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Department of Energy
"G.Ferraris"

2024

PhD Days
ENERGETICS

Annual Report

Editors: Massimo SANTARELLI, Daniela MISUL

December 2024

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Introduction

This document contains a series of one-page reports from the students enrolled in the Energetics PhD program at Politecnico di Torino, Italy, including the highlights of their research activity in 2024. The previous editions of the Annual Report can be downloaded from https://www.polito.it/en/education/phd-programmes-and-postgraduate-school/phd-programmes/energetics/annual-reports

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Building physics and energy systems in future buildings and communities

First name: Manuela **LAST NAME**: BARACANI

Topic: Occupant-centric and multi-domain design, operation and integration of advanced transparent envelopes in buildings

Course year: 3rd **Tutor(s)**: Fabio FAVOINO, Valentina SERRA

Highlights of the research activity

This research supports Europe carbon neutrality goals advancing energy-efficient buildings that minimize CO_2 emissions and enhance energy demand flexibility. The transparent envelope of buildings highly contributes to energy performance and occupant comfort. Advanced Fenestration Systems (AFS) can optimize both by adapting to changing boundary conditions, and influence multiple comfort domains, including thermal, visual, acoustic, and indoor air quality (IAQ). Integrating AFS into building operations requires a balance of design optimization, effective control systems, and occupant behavior considerations: this research tries to develop an occupant-centric approach for AFS integration in buildings. AFS are evaluated through both objective and subjective Key Performance Indicators (KPIs) and challenges in their simulation, real-world implementation and users integration in monitoring and actuation are explored. The need for comprehensive assessment tools to simulate AFS is investigated in a case study consisting in an openable double-glazed window with in-cavity venetian blinds. A co-simulation workflow to accurately capture its multi-domain effects was developed, focusing on visual and thermal comfort, energy demand, and IAQ. This allowed to develop rule- and model-based controls balancing contrasting objectives, based on multidomain KPIs. Results highlighted the potential of multi-domain control logics to optimize energy use and maximize human comfort. Real world assessment challenges were investigated in a Living Lab in Politecnico di Torino, equipped with advanced envelope components and a monitoring infrastructure combining high-accuracy wired and low-cost, low-invasive IEQ sensors. An IoT platform supporting real-time monitoring was also implemented. Field experiments analysed how data acquisition systems varying in cost, accuracy, and intrusiveness, affect variable measurement and KPIs calculation, showing that low-cost sensors could deliver acceptable accuracy for large-scale applications if combined with numerical models. Evaluation of AFS performance through subjective feedback was conducted through short-term monitoring experiments including more than 50 occupants. Participants were given full control of HVAC, lighting systems and a ventilated window, which they could operate in various modes. Multiple surveys were submitted to occupants to assess real-time perceived comfort, personal preferences and overall satisfaction. AFS components were also characterized by objective measurements and KPIs. The research advances methodologies for designing, controlling, and evaluating AFS in both simulated and real-world settings, showing the importance of integrating occupants to real-life performance assessments.

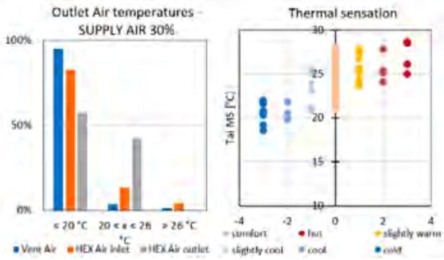

Fig 1: Objective and Subjective thermal assessment of environment and ventilated window

External collaborations

- ENEA - Agenzia nazionale per le nuove tecnologie, l'energia e lo sviluppo economico sostenibile
- Horizon 2020 Iclimabuilt project partnership

Academic context

[1] E. Taveres-Cachat, F. Favoino, R. Loonen, and F. Goia, "Ten questions concerning co-simulation for performance prediction of advanced building envelopes," *Build. Environ.*, vol. 191, p. 107570, Mar. 2021, doi: 10.1016/j.buildenv.2020.107570.

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[3] A. Ståhlbröst and M. Holst, "Reflecting on Actions in Living Lab Research," *Technol. Innov. Manag. Rev.*, vol. 7, no. 2, pp. 27–34, Feb. 2017, doi: 10.22215/timreview1055.

First name: Franz Giorgio Maria**LAST NAME**: BIANCO MAUTHE DEGERFELD

Topic: Implementation of Standard Calculation Models for the Assessment of Technical Building Systems and of the Whole Building Energy Performance

Course year: 3rd **Tutor(s)**: Vincenzo CORRADO, Ilaria BALLARINI

Highlights of the research activity

In the context of improving energy efficiency and reducing carbon emissions in buildings, a key strategy involves advancing design methodologies and tools. Simplified calculation procedures for building energy assessment face a critical challenge: achieving a balance between simplicity and accuracy. These methodologies must be user-friendly to minimize user errors while aiming to accurately represent a building's actual performance. However, existing simplified models, even though are user-friendly, often lack precision. To bridge this gap, the focus of this Ph.D. research is on enhancing simplified calculation methodologies for assessing the performance of HVAC systems. Following a comprehensive literature review of simplified procedures and an initial focus on the generation subsystem, the research expanded to include a detailed analysis of emission and control subsystems. Currently, simplified calculation procedures for modelling emitters and control systems lack flexibility and heavily rely on tabular fixed values. Complex phenomena within heated or cooled space − such as spatial variations in air temperature, non-uniform radiant temperature, and imperfect air temperature control − are often overlooked or oversimplified, highlighting the need for further enhancement. To address the gaps, the existing calculation methods were thoroughly analysed, with a focus on key parameters, including heat emitter properties. Using different methodologies, two comparative analyses were performed to assess the deviations in emission losses related to different emitters and control strategies. Sixteen case studies (indicated in Figure 1 as C1 – C16), with identical building geometries, but varying parameters such as emission terminal type (radiator or low-temperature radiant system), control strategy (on/off or proportional), climatic conditions, and building envelope properties, were tested. The analysis, as presented in Figure 1, confirmed previous results and highlighted the shortcomings of simplified methods. In some cases, the Mean Bias Error (MBE) exceeds 200%, while in other cases, the simplified procedures inaccurately predict energy needs for time steps where it should be zero (highlighted in orange in Figure 1). The findings of the research activity have led the proposal of an improvement in simplified methods. These enhancements include the substitution or modification of the correction factors, and the integration of advanced algorithms into the calculation process for control systems. For emission energy losses, new correction factors that vary on a time-step basis have been implemented to increase accuracy and reliability. The initial analysis was followed by a whole building analysis to assess the combined effect of different procedures on key performance indicators such as primary energy consumption.

