoc project "Design for metal additive manufacturing" has been supported partly. Currently, this project area involves 3 men and 2 women, reaching a good gender balance.

The two Ph.D. projects funded by the center are:

- PhD1: Metal Additive Manufacturing for Hydrogen Fuel Supply Systems. Erika Tuneskog was appointed to work in PhD1 project on 2022-12-01. She graduated from Linköping University. She is a student with strong gas turbine engine background and AM competence.
- PhD2: Characterization and Post-treatment of Metal Component Produced by Additive Manufacturing for Hydrogen Application. Vishnu Anilkumar was appointed to work in the PhD2 project on the same day (2022-12-01). Vishnu is a former Chalmers Master student. He has a background of engineering materials and competence in AM.

Saeed Khademzadeh was recruited as a post doc. starting from 2022-10-01. He has a background in additive manufacturing and Material science. In addition, the center funds efforts at RISE for spray testing and numerical modelling of various liquid hydrogen carrier fuels in fuel nozzle.

The research topics

The PhD1 project is targeting additive manufacturing (AM) as a means for high-performance metallic parts in the section of gas turbine and fuel cell with possible extension to internal combustion engine (under discussion). The focuses are the design, manufacturing, postprocessing, spray behavior of the fuel and final implementation and demonstration of the metal parts that would benefit significantly from the design freedom of AM. The goal is to develop novel approaches to produce the fuel nozzle; to optimize AM-processes for intended metal parts; to establish process parameter and quality control; and to manufacture a prototype demonstrator. The cross-correlation between these goals and the joint efforts targeting high performance metallic parts comprises the core of the project involving a constellation with key industrial partners (Siemens Energy, Volvo) and core research providers in additive manufacturing, materials science and fluid dynamics (Chalmers and RISE). The results developed in the project will be useful for electricity generation, aviation and shipping/heavy road and rail.

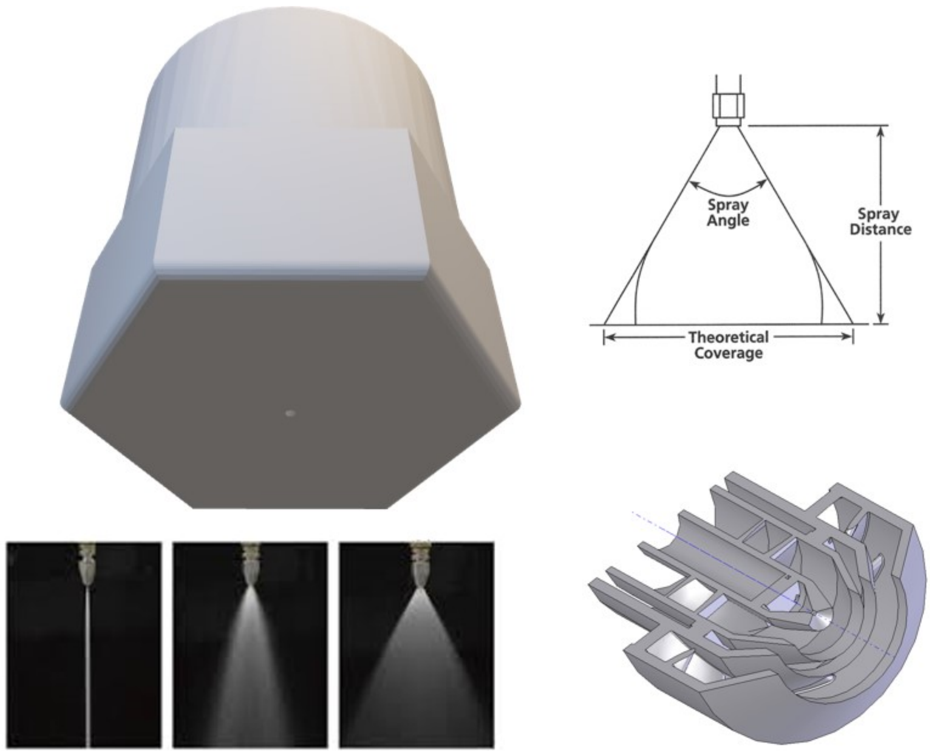

Figure 6: Hydrogen fuel nozzle and fuel spray

In PhD2 project, additive manufacturing (AM) is used as a means for high-performance metallic parts in the section of a gas turbine (possibly extended to the internal combustion engine) and fuel cell. The research focuses are **i)** Characterization of as-built and post processed components; ii) Environment impact which are relevant to the application condition of the metallic alloys, such as hydrogen embrittlement and oxidation/corrosion behaviour, iii) Surface engineering to improve material properties in hydrogen application. The goal is to gain improved understanding of material behaviour in hydrogen applications related to gas turbine and fuel cell usage; to establish efficient approaches for improving material properties in the conditions concerned; to build confidence to use additive manufacturing for high performance components that would benefit significantly from the design freedom of AM. Successful implementation of project results is expected to bring the TRL-level in these cases from TRL4 towards TRL6 for specific parts. The results developed in the project will be useful for electricity generation, aviation and shipping/heavy road and rail.

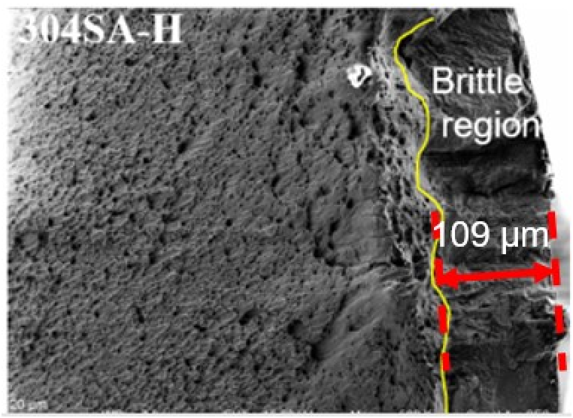

Figure 7: Brittle region formed due to hydrogen embrittlement

Activities since the start of TechForH2:

- Outlining a systematic literature review on issues associated with AM of spray nozzles including design concepts, nozzle performance, and surface integrity of internal complex channels made by AM.
- Systematic literature review on hydron embrittlement and material behavior when exposed to the hydrogen-related environment
- Design and additive manufacturing of a test model aiming at calibrating LPBF setup, printability assessment, and surface roughness investigation
- Evaluation of alternative AM processes
- Refining nozzle design for 1st test campaign at RISE in Piteå focusing on nozzle performance
- Setup of the test facility at RISE in Piteå has started, no exact timeline for when the test rig will be operational has been given but we estimate it will take between 3-6 months. The test setup will be calibrated by a 1st test campaign
- Production planning for the 1st test matrix is ongoing
- On-going characterization of samples exposed to ammonia
- Hydrogen embrittlement and corrosion resistance of 304 and 316L stainless steels
- The Chalmers funded post doc has so far mainly been involved in the activities commencing to work on the Siemens Energy AB use case, more specifically for the design and additive manufacturing of the spray nozzle

Progress in relation to project goals

The projects aim to manufacture nozzles that allows a gradual hydrogen introduction by additive manufacturing including postprocessing (R2a). Refining nozzle design and manufacturing planning is ongoing for the first test matrix. The first printing was performed. The roughness and outlet diameter were measured. Besides laser powder bed fusion, we also plan to use binder jetting for the production. It is too early to examine the effect at this stage. The project also aims for experimental validation of fuel nozzle at RISE in Piteå focusing on nozzle performance (R2b). Setup of the test facility has started, but this task is also premature. In the medium term, at the end of 2024, the first nozzle concept is supposed to be available (Miles 3). When the project is finalized, it should contribute to Swedish industry developing gas turbines usable for a range of future hydrogen scenarios (R2c). Another aim of the project is a more sustainable use of materials when using hydrogen as fuel for cleaner transportation in for instance fuel cell vehicles (R7a). As one type of commonly used material for bipolar plates, hydrogen embrittlement and corrosion resistance of 304 and 316L stainless steels have been tested. A better understanding of the material behavior has been obtained.

Current studies and publication plan

With respect to dissemination, four publications have already been planned for 2023 (D1). One of them has been drafted and it represents a collaboration between Chalmers, Bodycote Specialist Technologies GmbH, Germany, and Central South University, China (D3a). Two international conferences: i) TCT conference at Formnext 2023 (November 2023), and ii) ECHT – European Conference of Heat Treatment in Genova, Italy on 29-31 May 2023 have been planned (D2a). A presentation titled “Protection of austenitic stainless steel from hydrogen embrittlement by a surface engineering approach” was given in the 4th Swedish hydrogen seminar organized by Jernkontoret on 27th October 2022 (D7d).

List of planned publications for 2023:

- A review paper and presentation at a conference in the field: It is planned for the latter part of this year. The review paper will mainly look at the precision AM of metallic parts with internal channels. Planned to be finished in 6-8 months.
- A paper related to the first test campaign at RISE in Piteå. The objective will be to compare the spray performance depending on the additive manufacturing method. Paper is planned to be finished in 6-10 months depending on the rig and manufacturing.
- A paper related to the effects of cracked ammonia on the degradation of additively manufactured materials. The paper will focus on how the varying proportions of this gaseous atmosphere composed of

nitrogen and hydrogen impact the surface chemistry of a special grade of stainless steel and nickel superalloy widely used in gas turbines. The study is expected to be published in leading journals in the field of materials science.