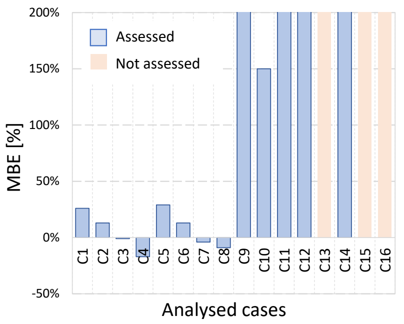

Figure 1. Mean bias error (MBE) of the annual monthly energy consumption calculated using simplified methods for emission and control systems, compared against reference detailed methods.

External collaborations

- Edilclima S.r.l. - Engineering & Software
- Eindhoven University of Technology

Academic context

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[3] Võsa K. V., Ferrantelli A., Kurnitski J. 2020. A novel method for calculating heat emitter and controller configuration setpoint variations with EN15316-2. Journal of Building Engineering, 31.

First name: Roberto **LAST NAME**: CHIOSA

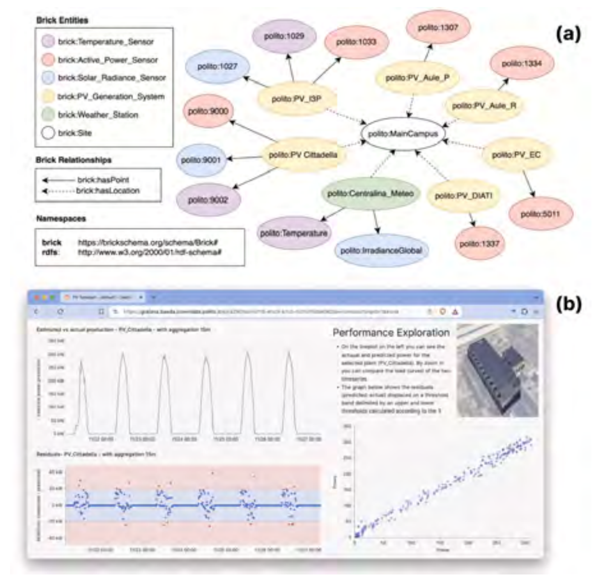
Topic: Artificial intelligence-based decision support systems for enhancing energy management in buildings

Course year: 3rd **Tutor(s)**: Alfonso CAPOZZOLI, Cheng FAN

Highlights of the research activity

During the 3rd year of my PhD, I dedicated my attention to the development of methodological processes for Decision Support Systems (DSSs) aimed at the development of Anomaly Detection and Diagnosis (ADD) algorithms that are scalable and interoperable among different buildings and systems configurations. With this aim, during my period at Lawrence Berkeley National Laboratory (Q2 2023), I deepened my knowledge of standard and flexible data and metadata organization (i.e., semantic schemas), which can handle the complexity and heterogeneity of building data. The introduction and adoption of such ontologies (e.g., Brick schema) enabled the development of a framework to deploy ADD processes in a standard and robust way across different buildings. The outcomes of this research lead to the development of an open-source Python package that was employed to demonstrate the scalability of such approaches which the results have been discussed in a published paper [2].

Figure 1. Semantic representation of the monitoring infrastructure of POLITO campus (a) used as case study for the implementation of a portable anomaly detection solution (b) for the installed photovoltaic plants.



The previous work has been adopted and implemented in the monitoring infrastructure of Polito Campus through the implementation of an online methodology to perform ADD on the campus photovoltaic plants as shown in Figure 1. By carefully designing DSS solutions like the one previously described, it is possible to deliver information in the most accessible and actionable manner to different stakeholders, such as energy managers, building owners, and energy service companies. Achieving this is essential for (i) enriching the informative output, (ii) enhancing predictive capabilities, and (iii) increase end users' trust in automated systems.

The approach is currently under validation against user requirements and expectations, the goal is to gain a deeper understanding of the essential variables, procedures and information needed to correctly support stakeholders' decisions and how needs may vary during the building lifecycle (especially during operation)

External collaborations

- IEA EBC - Annex 81 - Data-Driven Smart Buildings
- Lawrence Berkeley National Laboratory (LBNL)
- Shenzhen University

Academic context

[1] Lin, G., Kramer, H., & Granderson, J. (2020). Building fault detection and diagnostics: Achieved savings, and methods to evaluate algorithm performance. Building and Environment, 168, 106505.
[2] Chiosa, R., Piscitelli, M. S., Pritoni, M., & Capozzoli, A. (2024). A portable application framework for energy management and information systems (EMIS) solutions using Brick semantic schema. Energy and Buildings
[3] Chiosa, R.; Piscitelli, M.S.; Capozzoli, A. A Data Analytics-Based Energy Information System (EIS) Tool to Perform Meter-Level Anomaly Detection and Diagnosis in Buildings. Energies 2021, 14, 237.

First name: Davide **LAST NAME**: CORACI

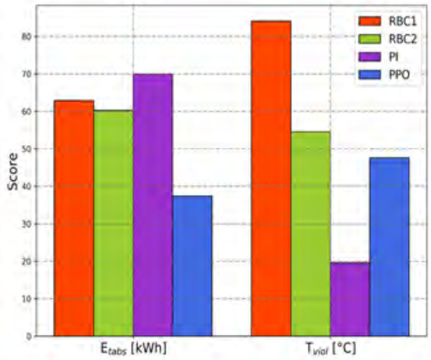
Topic: Transfer learning to enhance the scalability of artificial intelligence based control strategies in buildings

Course year: 3rd **Tutor(s)**: Alfonso CAPOZZOLI, Tianzhen HONG

Highlights of the research activity

Deep Reinforcement Learning (DRL) is an innovative approach to enhance energy efficiency in buildings, offering advanced control capabilities. However, its implementation in real buildings is often impractical due to economic constraints and the extensive effort required to develop surrogate models for pre-training. Knowledge-sharing strategies, such as Transfer Learning (TL) and Behavioral Cloning (BC), have emerged as viable solutions to address these challenges and enable DRL deployment in real-world scenarios. In 2024, my research focused on applying TL and BC in both simulated and real buildings. The first study developed an online heterogeneous TL methodology to transfer DRL controllers managing integrated energy systems (chiller, PV, electrical and thermal storage) in buildings with differing Envelope properties, weather, and electricity tariffs. The TL approach reduced electricity costs by 10% and improved temperature control by up to 40% compared to Rule-Based Controllers (RBCs) and online DRL, validating TL as an effective and model-free strategy for scaling DRL controllers. The second study evaluated TL real implementation in buildings, transferring DRL agents between two office spaces equipped with Thermally Activated Building Systems. The proposed TL approach allowed to reduce energy consumption up to 20% compared to RBC and online DRL while improving temperature control. Finally, the third study evaluated, for the same real building as in the second application, the implementation of a BC methodology coupled with online DRL training to ensure initial reliability and adaptive capabilities for DRL during the real implementation. By firstly mimicking the behavior of the real implemented RBC, the DRL controller based on Proximal Policy Optimization (PPO) reduced energy consumption by 40% and improved indoor temperature control by up to 40%. While Proportional-Integral controllers slightly outperformed DRL in temperature control, they required 45% more energy, highlighting DRL capabilities in multi-objective optimization processes. The two proposed real contributions demonstrated the feasibility of employing knowledge-sharing strategies to enhance the DRL controllers deployment in buildings, bridging the gap between simulation and real-world.

Figure 1. Performance comparison for RBCs, PI and PPO with Behavioral Cloning



External collaborations

- Lawrence Berkeley National Laboratory (Berkeley, USA)
- ABB s.p.a
- Architecture and Building System group (ITA Institute of Technology in Architecture - ETH Zurich)

Academic context

[1] Coraci, D.; Brandi, S.; Hong, T.; Capozzoli, A. An innovative heterogeneous transfer learning framework to enhance the scalability of deep reinforcement learning controllers in buildings with integrated energy systems. *Building Simulation* (2024), *17 (5), 739-770*. doi: https://doi.org/10.1007/s12273-024-1109-6.
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[3] Silvestri, A.; Coraci, D.; Brandi, S.; Capozzoli, A.; Schlueter, A. Practical deployment of Reinforcement Learning for building controls using an Imitation Learning approach. *19th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES), Rome* (2024).

First name: Virginia Isabella **LAST NAME**: FISSORE

Topic: Indoor environmental quality monitoring for the optimized management of the energy performance and comfort of the building

Course year: 3rd **Tutor(s)**: Arianna ASTOLFI, Anna PELLEGRINO, Stefano Paolo CORGNATI

Highlights of the research activity

The PhD research is carried out with the participation of C2R Energy Consulting, as company that co-finances the PhD, the Italgas and Geoside companies, the DET, DAUIN and CALOS Departments of Politecnico di Torino. The research focuses on Indoor Environmental Quality (IEQ) monitoring for the optimized management of the energy performance of the building and the enhancement of occupants' comfort and health. To this aim, a low-cost and accurate monitoring system was developed. It includes a multi-sensor device that monitors the main parameters of IEQ domains (thermal, visual, acoustic and indoor air quality), and a survey for the acquisition of occupants' subjective feedback on comfort perception. The monitored parameters (air temperature, relative humidity, carbon dioxide, carbon monoxide, nitrogen dioxide, particulate matter, volatile organic compounds, formaldehyde, illuminance and sound pressure level) were selected based on international standards and the sensors based on dimensions, cost and accuracy. The multi-sensor hardware components are integrated in a single-case 3D printed device. Calibration procedures of the sensors were done to ensure the measurements traceability. In addition, an online questionnaire to get users' feedback on comfort perception was developed based on the standard ISO 28802:2012. Measured data and calculated objective and subjective comfort indexes for each IEQ domain are displayed on an ad-hoc designed dashboard for an effective communication with users. Models for the calculation of the comfort indexes related to each domain were defined and applied for their validation in a two-semesters in-filed study in the "Aule P" of Politecnico di Torino. IEQ monitoring was performed through a commercial multi-sensor device and students' feedback on comfort perception was collected. The completed PROMET&O system was applied in two open-plan offices, and a BIM model was developed for the real-time spatialized visualization of the environmental conditions inside the offices monitored through the multi-sensor.

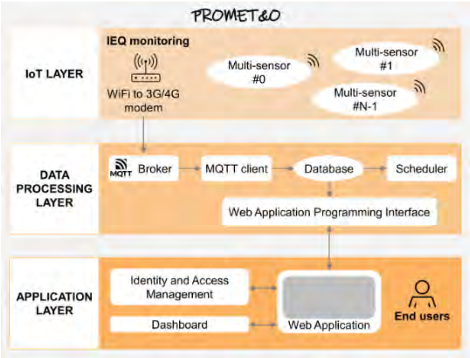


Fig.1: PROMET&O system for IEQ monitoring, occupants' feedback on comfort perception collection and data visualization.

External collaborations

- C2R Energy Consulting S.r.l.
- Italgas S.p.A.
- Intesa Sanpaolo S.p.A.