- A paper titled "Effects of Low-Temperature Carburizing on the Corrosion and Mechanical Behaviour of AISI 304 Austenitic Stainless steel after Hydrogen Charging" has been drafted. It will present at ECHT – European Conference of Heat Treatment in Genova, Italy on 29-31 May 2023. The paper might be published in the journal La Metallurgia Italiana.

Project area 3: Nanoplasmonic hydrogen sensor maturation

Industry stakeholders
This multidisciplinary area is configured by collaborating with materials technology and strong collaboration with Insplorion AB. Via the ties to materials technology, a collaboration with Oxeon AB is actively being explored.

Basic disciplines
The plasmonic hydrogen sensors discipline is of critical importance for the entire hydrogen energy value chain from both a safety and process monitoring perspective. Examples are safety sensors that detect leaks at ultralow concentrations to enable timely and effective leak control and process monitoring sensors in the high humidity environment of electrolyzers or fuel cells.

Key research challenges that we address are to develop ultrafast response sensors in the sub-second range that can detect hydrogen concentrations in the low ppm/ppb range in air or in high pressure hydrogen environments, to develop stable sensor operation at widely varying relative humidity conditions, to facilitate long-term (years) stable sensor operation without significant deactivation/ageing/sensitivity loss, to provide reduced sensor cross-sensitivity to other molecular species.

Joint projects and recruitment
During 2022 one Ph.D. project have been defined and one Ph.D. student, has been recruited.

The Ph.D. project funded by the center is:

- PhD1: Plasmonic hydrogen sensors

The PhD1 project was appointed in 2022-09-01 with Athanasios Theodoridis, a student with strong nanoscience and nanotechnology background with a corresponding master from Chalmers, as well as hands-on experience with industry collaboration via his master thesis project.

As part of one main research direction of this PhD project, we have during the fall successfully published the first collaborative work with Prof. Andrea Baldi at VU Amsterdam on exploring surface lattice resonances to push the limit of detection of plasmonic hydrogen sensors to the parts-per-billion (ppb) concentration range in air [3]. Furthermore, we have initiated a collaboration with Prof. Bernard Dam and Asst Prof. Lars Banenberg at TU Delft with the goal to develop PdTa alloy-based plasmonic hydrogen sensors with unprecedented dynamic range. Finally, the PI of this project area, C.L., has been granted a Lise-Meitner Sweden-Israel collaboration grant by the Swedish Foundation for Strategic Research on the topic of humidity tolerant plasmonic hydrogen sensors. The main aim of this collaboration with Prof. Elad Gross and Asst. Prof. Tamar Stein at Hebrew University in Jerusalem is to generate fundamental understanding of the deactivation processes of hydrogen sensors in humid and otherwise challenging chemical environments on the basis of in situ IR and X-ray spectroscopies (Gross) and first-principles calculations (Stein). This collaboration with significantly boost this PhD project by generating fundamental understanding of the sensors it develops by shedding light on short- and long-term deactivation mechanism. These insights then will constitute the foundation for the rational mitigation of the found deactivation mechanisms.

The research topics
The need for accurate and rapid sensing techniques both for measuring hydrogen contents in process monitoring and for taking safety measures by leak detection is high in all modes of transport. However, to date, no hydrogen sensor technology exists that can meet all the hydrogen (safety) sensor performance targets defined by the US DoE, despite significant global R&D efforts. Hydrogen detection in complex chemical and/or humid conditions, as well as in the ultralow and high-pressure ranges constitute the toughest challenges here. This development is driven, among other, by the US DoE hydrogen sensor performance targets summarized in the Figure 8 below.

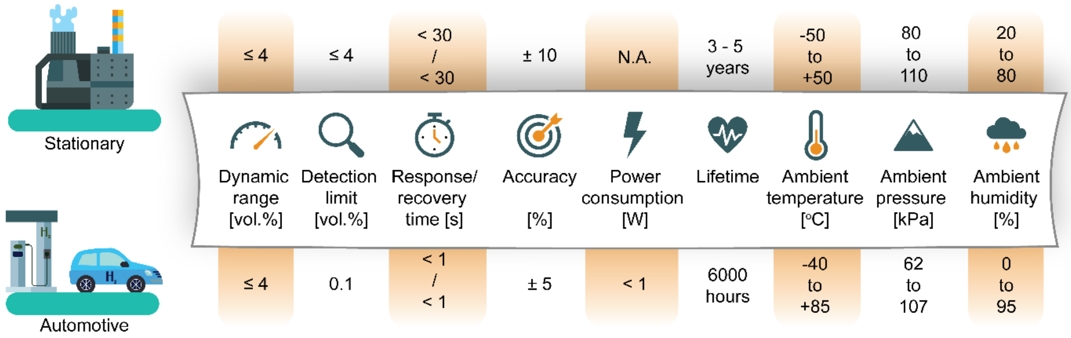

Figure 8: The DoE hydrogen safety sensor performance targets for stationary and mobile applications.

This PhD project is focusing primarily on developing nanoplasmonic hydrogen sensors that have the capability to operate in complex gas environments that, e.g., contain hydrocarbons, ammonia, O_2 and H_2O, by exploring a new generation of carbene-based H_2-transparent nanolayers to prevent competitive H_2O adsorption on and ageing of the plasmonic nanoparticles, and to spatially separate hydrogen dissociation from hydride formation and detection by developing catalytic adlayers based on Pt that will alleviate deactivation by water. Here, preliminary results generated in this PhD project and displayed in Figure 9 below show promising sensor response in up to 80 % RH when exploring the Pt-approach. The carbene-adlayers will be explored later during the project.

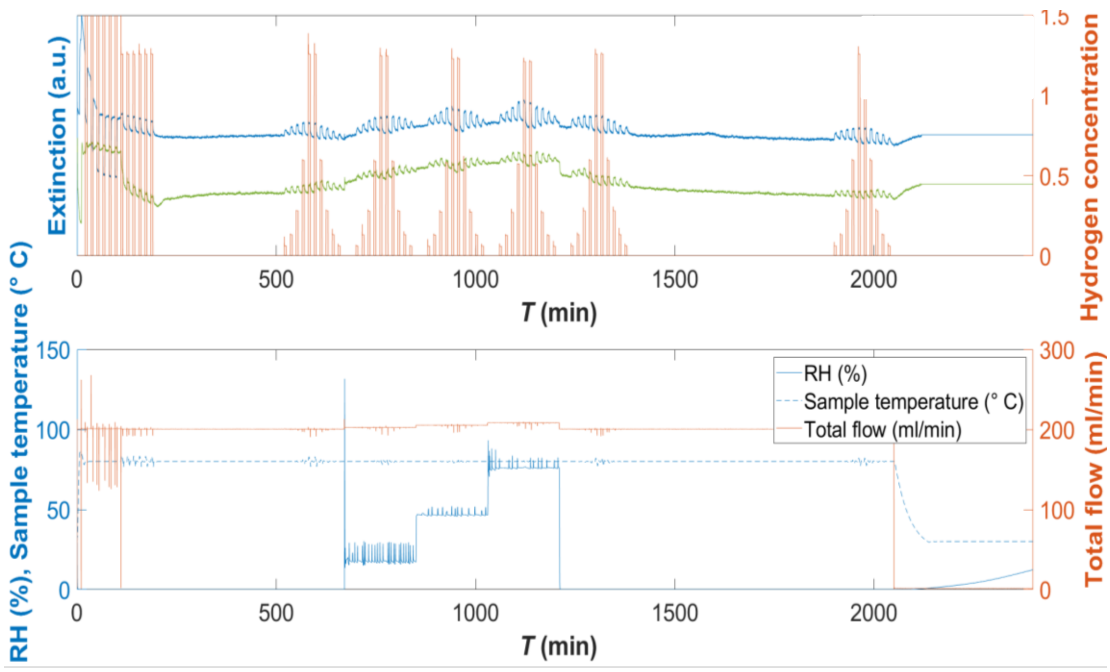

Figure 9: Preliminary results for a plasmonic hydrogen sensor with Pt co-catalyst operated in up to 80 %RH in air that demonstrates distinct response also at the highest humidity conditions.

As the second main aspect, this PhD project will focus on the development of sensors in the low (10-5 - 10-3 bar) pressure range, by implementing new nanoparticle array designs that, for example, explore surface lattice resonances to improve the limit of detection and develop protocols to implement SLR-based sensors based noble-metal and rare-earth metal alloy nanoparticles. Here, a first study we have executed together with collaborator prof. A. Baldi at VU has demonstrated that detection limits in the ppb range become available already when using pure Pd as sensing material (see Figure 10below from Nature Communications 2022, 13

(1), 5737). This is a very strong foundation to further explore this concept using better sensing materials, such as our own PdAu alloys or PdTa alloys developed together with our collaborators at TU Delft.