Academic context

[1] T. Parkinson, A. Parkinson, R. de Dear, Continuous IEQ monitoring system: Context and development, Build. Environ. 149 (2019) 15–25.
[2] N. Lassen, T. Josefsen, F. Goia, Design and in-field testing of a multi-level system for continuous subjective occupant feedback on indoor climate, Build. Environ. 189 (2021) 107535.
[3] M. Schweiker, E. Ampatzi, M.S. Andargie, R.K. Andersen, E. Azar, V.M. Barthelmes, C. Berger, L. Bourikas, S. Carlucci, G. Chinazzo, L.P. Edappilly, M. Favero, S. Gauthier, A. Jamrozik, M. Kane, A. Mahdavi, C. Piselli, A.L. Pisello, A. Roetzel, A. Rysanek, K. Sharma, S. Zhang, Review of multi-domain approaches to indoor environmental perception and behaviour, Build. Environ. 176 (2020) 106804.

First name: Antonio **LAST NAME**: GALLO

Topic: Data-driven energy management strategies for Renewable Energy Communities

Course year: 3rd **Tutor(s)**: Alfonso CAPOZZOLI

Funded by ABB s.p.a.

Highlights of the research activity

Renewable Energy Communities (REC) offer benefits to both community members and grid operators through Shared Energy (SE) incentives, encouraging behaviors like reducing peak imports and increasing self-consumption. However, the effectiveness of these incentives depends on REC configurations, such as the number of prosumers, storage capacity, and energy patterns.

An MPC optimizer was used to minimize REC energy costs, incorporating thermal demand, heat pump efficiency, and PV generation. Simulations over a 4-day heating period analyzed scenarios with 5–50 prosumers, both with and without incentives. The effectiveness of SE incentives was measured using cost/benefit ratios for reducing energy imports, exports, and peak loads, and highlighted the following considerations:

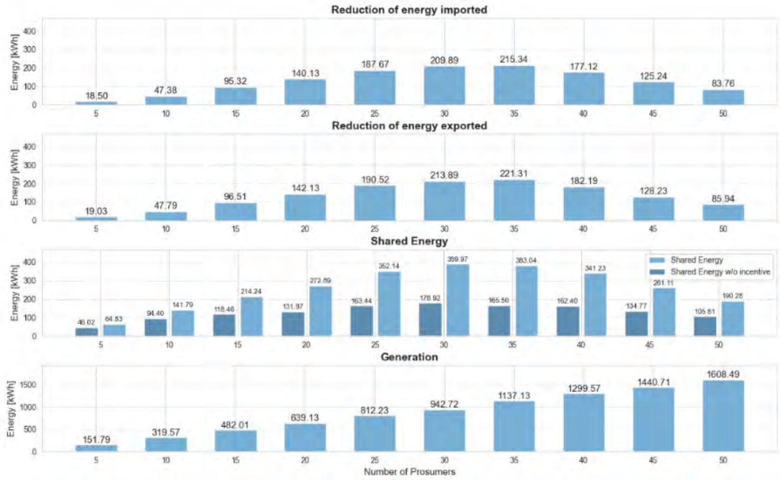


Figure 1. Comparison between incentivized and no-incentivized scenario

- Energy reductions peaked at 35 prosumers, the most cost-efficient configuration.
- SE incentives significantly increased energy self-consumption but benefits decreased after 30 prosumers.
- Costs for reducing negative peak loads spiked after 40 prosumers, highlighting reduced cost-effectiveness.
- Positive peak loads were unaffected due to low PV generation during those periods.

This analysis guides resource allocation to maximize grid stability benefits within budget constraints.

External collaborations

- IEA EBC Annex82
- ABB s.p.a.
- Aarhus University

Academic context

[1] Kathryn Kaspar, Mohamed Ouf, Ursula Eicker, A critical review of control schemes for demand-side energy management of building clusters, Energy and Buildings, Volume 257, 2022, 111731, ISSN 0378-7788, https://doi.org/10.1016/j.enbuild.2021.111731

[2] Flora Charbonnier, Thomas Morstyn, Malcolm D. McCulloch, Scalable multi-agent reinforcement learning for distributed control of residential energy flexibility, Applied Energy, Volume 314, 2022, 118825, ISSN 0306-2619, https://doi.org/10.1016/j.apenergy.2022.118825

[3] Aihua Jiang, Huihong Yuan, Delong Li, Energy management for a community-level integrated energy system with photovoltaic prosumers based on bargaining theory, Energy, Volume 225, 2021, 120272, ISSN 0360-5442, https://doi.org/10.1016/j.energy.2021.120272

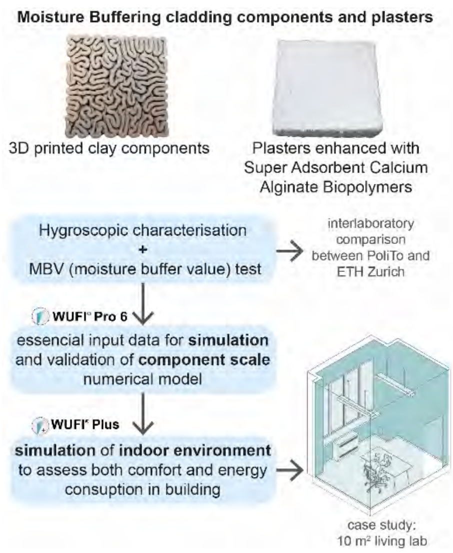
First name: Giorgia **LAST NAME**: AUTRETTO

Topic: Thin layers for indoor climate control in advanced multifunctional building envelopes

Course year: 2nd **Tutor(s)**: Stefano Fantucci, Valentina Serra

Highlights of the research activity

The construction industry is increasingly adopting innovative solutions for energy-efficient building refurbishments, addressing growing energy demands and the need to mitigate cooling loads, particularly in Mediterranean regions. Multifunctional materials like Phase Change Materials (PCM), Super Insulating Materials, advanced coatings, and moisture-buffering cladding components offer substantial energy efficiency potential without significantly increasing envelope thickness. However, current methods for evaluating these materials often rely on simplified procedures, resulting in inaccurate assessments of their transient hygrothermal performance. Research focuses on thin-layer advanced surface technologies that integrate multiple functionalities, such as thermal and moisture buffering, and insulation. Objectives include accurately measuring properties, analyzing dynamic behavior, and establishing reliable performance indicators to assess their impact on energy efficiency, indoor environmental quality, and occupant comfort. During the second year of the PhD programme, significant progress was achieved on 3D-printed clay components and plasters enhanced with Super Adsorbent Polymers (SAPs). For 3D-printed components, Moisture Buffering Value (MBV) tests conducted in two laboratories revealed air velocity as a critical factor for accurate measurements of complex geometries. Simulations validated the moisture buffering behaviour of these components for real-world applications using an equivalent material approach, matching the modeled results with the experimental one. SAP-enhanced plasters demonstrated improved moisture buffering (up to 9 g/m² %RH) and potential for stabilizing indoor humidity while reducing HVAC energy demand. Simulations in a 10 m² room confirmed their effectiveness in enhancing comfort and dehumidification savings. Future research will further optimize the performance of these materials by examining variables like ventilation rates, occupant behavior, and application area extension, supporting their integration into sustainable building designs. This work highlights the potential of advanced materials to improve energy performance and indoor quality, promoting their use in innovative, energy-efficient building practices.



Research workflow on Moisture Buffering cladding components and plasters

External collaborations

- ETH | Zurich | Switzerland
- STU Bratislava | Bratislava | Slovakia
- KU Leuven | Campus Brussels and Ghent | Belgium

Academic context

[1] V. Cascione, D. Maskell, A. Shea, P. Walker, M. Mani, Comparison of moisture buffering properties of plasters in full scale simulations and laboratory testing, Construction and Building Materials (2020), doi: https://doi.org/10.1016/j.conbuildmat.2020.119033
[2] V. Gentile, J.D. Vargas Velasquez, S. Fantucci, G. Autretto, R. Gabrieli, P.K. Gianchandani, M. Armandi, F. Baino, 3D-printed clay components with high surface area for passive indoor moisture buffering, Journal of Building Engineering (2024), doi: https://doi.org/10.1016/j.jobe.2024.109631
[3] M. Posani, V. Voney, P. Odaglia, D. Eschbach, G. Habert, High-tech, low-carbon material fabrication: 3d-printed geopolymers for indoor hygrometric comfort improvement. CEES 2023 - The second International Conference on Construction, Energy, Environment and Sustainability (2023).

First name: Giacomo **LAST NAME**: BUSCEMI

Topic: Artificial Intelligent based Energy Management of Building-integrated Microgrid and Energy Hubs

Course year: 2nd **Tutor(s)**: Alfonso CAPOZZOLI, Marco Savino PISCITELLI

Highlights of the research activity

Research activities during the 2nd year of the PhD focused on developing advanced methodologies and tools to optimize energy management in buildings and microgrids, aligning with the PRIN 2020 project *Optimal refurbishment design and management of small energy micro-grids.* Key efforts addressed the challenges of integrating renewable energy, enhancing flexibility, and improving the performance of building energy systems. In the end of my first year, a methodological framework applied to buildings modeled as microgrids, was developed to extract typical demand load profiles of buildings using pattern recognition, data mining, and time series analytics. A TRNSYS-Python co-simulation environment was developed to connect proprietary simulation tools with scalable control systems. Applied at Politecnico di Torino, it used Deep Reinforcement Learning (DRL) to optimize rooftop units, enhancing energy efficiency and thermal comfort. Explainable Artificial Intelligence (XAI) techniques were explored to increase trust in AI-based solutions, providing interpretable insights into building energy performance based on data from Energy Performance Certificate. Contributions to the CityLearn platform involved integrating data-driven thermal dynamics models for more realistic simulations of energy systems. In 2024, research focused on Energy Hubs, multi-energy systems that optimize different kind of energy flows. Safe DRL, which integrates safety constraints into control strategies, was investigated as an alternative to traditional optimization techniques. Case studies included an Energy Hub with borehole thermal storage and the Miulli Hospital in Bari, featuring Solid Oxide Fuel Cells and photovoltaics. Further work extended the TRNSYS platform's capabilities, enabling the management of HVAC in non-residential buildings and advancing strategies for fault detection and control optimization.

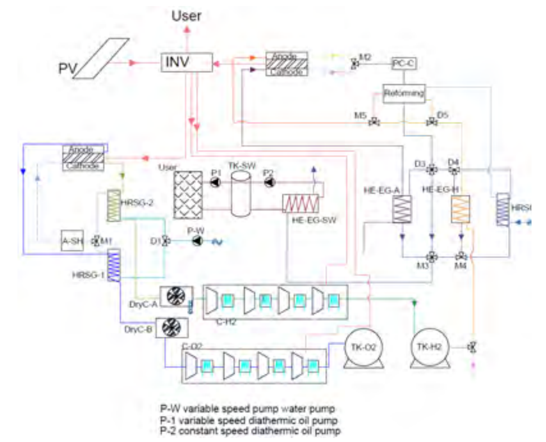


Figure 1 Layout of the generation system that serves the Miulli Hospital

External collaborations

- Participation in **IEA-EBC Annex 82:** Energy Flexible Buildings Towards Resilient Low Carbon Energy Systems (2020-2025)
- University of Texas at Austin and University of Montreal
- Aarhus University

Academic context

[1] Fontenot, H.; Dong, B. ***Modeling and control of building-integrated microgrids for optimal energy management – A review***. Elsevier, Applied Energy. 2019. https://doi.org/10.1016/j.apenergy.2019.113689
[2] Qiu, D., Dong, Z., Zhang, X., Wang, Y., Strbac, G. **Safe reinforcement learning for real-time automatic control in a smart energy-hub**. Elsevier, Applied Energy, 2022. https://doi.org/10.1016/j.apenergy.2021.118403
[3] Zhang, G., Hu, W., Cao, D., Zhang, Z., Huang, Q., Chen, Z., Blaabjerg, F. ***A multi-agent deep reinforcement learning approach enabled distributed energy management schedule for the coordinate control of multi-energy hub with gas, electricity, and freshwater***. Energy Conversion and Management, 2022. https://doi.org/10.1016/j.enconman.2022.115340