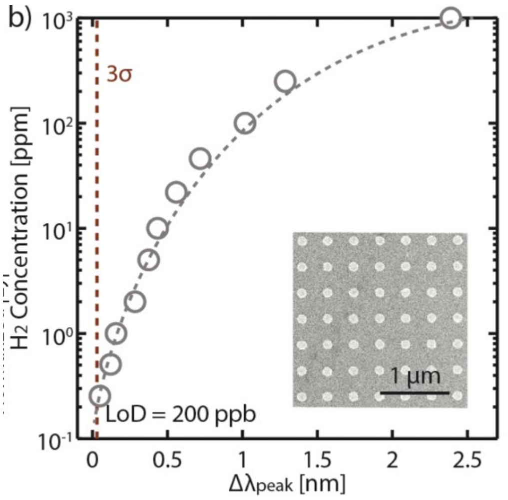

Figure 10: an SLR-based plasmonic hydrogen sensor with a limit of detection (LoD) of 200 ppb. Adopted from Nature Communications 2022, 13 (1), 5737

As further important aspect, the above main research efforts of this PhD project also tie into the Vinnova-funded project entitled “hAIdrogen sensors” that also is coordinated by the PI of this project area, C.L., and executed with Insplorion AB as industry partner. It explores deep learning methods for the treatment of data generated by plasmonic hydrogen sensors as an alternative and complementary means to materials engineering to improve limit of detection, response time and long-term stability. Here, we have recently demonstrated (see Figure 11 below) in a manuscript currently under peer-review that for a PdAu alloy plasmonic sensor a limit of detection of 200 ppm in highly humid air can be achieved (this exceeds the corresponding DoE target) and that the ISO 26142:2010 standard for sensor robustness can be met at 80 %RH. This an important breakthrough for the field that paves the way for further efforts in the direction of using machine learning techniques for the development of next generation hydrogen sensors.

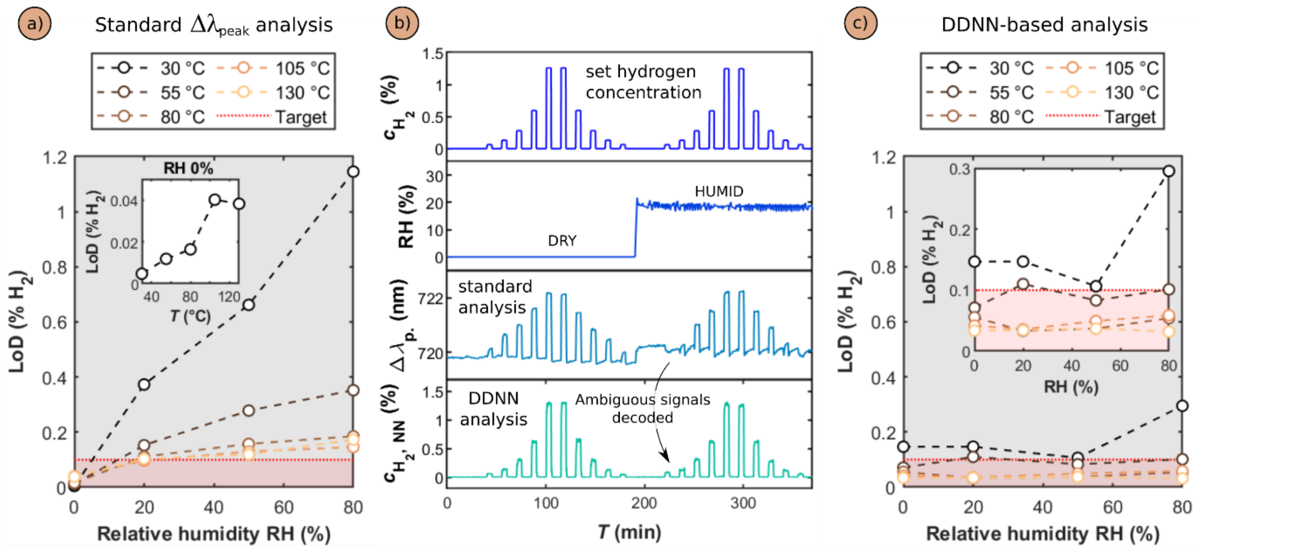

Figure 11: a) Sensor limit of detection (LoD) as obtained by the standard Δλpeak readout for different sensor operating temperatures and RH. Note that above 20% RH all sensors fall short on the US DoE target of LoD < 0.1% H2. b) Comparison of sensor response to c_{H_2} pulses at dry and 20% RH conditions at 80°C operating temperature, as obtained by the standard Δλpeak readout and the deep dense neural network (DDNN) architecture-based readout, $c_{H_2,NN}$. c) Sensor LoDs obtained by the DDNN architecture-based readout revealing that an essentially RH-independent LoD that lies significantly below the DoE target of 0.1% H2 is obtained for sensor operating temperatures of 80°C and above. Adopted from Tomecek et al., a manuscript currently under peer-review.

Progress in relation to project goals

This PhD project addresses the *research goals*:

- R6a. Develop ultrafast sensor response technology in the sub-second range at hydrogen concentration in the low ppm/ppb range in air and air-starved environments. (M36)
- R6b. Demonstrate reduced cross-sensitivity to other species present in the sensor environment. (M48)
- R6c. Survey and propose hydrogen sensor integration solutions for competing technology in collaboration with R1 (M60)
- Mile8. First ultrafast sensor concept demonstrated

This early in the project we have not jet completely fulfilled any of these goals. However, we have already made significant progress on R6a and R6b, as summarized above. Specifically, we have demonstrated a sensor that has set a new limit of detection record for optical hydrogen sensors (200 ppb in air) and we have (preliminarily) demonstrated that plasmonic hydrogen sensors can be made functional in high humidity environments using both a materials engineering strategy and deep learning-based sensor response treatment.

This PhD project also addresses the following *innovation goals*:

- I2b. operation in high humidity (M36)
- I2d. ultrawide dynamic range. (M60)
- I2e. explore the plasmonic hydrogen sensor technology for application in hydrogen energy related process monitoring. (M60)
- Mile11. Demonstration in high humidity. (M24)

Also here, this early in the project, no innovation goal has yet been completed in its entirety, but we have made significant progress in relation to I2b and thus also I2e, as summarizes above.

In terms of *dissemination*:

- we have published a first paper in collaboration with VU Amsterdam [3].
- this work is also the basis for a joint patent application, which is currently being discussed with TechForH2 industry partner Insplorion AB.
- This work is also the basis for international press releases by VU Amsterdam (https://vu.nl/en/news/2022/physicists-make-optical-hydrogen-sensor-with-record-sensitivity) and Chalmers (https://www.chalmers.se/aktuellt/nyheter/f-ultrakanslig-sensor-kan-minska-vatgasens-risker/), that have received a lot of national and international attention
- we have submitted a second manuscript entitled "A nanoplasmonic hydrogen sensor with 200 ppm limit of detection in highly humid air" that currently is under peer-review
- we have included some of these results in the master level course TIF120 "Surface and Nanophysics" for which C.L. is examiner.

Current studies and publication plan

The PhD1 project was appointed in 2022-09-01 with "Athanasios Theodoridis". He is currently investigating Pt-co-catalyzed hydrogen sensors for operation in highly humid air, developing PdTa alloy-based sensors with ultrahigh dynamic range in collaboration with the Bannenberg/Dam team at TU Delft and is investigating the impact of sulfur on the deactivation of plasmonic hydrogen sensors in collaboration with the group of Prof. Elad Gross at Hebrew University in Jersualem.

In terms of publications and publication plan:

- we have 2022 published *Nature Communications* **2022,** *13* (1), 5737 [3]
- and have Tomecek et al. "A nanoplasmonic hydrogen sensor with 200 ppm limit of detection in highly humid air" in peer review.
- for the upcoming year, we plan to submit

- (i) a paper on the topic of the impact of sulphur species on the deactivation of plasmonic hydrogen sensors in collaboration with the group of Elad Gross in Israel,
- (ii) a paper on the topic of Pt-co-catalyst for plasmonic hydrogen sensor operation in high humidity environments and
- (iii) a paper on the topic of PdTa alloy plasmonic hydrogen sensors with ultrawide dynamic range in collaboration with the Dam/Bannenberg team at TU Delft.

Project area 4: Fuel cell development and integration

Industry stakeholders

This multidisciplinary area combines low-level understanding of fuel cell materials, fuel cell stack modeling and validation testing, and powertrain system modeling to enable comparison of component sizing choices, control strategies, and optimal operating conditions for proton exchange membrane fuel cell (PEMFC) hybrid powertrains. The methods developed focus primarily on heavy road transport, but the results and model framework should be adaptable for use also for shipping/rail and aviation applications Initially Chalmers, Volvo AB, Volvo Penta, and Scania collaborated to define the content. As the work has progressed increased interest from Johnson Matthey and PowerCell has also been noted.