First name: Davide **LAST NAME**: FOP

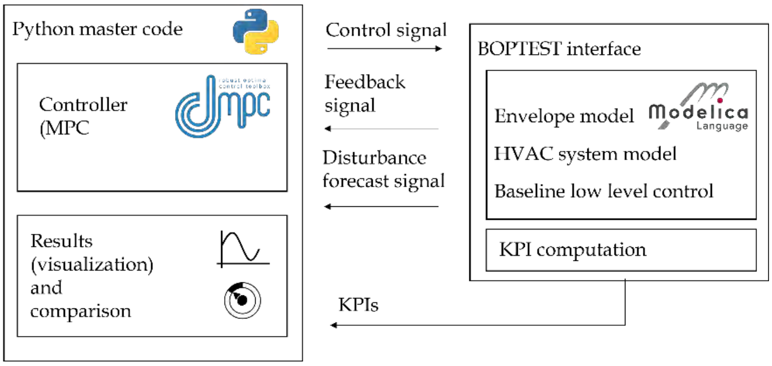
Topic: Development of simulation platforms for the testing of building energy systems advanced control strategies

Course year: 2nd **Tutor(s)**: Prof. Alfonso CAPOZZOLI, Prof. Stefano Paolo CORGNATI, Prof. Cristina BECCHIO

Highlights of the research activity

Research has in recent years proven how advanced controllers for energy management in buildings can provide benefits in terms of energy savings for individual buildings. At the same time, proper control strategies can enable the exploitation of buildings' energy flexibility, thus providing ancillary services to the power grid. Novel controllers require extensive testing to assess their feasibility and performance with respect to the current state of the art strategies. However, in field testing can be costly, time consuming, and result int improper operation, leading to equipment wear and occupants' discomfort. Simulation offers an alternative to real world implementation. Literature highlights an increasing need for detailed, reliable emulators that can reproduce the dynamic behaviour of the building. These emulators can serve for research purposes, allowing to test novel control strategies, or they can be used as digital twins of the real buildings, enabling the exploration of scenarios and the benchmarking of new controllers against state of the art solutions.

Co-simulation framework



In this context, the potential of building emulators has been investigated. In particular, the Building Optimization Testing Framework (BOPTEST) was employed since it offers a set of shared, open-source building models on which to test control strategies, so that different control solutions can be benchmarked with each other on the same testcases. An optimal, model-based controller, specifically belonging to the Model Predictive Control (MPC) class, has been tested on a detailed building emulator of a single zone served by a heat pump and a heating floor emission system. Different MPC formulation were tested on the system, highlighting the capability of advanced controllers to handle multiple control objective, including ensuring thermal comfort for occupants, energy consumption minimization, and the attainment of requirements from the energy grid.

Academic context

[1] Fop, D.; Yaghoubi, A.R.; Capozzoli, A. Validation of a Model Predictive Control Strategy on a High Fidelity Building Emulator. *Energies* 2024, *17*, 5117. https://doi.org/10.3390/en17205117
[2] D. Blum, J. Arroyo, S. Huang, J. Drgona, F. Jorissen, H.T. Walnum, Y. Chen, K. Benne, D. Vrabie, M. Wetter, and L. Helsen. (2021). "Building optimization testing framework (BOPTEST) for simulation-based benchmarking of control strategies in buildings." Journal of Building Performance Simulation, 14(5), 586-610.
[3] J. Drgoňa, J. Arroyo, I. Cupeiro Figueroa, D. Blum, K. Arendt, D. Kim, E. Perarnau Ollé, J. Oravec, M. Wetter, D. L. Vrabie, L. Helsen, All you need to know about model predictive control for buildings, Annual Reviews in Control, Volume 50, 2020, Pages 190-232, ISSN 1367-5788, https://doi.org/10.1016/j.arcontrol.2020.09.001.

First name: Rocco **LAST NAME**: GIUDICE

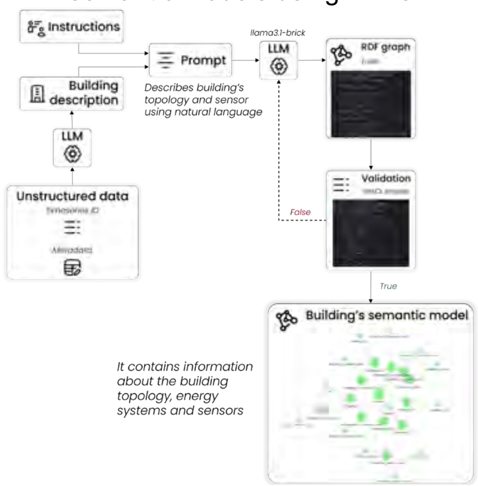
Topic: Scalable and Interoperable Decision Support Systems for enhancing energy management in buildings

Course year: 2nd **Tutor(s)**: Alfonso CAPOZZOLI, Marco Savino PISCITELLI

Highlights of the research activity

The increasing digitalization of buildings highlights the importance of Decision Support Systems (DSSs) in optimizing energy use, improving system performance, and enhancing occupant comfort. However, the growing complexity of modern buildings, with their interconnected systems (e.g., HVAC, lighting, and security), presents significant challenges for DSSs in terms of interoperability, portability and transferability. Current DSSs solutions often lack standardized data models, resulting in inefficiencies, high costs, and prolonged when developing the same DSS solution in multiple buildings. Semantic metadata models based on ontologies offer a promising solution to these challenges by providing machine-readable frameworks to describe building equipments and their relationships in a standardized way. However, the manual creation of these models remains a significant bottleneck due to its labor-intensive nature and the expertise required.

Pipeline for generating building's semantic models using LLMs



Building on this context, the research conducted focused on developing robust DSS solutions using real Renewable Energy Communities (REC) as the main case study, resulting in a methodology for a fairest allocation of the incentive derived from the shared energy among memebers. The methodology developed is based on an energy benchmarking approach where the members of the community are remunerated based on their performance, evaluated in line with the objectives of the community, i.e. the maximization of the self-sufficiency. To achieve portability and interoperability objectives of DSSs, a methodology that employes Large Language Models (LLMs) for the automatic development of semantic metadata models of buildings using the Brick ontolgy was introduced, starting from the natural language description of the building and its equipments and senors. A multi-agent system was employed, where each step of the semantic model development is executed by a LLM agent, such as entities identification, hierarchy construction, relationships mapping, etc.. This approach is highly general, allowing the construction of semantic models for various types of buildings and equipments. Furthermore, a fine-tuned LLM was developed for enhancing the performance of semantic metadata model development when examples of semantic models are available, resulting in a less general but more DSS-oriented solution.

External collaborations

- EURAC Research, Bolzano, Italy
- Italian National Agency for New Technologies, Energy and Sustainable Economic Development
- Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia

Academic context

[1] Piscitelli, M. S., Giudice, R., & Capozzoli, A. (2024). A holistic time series-based energy benchmarking framework for applications in large stocks of buildings. Applied Energy, 357, 122550.
[2] Perini, M., Antonucci, D., Giudice, R., Piscitelli, M.S., & Capozzoli, A. (2024). BrickLLM: A Python library for generating Brick-compliant RDF graphs using GenAI, *Submitted in SoftwareX*.
[3] Giudice, R., Piscitelli, M.S., Chiosa, R., & Capozzoli, A. (2024). A Data-Driven Process for Optimal Incentive Sharing in Collective Self-Consumption Groups of Residential Users, Multiphysics and Multiscale Building Physics. Lecture Notes in Civil Engineering, 553, Springer, Singapore.

First name: Matteo **LAST NAME**: PIRO

Topic: Advanced energy performance assessment of building stocks

Course year: 2nd **Tutors**: Ilaria BALLARINI, Vincenzo CORRADO

Highlights of the research activity

The recently issued EPBD recast (EU 1275/2024) highlights the need for national building renovation plans to improve building stock energy performance, driving large-scale urban renovations. The enhancement of building stock energy efficiency depends on the adoption and advancement of the Urban Building Energy Model (UBEM). The high level of uncertainty in urban energy analysis, due to outdated and obsolete local databases, privacy concerns, and a lack of digitalized data, often result in unvalidated and uncalibrated UBEMs.

This Ph.D. activity aims to improve the reliability of urban-scale energy model outputs. To bridge the data uncertainty gap and enhance UBEM validity, several actions have been implemented.

Nowadays, a core source of information for UBEM is represented by the energy performance certificates (EPCs) of buildings. However, EPC data currently lack credibility and reliability, necessitating a data quality checking procedure. To address this issue, a procedure to score and rank the reliability of energy certificates has been developed and applied. This experience, which was performed within the context of the H2020-TIMEPAC project, will be also used to improve control measures in the Piedmont EPC database, ensuring higher-quality certificates.

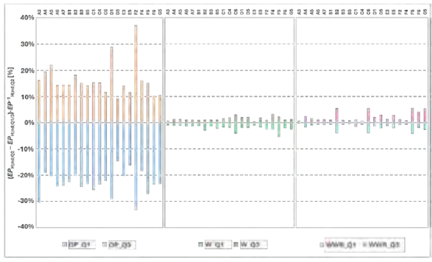


Figure 1. Impact of the variations of key inputs in assessing the overall energy performance of the building stock (Piro et al., 2024).

Starting from a comprehensive survey of data sources besides EPCs, probabilistic building archetypes to be used in UBEM have been developed for residential and non-residential use categories in Piedmont and Aosta Valley regions, balancing reduced model complexity with improved accuracy. These archetypes capture the non-geometric properties required to characterise the energy performance of similar buildings, segmented by climatic zone, building use category, and construction period. Moreover, a paradigm shift is underway: it consists in transitioning from single-building archetypes to typical district archetypes. Representative city blocks in three distinct Italian climatic zones are going to be developed, in such a way to combine single-building archetypes to analyze energy interactions between buildings and to increase the spatial coverage of the outcomes by deploying the concept of urban typology. These activities are carried out in the context of two PRIN projects, respectively, URBEM and CRiStAll.

Current and future work will focus on calibrating archetype-based UBEMs and validating the data in the generated building archetype schema. Individual building calibration will involve iterative optimization of archetype inputs within their confidence intervals. From this perspective, preliminary results showing how variations in key inputs affect the overall energy performance of the building stock are presented in Figure 1. This activity is under development at Idiap Research Institute in Martigny (Switzerland).

In conclusion, the combined efforts undertaken in this Ph.D. will enable improved modeling and planning for the energy performance of future cities.

External collaborations

- Idiap Research Institute – Martigny (Switzerland)
- La Salle – Ramon Llull University – Barcelona (Spain)

Academic context

[1] Reinhart, C. F., & Cerezo Davila, C. (2016). Urban building energy modeling – A review of a nascent field. *Building and Environment, 97*, 196-202.

[2] Johari, F., Peronato, G., Sadeghian, P., Zhao, X., & Widén, J. (2020). Urban building energy modeling: State of the art and future prospects. *Renewable and Sustainable Energy Reviews, 128*, 109902.

First name: Lorenzo **LAST NAME**: RAPONE

Topic: Towards digital twins enhanced services for high performing facades

Course year: 2nd **Tutor(s)**: Prof. Fabio Favoino, Prof. Valentina Serra

Highlights of the research activity

The PhD project focuses on developing digital twin (DT) services for transparent building envelope technologies to enhance energy efficiency while maintaining indoor environmental quality (IEQ). Over the past year, the research extended the literature review and initiated the first case study to understand DT's potential in building facades. The guiding research questions were: "what is an effective DT development structure for transparent building envelope systems aimed at improving energy flexibility and IEQ in buildings?" and "Would it be beneficial to create distinct DTs for building façade components and the overall building to address different tasks?".