Basic disciplines

The development of fuel cell systems that can operate at the scales and power densities required for vehicle powertrains requires linking the understanding of ion transport, gas-exchange, electrochemical and catalytic action at the cell level to the fuel cell stack response in the context of the power demands of the vehicle. This calls for a combined approach integrating input from low-level physics and thermodynamic and electrochemical system modeling to address FC stack level challenges, such as how alternate cooling or humidity profiles will impact stack power and longevity and how time-dependent stack temperature and relative humidity will modulate heat production, cell impedance and losses, as well as durability/degradation of the membrane and catalyst structures.

Key research challenges are to develop proton exchange membrane fuel cells (PEMFCs) solutions that radically reduce the use or entirely remove the use of scarce noble metals, as well as to develop novel PEMFCs that can substitute perfluorinated polymers, like Nafion, which are costly to produce and difficult to recycle. A correlated aspect is the need for finding non-volatile proton conducting electrolytes alternative to acidic water, able to operate at intermediate temperatures (80 – 200 °C) and thus enable the use of cheaper and more abundant catalysts.

The detailed PEMFC cell-level and stack-level understanding in turn must be integrated with a system model for fuel-cell hybrid electric powertrains in order to address the tradeoffs and performance of specific hardware choices and the energy balance of a powertrain for relevant vehicle operating conditions and power demand. The long-term research ambition is to develop models to optimize and experimentally validate the impact of design choices and predict top-level vehicle performance for hydrogen propelled vehicles and to develop low cost, durable fuel cell stacks with a high degree of sustainability.

Joint projects and recruitment

During 2022 two Ph.D. projects have been defined and two Ph.D. students have been recruited. In addition, Chalmers has supported the project by defining and funding the postdoctoral research project Systematic control of PEM fuel cells for vehicle applications.

The two Ph.D. projects funded by the center are:

- PhD1: PEMFC time-response and lifetime analysis
- PhD2: PEMFC temperature management for high performance

The PhD1 project has provisionally accepted Mina Bahraminasab for the position. Her work-visa application is still being evaluated by Migrationsverket, so her start date has been postponed to 2023-03-01. Mina is a graduate of AL-Zahra University, Iran with a strong background in mechanical engineering and experience with biological fuel cells.

The PhD2 project was launched on 2022-10-10, the with Christian Bosser appointed to the position. Christian is a graduate of RWTH Aachen, Germany with a specialization in propulsion technology. He has experience in powertrain modeling and experience with fuel cells from his Erasmus work at Aalto University, Finland.

The research topics

Polymer electrolyte membrane fuel cells (PEMFC) are currently the most promising fuel cell design for flexible, robust, and cost-effective use of hydrogen fuel for transport applications. PEMFCs operate at low temperatures which ease handling and enable reasonable system response times, as well as idling, and cold-start which are comparable to conventional ICE vehicle capabilities. In addition, PEMFCs produce only water and excess heat under normal operation and directly generate electrical power which can yield peak efficiencies in excess of 60%. While this efficiency and emissions profile is highly favorable, a number of challenges remain in order to compete with conventional heavy-duty powertrains, especially with regard to durability which factors heavily in vehicle total cost of ownership.

The current state of PEMFC stack durability and lifetime for automotive powertrains varies widely by application, with assessments ranging from 1200 to 12000 hours. Figure 12 shows the disparity of estimated run-time durability reported (A) or predicted (B, C, D) by experts elicited from academia, government, and industry, with a median reported value at roughly 4000 hours.

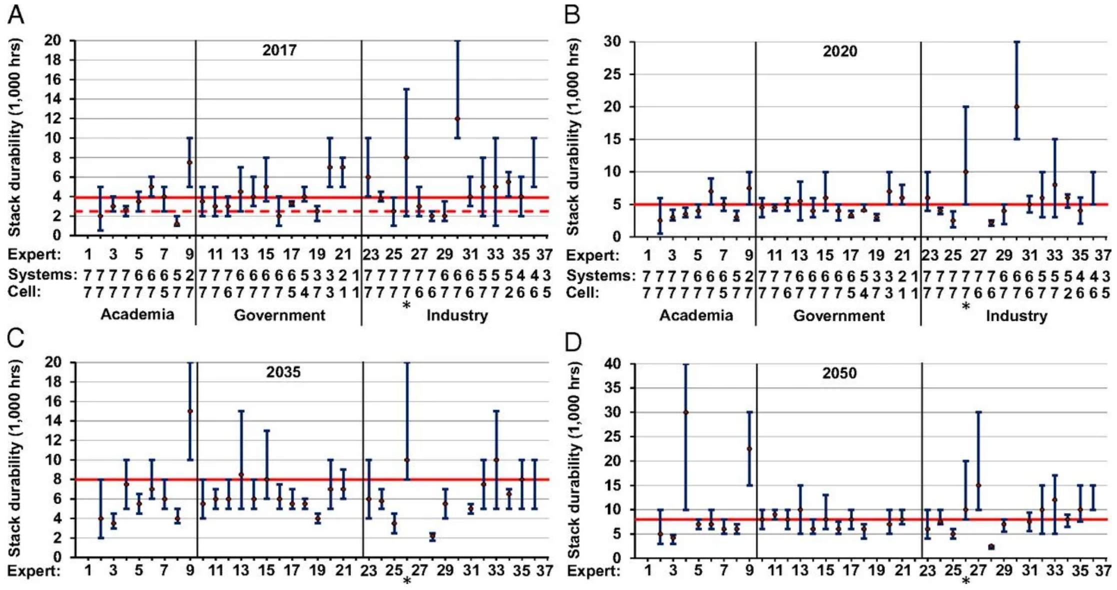

Figure 12: Assessment of PEMFC stack durability (A) 2017 values. (B) 2020 values. (C) 2035 estimate. (D) 2050 estimates. The solid lines represent DOE targets for stack durability. Courtesy of PNAS 2019, 116(11) 4899-4904.

It is clear that transients can severely impact the useful lifetime of PEMFC systems. In general, unsteady conditions promote imbalances in the chemistry, temperature, pressure, and humidity control which lead to small scale changes in the fuel cells which gradually contribute to performance degradation.
A large body of individual mechanisms which can lead to degradation in fuel cells are covered in the literature, especially reactions and physical changes which reduce electro-catalyst surface area. However, the combined MEA disturbances distributed throughout the stack which interfere with the system performance over time often depend strongly on historical as well as present conditions. This complicates lifetime prediction of fuel cells and limits the utility of physical-model based prediction methods, while data-driven (or hybrid) approaches which can be tailored more specifically to the stack hardware appear to be a promising way forward.

The PhD1 project is targeted to link the understanding of the causes and relative importance of degradation mechanisms in the membrane electrode assembly (MEA) to a vehicle configuration and control strategies which balance the need for agile stack response and durability. Empirical data from fuel cell testing will be used to develop a data-based stack model which will track probable deterioration and provide state-of-health information which can inform control of the vehicle. This model can then be applied to adjust the vehicle control strategy based on current state-of-health to further increase the lifetime of the stack. The start date for this project has been changed to 2023-03-01, to allow extra time in the work-visa application to Migrationsverket.

The fragility of the perfluorinated polymer membranes used in PEM fuel cells is a significant drawback that contributes to the cost and reduced durability of PEMFC powertrains. Alternative fuel cell arrangements that replace the membrane with an ionic liquid offer huge opportunities for improving lifetime and reducing cost. An upcoming PhD project, led by Anna Martinelli is planned to explore this approach. On a systemic level, the focus will be fuel cell stack design and optimization, including scaling aspects to larger fuel cell systems, maximizing power density, detection of poisoning agents, and close control of fuel and oxidant flows.

For now, stacks based on PEMFCs remain the most compelling choice for long-haul and regional transport, where the diminishing returns of increasing battery capacity severely impact the operational range, time in service, and payload capacity of battery electric powertrains. Fuel cell power systems based on PEMFCs rely on thin solid-state electrolytes for ion transport and their effective operating range is constrained to lower temperatures to maintain the water balance in the membrane. The heat generation and relatively strict temperature requirements of PEMFCs present difficulties for efficient thermal management,[1] but also some opportunities to repurpose waste heat for battery management and auxiliary use with a comprehensive temperature control strategy.

High-load operation of a PEMFC stack presents a number of challenges in balancing the heat dissipation and contrasting water management demands on the anode and cathode sides of the MEA unit cells, especially under more extreme environmental conditions. The power of the fuel cell stack for vehicle applications must be matched by the heat rejection capability of the powertrain. Here, the changes in power demand, time-varying stack response, and external temperature variation result in complex interactions that require adaptive control.

The PhD2 project targets development of a system model that combines the mass flow and heat dissipation of an active cooling system to the temperature dependent behavior of the PEMFC electrochemistry and heat transfer within a physics-based stack model. This approach is intended to enable closer, faster heat control which can drive efficiency savings in some conditions, but also allow for better performance and a wider performance envelope for a given PEMFC system.

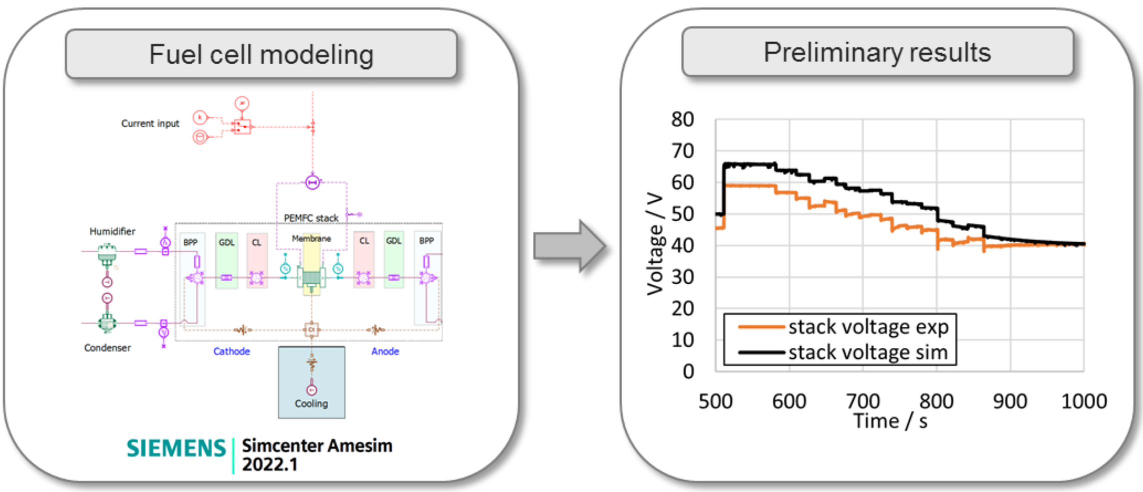

Figure 13: Preliminary model results, together with PEMFC experimental data (5 kW short stack).

[1] Kandlikar, et al., Thermal management issues in PEMFC stack – a brief review of current status, *Applied Thermal Engineering*, **29** (7), 1276-1280, 2009.

A preliminary model with an idealized cooling setup has been implemented in Simcenter Amesim. Figure 13 shows a view of the PEMFC membrane electrode assembly from the simulation setup and a comparison of model results targeting a 5 kW test bench stack and experimental results measured from the 5 kW PEMFC stack.

Progress in relation to project goals

The projects aim to contribute to developing design methods for hydrogen driveline integration in powertrains relevant to road, air, and sea vehicles (R4a). Here, progress has been made in implementing simplified PEMFC stack models, including a Matlab/Simulink model with idealized cooling and boundary conditions, and a Simcenter Amesim model with a simple cooling loop.

A further aim is to develop quantitative models for usage vs. durability (R4b). This will be addressed in the PhD1 project which is slated to begin 2023-03-01.

An important project aim is to demonstrate next generation fuel cell concepts (R7c and R4c). This should be addressed in the future fuel cell work led by Anna Martinelli and informed by PEMFC system modeling results from more advanced system models developed in year two or three of the PhD1 and PhD2 projects.

Another aim is to demonstrate concepts for more sustainable use of materials on the stack level (R7a, R7b and R4c). This goal requires the expansion of the fuel cell testing capabilities leveraged by TechForH2 at Chalmers. Design of the test-bench hardware is underway, with plans for installation of the implemented design in the Nov/Dec. 2023. This aim also served by the upcoming work led by Anna Martinelli.

With respect to dissemination two conference contributions and one journal paper is underway for 2023. The projects are slightly behind due to delayed starts. Notice that the Ph.D. projects have run 6 months in total at the time of writing (plan for first year was 24 months).

With regard to teaching impact (D6), both David Sedarsky and Anna Martinelli have contributed with invited lectures in a Chalmers course: TRA105, Fuel Cell Systems.

Current studies and publication plan

In 2022-08-01, Ahmed Zoukit was recruited as post doc in the project "Systematic control of PEM fuel cells for vehicle applications". Ahmed has a background in electrical engineering from Cadi Ayyad University, Morocco and experience with PEM fuel cell systems working at PSL University, France.
So far work on one papers has been conducted, "Takagi-Sugeno fuzzy approach for PEM fuel cell system modeling", and presentation of a related work at the conference, European Fuel Cell Forum (Lucerne, Switzerland) is planned for July 2023.

The PhD2 project was launched on 2022-10-10, the with Christian Bosser appointed to the position. Initial work in the project is focused on implementing and validating a simplified PEMFC stack model. A conference presentation at the Thermal and Fluids Engineering Conference (Maryland, USA) is planned for March 2023.

Project area 5: The future of hydrogen – societal challenges

Industry stakeholders

This multidisciplinary research area is assessing the role of future hydrogen in society from a systems perspective. Volvo, Scania, Siemens Energy, PowerCell, GKN Aerospace, Johnson Matthey and Stena Rederi have all been involved in the initial phase of formulation this project and more intense collaboration be initialized during 2023.

Basic disciplines

The energy and environmental systems analysis discipline evaluates the role of different energy carriers in the energy system based on energy systems modelling and environmental systems analysis. Hydrogen can play an important role in a future sustainable low-carbon energy system. However, there are challenges to overcome during the transition period from today until used in large scale. Key factors are the amount of excess electricity, availability of infrastructure, capital cost of fuel cells and electrolysers, the lower round-trip efficiency compared to direct electrification, geopolitical and limitation risks connected to the use of scare metals, the relatively costly hydrogen distribution and storage and issues related to consumers' preferences. The role of hydrogen in the transport sector is in focus, but other parts of the energy system are also considered.

Key research challenges connected to the role of hydrogen in a future sustainable low-carbon energy system are to detect and model potential show-stoppers from for instance resource limitations, cost-competitiveness, environmental performance, social acceptance, synergies and competition with other energy sectors, the supply potential, localization and hydrogen infrastructure and storage demand, interlink transport hydrogen and future systems scenarios, predict and optimize policy and regulations of transport and society in general.

Joint projects and recruitments

During 2022 one Ph.D. project has been defined and one Ph.D. students has now been recruited and will start 1st of March, 2023. In addition, Chalmers has supported the project by two postdoc projects Hydrogen in transport – Global, European, and Nordic perspectives (Chalmers AoA Transport) and Systems assessment of hydrogen and electrofuels in transports (Chalmers Genie). The two postdocs are also engaged in the community of the competence center on catalysis (KCK).

The Ph.D. project funded by the center is:

- PhD1: The future of hydrogen – societal challenges.

The PhD1 project has recruited PhD student Joel Löfving, a former Chalmers student with strong knowledge in environmental systems assessment and modelling. Joel will start 2023-03-01. In addition to the centre funds this project will collaborate with Energiforsk's hydrogen program (Vätgasens roll i energi- och klimat-omställningen (VREK)) to increase knowledge transfer about the role of hydrogen in the energy system. The collaboration will first and foremost occur within an associated 3-year project funded by the Swedish Energy Agency with the long Swedish title: "Vätgasens samlade påverkan på elsystemet och dess roll i energi- och klimatomställningen: En system- och syntesstudie om vätgas och elektrobränslens roll i framtidens sektorkopplade energisystem". Project leader: Maria Grahn. Another project with close links is the Nordic roadmap for sustainable fuels for shipping (https://futurefuelsnordic.com/). It is a Nordic collaboration project centered around the establishment of a Nordic Cooperation platform to facilitate knowledge sharing, alongside the launch of pilot projects and studies that will build experience in new fuels, to establish "green corridors" and the enabling infrastructure, hydrogen is among the fuels investigated. Project leader at Chalmers: Selma Brynolf.

Developing a transnational network of hydrogen refuelling stations for trucks (HyTruck) is an EU Interreg (Baltic Sea Region) project coordinated from Germany. In WP1, GoA 1.2, Chalmers will lead the work on techno-economic assessments, energy economic modelling and life cycle environmental impact aiming to shed some light to questions as: Where does hydrogen come from? What is the environmental impact depending on the distance from the place of production to the point of refuelling, and for different outlines of hydrogen refuelling stations for trucks, e.g., compare 300 bar, 700 bar, or liquified H2? Under what circumstances (battery price, fuel cell price, hydrogen storage costs, fuel station cost, electrolyser cost, efficiencies, capacity factors etc) do the model show that hydrogen plays a dominating role in the fuel mix for trucks? WP1 leader: Maria Grahn.

The research topics

The first phase of the PhD project *"The future of hydrogen – societal challenges"* (starting 1 March 2023) includes the development of a model for hydrogen production and distribution infrastructure in Europe based on demand scenarios for shipping, aviation, road transport and industry. The model will consider centralized and decentralized production in Europe as well as in other locations outside Europe with potentially even lower cost of producing renewable electricity, hydrogen and electrofuels, however with higher cost for fuel distribution.

The European model to be developed (H2-Infra) for hydrogen production and distribution infrastructure will consider different future hydrogen demand scenarios at NUTS 2[1] regions level. The model will consider cost, efficiency, small scale versus large scale hydrogen production, amount, and scale of tank stations/bunker terminals etc. as seen in Figure 14. Results from this model will be used to analyze cost-effective implementation of hydrogen in Europe. In addition to this it will also be used as input data to existing models such as the Global Energy Transition (GET) model and the European energy systems model ELIN EPOD for example in collaboration with the postdoc project "Hydrogen in transport – Global, European, and Nordic perspectives".

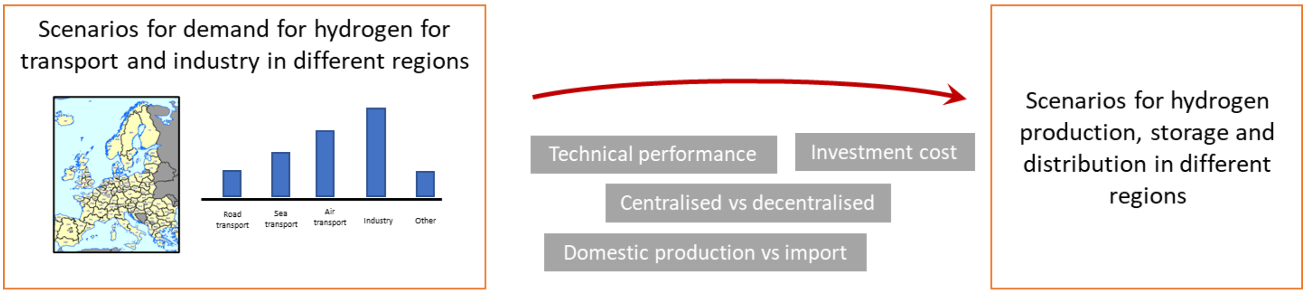

Figure 14: Overview of the main features that the European model to be developed (H2-Infra) will consider.

The two postdocs*, Jorge Velandia and Hadi Farabi,* started their work in early autumn 2022 and below are summaries of their ongoing work:

Postdoc: Jorge Velandia
Project: Hydrogen in transport – Global, European, and Nordic perspectives
Funder: Chalmers Area of Advance Transport (Competence center TechForH2), and Swedish Energy Agency (FFI) project No 51458-1 "Reducering av emissioner från vätgasmotorer (HEER)
Partners: Chalmers University of Technology, Volvo Technology AB, Scania, Johnson Matthey

Project summary and status: The aim of this project is to quantify the environmental burden of using green and blue hydrogen in fuel-cell trucks (FCT) and on internal combustion engine trucks (ICET) via life cycle assessment (LCA). Moreover, as transport and distribution of hydrogen is expected to represent a significant share of the environmental burden, we evaluate both centralized and on-site production of hydrogen. The production on-site eliminates the need for transport of hydrogen. In contrast, on-site production is not able to take advantage of improvements related to large-scale production. In terms of data collection and computing time, it is usual practice to use LCA databases to model the so-called background processes. In opposition, the foreground processes are those in which the decision-maker has influence. As an example, Figure 15 depicts the boundaries of the centralized production case.

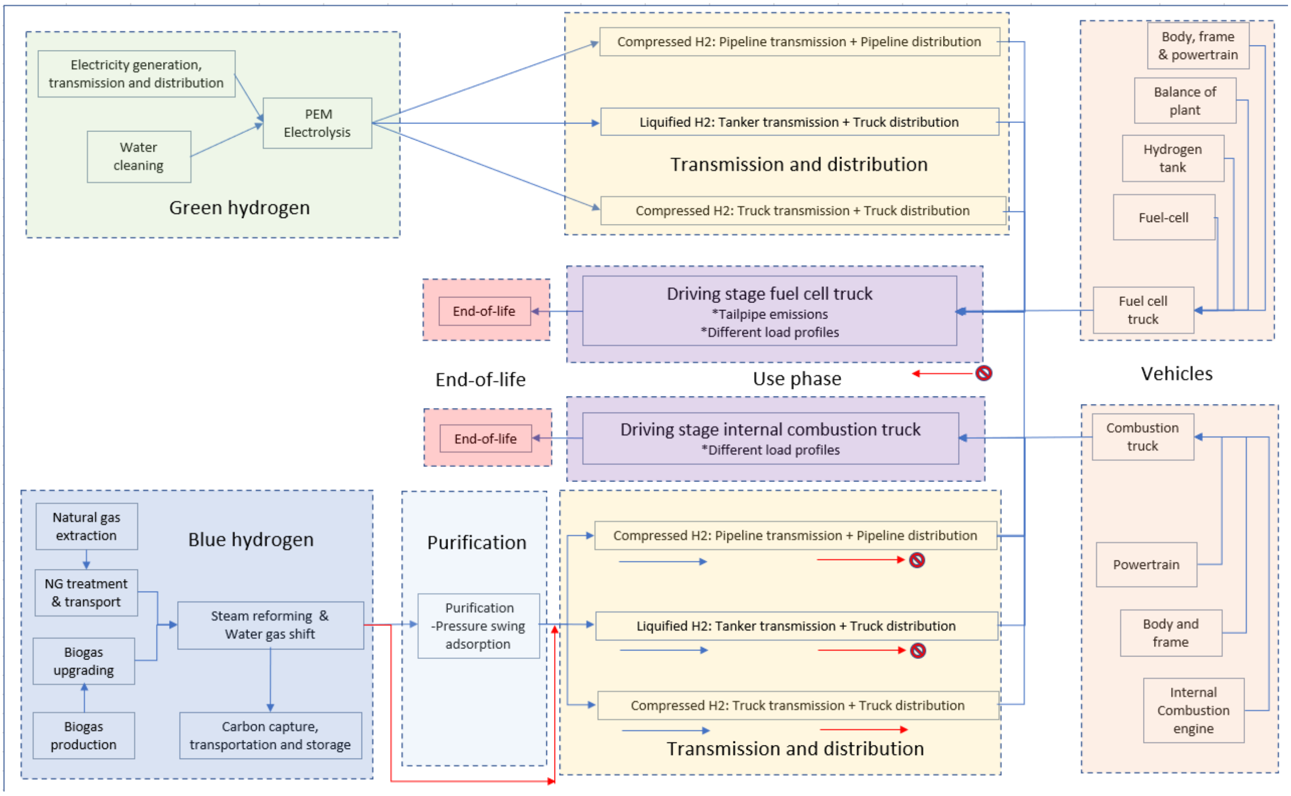

Figure 15: System boundaries hydrogen production on a central plant.

As of February 2023, we have managed to complete the initial literature review which provided raw data for the initial modelling in the software OpenLCA. The construction of the environmental model for the hydrogen production, both green and blue, has been completed and the initial results are in validation process. At the same time, we are advancing in discussions with stakeholders to construct a more realistic approach on the transmission and distribution of hydrogen and the features of the FCTs and ICETs. The partnerships allow us to obtain more accurate data, improving our model and decreasing uncertainties.

Postdoc: Hadi Farabi
Project: Systems assessment of hydrogen and electrofuels in transports.
Funder: Chalmers Genie.
Partners: Chalmers University of Technology, and IVL Svenska Miljöinstitutet AB (more to join)

Project summary and status: The aim of this project is to assess the suitability of different global policy instruments for reducing greenhouse gas emissions from shipping and their potential impact on cost-effective fuels and propulsion choices up to 2050. A literature review of various policy instruments potentially possible for the shipping sector has been carried out. In a next step, we assessed a selection of policy instruments considered interesting for the global shipping sector using global energy systems modeling. We have analyzed the impact of the selected policies on carbon budget, carbon prices, and cost-effective fuel and propulsion technology using the global energy transition (GET) model. GET is a cost-minimizing “bottom-up” systems engineering model of the global energy system set up as a linear programming problem in time steps of 10 years to minimize the discounted total energy system cost for the period under study while meeting both a specified energy demand and a carbon constraint.

Preliminary results for the ten different policy cases assessed are, e.g., that comparing Cases A (a global emission trading system covering several sectors without specific targets for shipping) and D (a moderate global marine carbon levy) shows that applying a carbon levy facilitates the introduction of hydrogen and earlier phase-out of heavy fuel oil. In 2050, the contribution of hydrogen in meeting shipping energy demand is 4% in Case A and 35% in Case D. A higher carbon levy (Case E) results in 65% hydrogen in the global fuel mix by 2050. Applying the marine ETS policy (Case B) resulted in meeting 55% of shipping energy demand by hydrogen by 2050. Implementing the fuel quota limitation (Case H) changes this value to 21% and also the share of bio- and electrofuels increased.

The main insights so far include that for all scenarios analysed, the increase in total system cost (for the whole energy system, not just the shipping sector) is in the range of 0.4%-0.8%.

Progress in relation to project goals

This project area 5: The future of hydrogen – societal challenges (initiated within the centers research discipline Transport and Society) have two main research goals: R5a. Develop comparative cost and sustainability methods for hydrogen use scenarios and its relation to transport and hydrogen society as a whole, and R5b. Interlink market needs and support innovation owners by surveying and trending technology usage in different hydrogen use fields. The work towards R5a will start first of March, 2023, and R5b will be continuously worked on throughout the project. The milestone Mile6 with a first scenario defined by M12 is expected to be somewhat delayed due to the delayed start of the PhD student. This project has no specific innovation goal, but the knowledge and insights generated from the project will support the industry including small and medium enterprises when taking decision about areas of innovation to focus on.

The project aims to contribute to all of the dissemination goals, what was accomplished during 2022 can be seen in italic, below:

• D1a. The aim is to publish one paper per year in the project "The future of hydrogen – societal challenges". Additionally, we aim to publish about 10 collaborative papers during the five years of the project. In connection to the research collaboration network first and foremost together with the identified research group at Aalborg University. *See publication plan below.*

• D2a. Attend the centre's annual conference presenting results from the project. Project leader will further help out in organizing the conference including invite speakers. *Not applicable for 2022.*

• D2b. Arrange at least one workshop at an industrial partner of the centre to ensure interaction across TechForH2. *No such workshop was arranged during 2022* for this multidisciplinary research area.

• D3a. Co-publishing with the research collaboration network. Yes, two hydrogen-related papers were published in collaboration with Aalborg university during 2022, [10, 11],

Grahn M, Malmgren E, Korberg AD, Taljegard M, Anderson JE, Brynolf S, Hansson J, Skov IR, Wallington TJ (2022). Review of electrofuel feasibility - Cost and environmental impact. Progress in Energy 4 (3), 032010. doi.org/10.1088/2516-1083/ac7937

Brynolf S, Hansson J, Anderson JE, Skov IR, Wallington TJ, Grahn M, Korberg AD, Malmgren E, Taljegård M (2022). Review of electrofuel feasibility - Prospects for road, ocean, and air transport. Progress in Energy, 4 (4), 042007.

• D3b. Develop a visiting researchers' strategy through the international research collaboration network, where recruited Ph.D. student is encouraged to spend time at relevant international university. At least one postdoc, with a non-Swedish citizenship, will be connected to the project. *Not applicable for 2022.*

• D4a. Contribute to at least 2 invited/panel talks *(1) Maria Grahn was invited as key-note speaker and panelist at Port of Ystad conference: "The goal is delivering sustainable fossil free transports". She presented the TechForH2 center and hydrogen related research results (2022-10-05). (2) Maria Grahn was invited as plenary speaker at the International Workshop of the BEST project in Brussels. She presented the TechForH2 center and hydrogen related research results (2022-09-09) (3) Selma Brynolf was invited as a panelist at "SamspEL Arena: Framtidens elbehov.". She presented the TechForH2 center and hydrogen related research at Chalmers (2022-12-08).*

• D5a. Meet experts at the Swedish transport administration, as well as the Swedish Energy Agency, to discuss the future of hydrogen in Sweden. *No such meeting was arranged by this multidisciplinary research area during 2022.*

• D6a. Through the technology and innovation advisory group arrange at least 1 hydrogen related invited lecture at Chalmers courses. *No such lecture was arranged by this multidisciplinary research area during 2022.*

• D6b. Disseminate new knowledge through existing and new courses, e.g., the courses "TRA105: Fuel cell systems", "TEK: Sustainable transport", "SJO851: Towards Sustainable Shipping", and "MVKF25: Hydrogen, Batteries and Fuel Cells (in Lund)" *Maria Grahn and Selma Brynolf presented the aim of the TechForH2 center at all mentioned Chalmers' courses listed above.*

• D7a. Disseminate research results and other relevant news from the project through Chalmers different media platforms, e.g., the newsletters of Area of Advance Energy and Area of Advance Transport. *Not during 2022.*

• D7b. Use the Chalmers Area of Advance as well as the linked-in platform to spread and discuss center activities such as recruitment and dissemination events. *The recruitment announcement was spread through Area of Advance Energy's newsletter. A joint linked-in-post collecting five simultaneous applications was performed.*

• D7c. Publish at least 2 times in newspapers and/or popular science forums to increase public interest for project results and TechForH2 activities. Involved researchers in the project will at least 3 times speak about research results in local and/or national radio, as well as while being guest in different podcasts. *Maria Grahn was co-authoring a debate article, published in Göteborgsposten 2022-10-18 "Reduktionsplikten måste utvecklas – inte försämras" https://www.gp.se/debatt/reduktionsplikten-m%C3%A5ste-utvecklas-inte-f%C3%B6rs%C3%A4mras-1.82975045*

• D7d. Involved researchers in the project will carry out at least 20 presentations at industry and/or society presenting the center and discussing project results. *(1) Maria Grahn was giving a speech at the maritime industrial network day arranged by Svensk Sjöfart in Helsinki, Finland. She presented the TechForH2 center and hydrogen related research results focusing on hydrogen as a marine fuel (2022-09-01), (2) Maria Grahn was giving a speech at a meeting with Stena Teknik. She presented an overview of research topics carried out at Chalmers Team Brynolf& Grahn including the TechForH2 center (2022-12-12), (3) Maria Grahn was giving a speech at the industrial network day "f3 Innovationskluster för hållbara biodrivmedel", in Lund. She presented the TechForH2 center and hydrogen related research results (2023-02-01). (4) Selma Brynolf was invited to Johnson Matthey to present hydrogen research and the TechForH2 center (220908). (5) Maria Grahn and Selma Brynolf was invited to Volvo Penta to discuss Future fuels and energy carriers. The TechForH2 center and the potential role of hydrogen in shipping was discussed (220902)*

• D8a. Launch and examine 1 Ph.D. student within this project. *Not applicable for 2022.*

• D8b. One licentiate thesis defense. *Not applicable for 2022.*

• D8c. Develop common activities and arrange seminars for the postdocs involved in all the centre's suggested projects. *No such seminar was arranged during 2022.*

• D9a. Senior researchers involved in this project will constantly contribute to the discussions on how to involve potential new partners to TechForH2. *Yes, three potential new partners have presented themselves at board meetings.*

Current studies and publication plan

During 2022 work on the following publications connected to the centre was initiated and submission during 2023 is planned.

- A paper on hydrogen area-efficiency: Winther-Mortensen A, Dalgas-Rasmussen K, Grahn M (20xx). How replacing fossil fuels with electrofuels could influence the demand for renewable energy and land area. Submitted to the Journal Smart Energy in Dec 2022, revised manuscript to be submitted latest 2023-03-03.
- LCA of multiple ways of producing and distributing hydrogen used in trucks (Velandia et al, Brynolf and Grahn co-authors),
- "Global policy instruments for a fossil free shipping sector and potential impacts on cost-effective fuel choices." This paper assesses the effect on fuel mix for the marine sector depending on different

CO_2 reduction policies, hydrogen is one of the alternatives in the fuel mix (Farabi et al, Brynolf co-author).
- “How do variations in ship operation impact the techno-economic feasibility and life cycle environmental performance of fossil-free fuels? a life cycle study”. The article evaluates among other things costs and environmental aspects from using either compressed or liquid hydrogen as fuel for shipping, compared to e-fuels and ammonia (Kanchiralla et al, Brynolf and Grahn co-authors).
- A common publication with Alexandre Capitao Patrao postdoc in the project “Pathways for a sustainable introduction of hydrogen into the aviation sector” on the possibility and life cycle impact or using hydrogen in aviation. Alexandre are more closely collaborating with the project Lightweight composite storage solutions for cryogenic hydrogen as mentioned earlier.
- “The future role of liquid fuels - Insights from global energy systems modeling and views from a Swedish local energy cluster in transition.” This article assesses global scenarios of future fuels including hydrogen for different transport modes (Johansson et al, Brynolf and Grahn co-authors),

The PhD student Joel Löfving starting 2023-03-01 will work on development of H2-Infra model and first publication connected to this is expected to be submitted early 2024.

DISSEMINATION AND COMMUNICATIONS EFFORT

Research publications achievements

With respect to dissemination the projects are generally behind schedule, mostly due to delayed starts of the individual projects. Notice that the Ph.D. projects have, as a maximum, run a bit more than six months at the time of writing. This delay is expected to be improved upon by the collaboration of the post docs, but not to the originally planned extent. Collaborative publications are being planned with the international network.

For detailed publication achievements and plans see the presentations of the five multidisciplinary research areas above.

Public/popular science activities

The center tries to increase its visibility by becoming active in a wide range of public/popular science activities.

The center has been mentioned and/or presented more in detail in the following events:

- Chalmers press release, 2022-12-01 [12].
- Chalmers press release on sensor research, 2022-12-01 [13]
- Energigas, Tomas Grönstedt, Interview, NR3, 2022 [14].
- Green Fly Way, Tomas Grönstedt, WP3 – focus area solar cells and hydrogen [15].
- P4 Göteborg, Maria Grahn, Interview – NYTT VÄTGASCENTRUM [16]
- UK – Sweden Aerospace workshop, Tomas Grönstedt – 2022-05-16
- Vätgas Sverige – Seminar, Tomas Grönstedt – Ny flyger vätgas – 2022-10-26
- Maria Grahn was invited as key-note speaker and panelist at Port of Ystad conference: "The goal is delivering sustainable fossil free transports". She presented the TechForH2 center and hydrogen related research results (2022-10-05).
- Maria Grahn was invited as plenary speaker at the International Workshop of the BEST project in Brussels. She presented the TechForH2 center and hydrogen related research results (2022-09-09)
- Selma Brynolf was invited as a panelist at "SamspEL Arena: Framtidens elbehov.". Selma presented the TechForH2 center and hydrogen related research at Chalmers (2022-12-08).
- Maria Grahn was co-authoring a debate article, published in Göteborgsposten 2022-10-18 "Reduktionsplikten måste utvecklas – inte försämras" https://www.gp.se/debatt/reduktionsplikten-m%C3%A5ste-utvecklas-inte-f%C3%B6rs%C3%A4mras-1.82975045
- Maria Grahn was giving a speech at the maritime industrial network day arranged by Svensk Sjöfart in Helsinki, Finland. Maria presented the TechForH2 center and hydrogen related research results focusing on hydrogen as a marine fuel (2022-09-01),
- Maria Grahn was giving a speech at a meeting with Stena Teknik. She presented an overview of research topics carried out at Chalmers Team Brynolf& Grahn including the TechForH2 center (2022-12-12), (3) Maria Grahn was giving a speech at the industrial network day "f3 Innovationskluster för hållbara biodrivmedel", in Lund. She presented the TechForH2 center and hydrogen related research results (2023-02-01).
- Yu Cao gave a speech on "Protection of austenitic stainless steel from hydrogen embrittlement by a surface engineering approach" was given in the 4th Swedish hydrogen seminar organized by Jernkontoret on 27th October 2022.

In addition, TechForH2 has participated at internal meetings with a wider scope than the normal TechForH2 participants at Scania, Volvo, Göteborgs Energi and ABB and Johnson Matthey.

The center has also committed to participate in the SHDC [17] as decided by the board on 2023-12-01. SHDC is a forum for hydrogen professionals addressing industrial needs and development. It is coordinated by RISE aiming to link industry innovation and research in the area of hydrogen development. Its scope is obviously broader than the current scope of TechForH2 but it is seen as an excellent platform to disseminate material and run activities through.

To increase the center visibility TechForH2 has adopted an official acknowledgement for research output:

The Competence Centre for TechForH2 is hosted by Chalmers University of Technology and is financially supported by the Swedish Energy Agency (Project No. 52675-1) and the member companies Volvo, Scania, Siemens Energy, GKN Aerospace, PowerCell, Oxeon, RISE, Stena Rederi, Johnson Matthey and Insplorion.

The aim is also to share the center affiliation as part of publications.

GOALS VISION AND THE CENTER DEVELOPMENT

Vision, strategy and goals

The TechForH2 vision is:

TechForH2 continues to contribute to the decarbonization of the energy and transport system by pursuing new innovations, stimulating enterprise sector investment and expands collaboration with the highly trained researchers and the engineers that continue to develop the hydrogen economy.

To accomplish this vision the center has a number of strategic commitments in the different research disciplines. These are:

- **Materials:** to create tailored, optimized, and sustainable material solutions to implement hydrogen propulsion across the transportation modes.
- **Production:** develop and experimentally verify novel manufacturing and product solutions for hydrogen use, required for manufacturability in terms of materials, geometrical capabilities, and product performance.
- **Cryo- and heat management:** to design and experimentally verify synergies between the cryogenic hydrogen storage and the fuel system and enable the use of cryogenic hydrogen across a number of transport modes.
- **Vehicle level research ambition:** to develop models and methods to understand, optimize and experimentally validate the impact of design choices and predict top-level vehicle performance for hydrogen propelled vehicles.
- **Transport & society research ambition:** to relate activities in TechForH2 with how to best introduce hydrogen and transit to a hydrogen economy by interacting and modelling larger societal activities including policies and regulation.
- **Safety & sensors:** to explore new classes of materials and develop their nanofabrication for hydrogen sensors with ultrawide dynamic range.

Strategic activities that are on a short list to support the above-mentioned technical ambitions are.

- Develop a visiting researchers' strategy through the international research collaboration network, preferably to further gender balance. Support mobility activities through Ph.D. students, post docs and senior researchers.

Strategic gender activities commitment:

TechForH2 is involved in a number of activities intended to advance gender balance, inclusion, and diversity:

- Genie will review the center's annual reports from a gender perspective.
- Initiate a dialogue with Genie (Chalmers Gender Initiative for Excellence) supporting the board and the director with advice on gender matters.
- The board, research leaders and key personnel will be offered a basic gender perspective course. This course is part of a sequence of courses being developed through the Genie initiative.
- TechForH2 may collaborate financially with Genie or independently take initiatives to stimulate mobility for female key researchers associated with the center.

The first two bullets have been achieved/will be achieved. There have been some delays due to that the Genie organization has been partly changed with new staffing between 2022/2023. The third and the fourth bullets are key activities planned for 2023 as listed below.

Selected strategic soft commitments for 2023:

- Work actively and extensively to use the international network. Some travels and research activity is already in place.
- Launch a seminar series for TechForH2 relevant researchers with the aim to:
    - Expand publication collaboration within the network.
    - Increase industry involvement across research topics
    - Launch a very condensed newsletter where SHDC activities are cross-promoted.
- Develop at and ideally also run the Genie initiative course.
- Actively use and develop the TechForH2 homepage.
- Boost mobility with a diversity focus, cross collaborate with Genie.
- Develop a relatively extensive power point material for potential use at conferences available to all partners and research leaders.

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TechForH2: who are we?

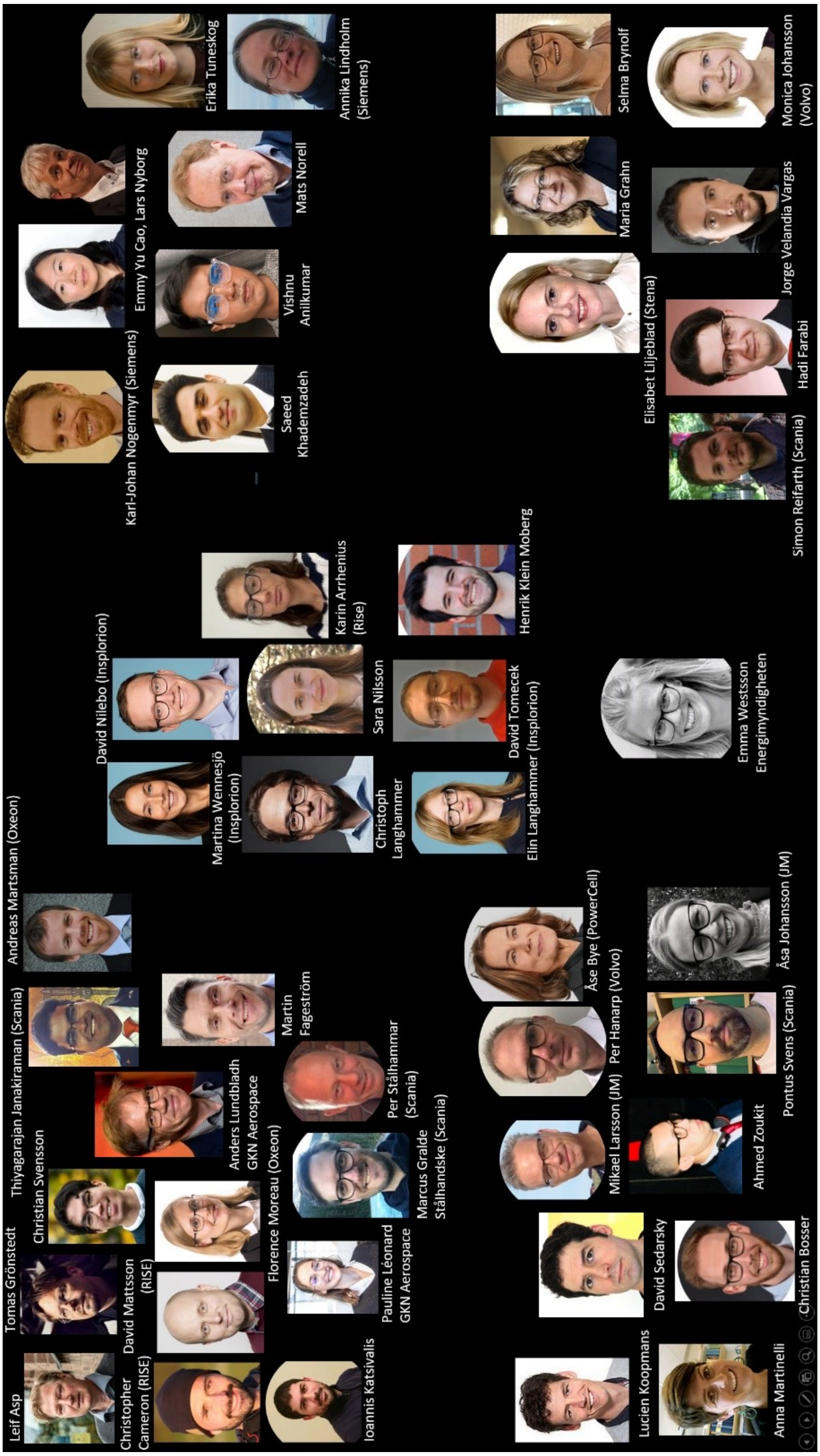

Figure 16: People involved in 2022 TechForH2 kick-off. Chalmers affiliation unless otherwise stated.