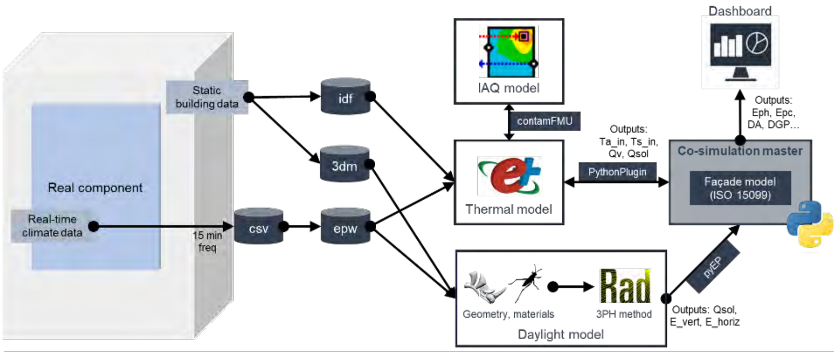


Figure 1. Summary of the co-simulation workflow for the first case study (TWINS test cell facility).

Key findings of the literature review indicate that DT application to building facades can significantly improve energy performance and IEQ, particularly through dynamic control systems. The most common DT services identified were: (1) automation of improved controls, (2) what-if scenarios, (3) predictive maintenance.

The first case study involved the TWINS (Testing Window Innovative Systems) facility at the Department of Energy, Politecnico di Torino. TWINS evaluates advanced façades under real-world conditions. The current mock-up, Test Case 1 (TC1), developed under the iClimabuilt H2020 EU project, is a dynamic façade system enhancing energy flexibility and occupant comfort. Key components include a Triple Glazed Unit (TGU) and a heat Exchanger (HEX) with PCM-based plates. The virtual case study uses a digital twin of the TWINS facility to run scenario analyses, comparing a static benchmark (simple TGU) with dynamic systems like TC1. The goal is to assess the impact of design choices and operational parameters on energy efficiency and IEQ. A co-simulation framework captures interactions across various domains: thermal (Simulated with EnergyPlus and Python-based models), daylight (simulated with Radiance, coupled with EnergyPlus for accurate solar impact representation) and Indoor Air Quality (simulated with Contam, integrated with EnergyPlus via a Functional Mock-up Interface). The system benefits from both a local DT for the façade and a general DT for the entire building. The co-simulation workflow integrates thermal, daylight, and IAQ simulations, with Python as the supervisory system, allowing iterative data exchange between EnergyPlus, Radiance, and Contam. Next steps include integrating Radiance simulations into the FMI framework and achieving real-time data updates from in-field sensors.

External collaborations

- Norwegian University of Science and Technology (NTNU)
- Eurecat Centre Tecnologic

Academic context

[1] Fabio Favoino et al. "5-Advanced fenestration - technologies, performance and building integration". In: Rethinking Building Skin - Woodhead Publishing Volume 26 (2022), pp. 117–154.
[2] Fabio Favoino et al. "Experimental analysis of the energy performance of an ACTive, RE-Sponsive and Solar (ACTRESS) façade module". In: Solar Energy 133 (2015), pp. 226–248.

First name: Yasemin **LAST NAME**: USTA

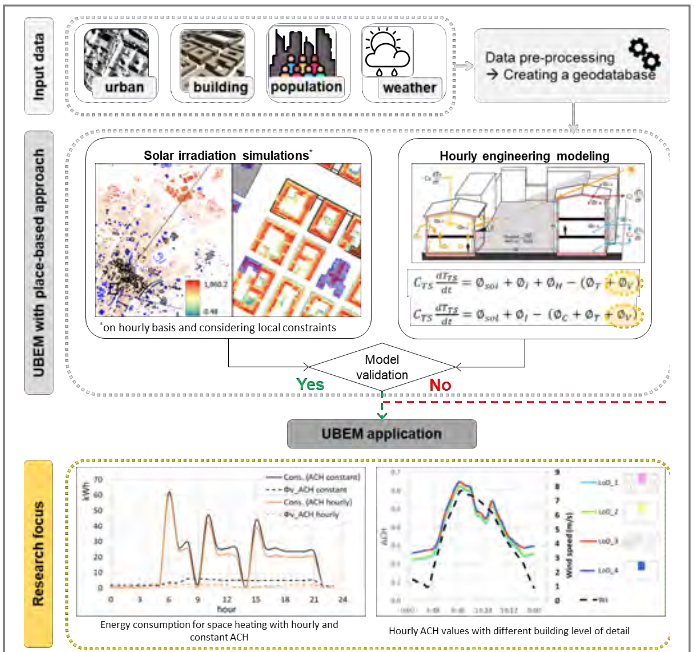
Topic: Buildings' Energy Modeling and Platforms for a Sustainable Development of Cities and Communities

Course year: 3rd **Tutor(s)**: Guglielmina MUTANI, Cristina BERTANI

Highlights of the research activity

Decarbonizing cities with existing building stock requires a detailed understanding of how buildings interact with their environment, as the building sector accounts for a significant share of urban energy use. Urban Building Energy Modeling (UBEM) is an important tool for analyzing energy performance and identifying strategies to reduce consumption, enhance efficiency, and integrate renewable energy sources. By connecting building-specific characteristics with urban parameters, UBEM offers critical insights into how the local environment affects each building's energy behavior. The current focus of this research is to analyze the impact of ventilation loads on the energy consumption of residential buildings. Wind speed is corrected based on the geometry of urban canyons and building orientation to accurately calculate airflow rates at certain heights. These airflow rates are used to calculate the air change per hour (ACH) values, which will be integrated into our existing hourly engineering model developed by our research group.

Currently, the hourly engineering model uses ACH values derived from a three-zone lumped parameter modeling [1]. This year, my work was directed toward validating the lumped parameter model using Contam, a software developed by NIST, to ensure the accuracy of our model. The next objective is to scale this approach to an urban level, using Contam to represent buildings with multiple zones for greater precision in energy and airflow analysis. This work aims to deepen our understanding of urban ventilation effects on the energy consumption of residential buildings.



UBEM approach and current research focus on hourly ACH as a function or urban and building geometry

External collaborations

- NIST – The National Institute of Standards and Technology, Maryland/USA
- Gruppo Iren,Torino, IT

Academic context

[1] Santantonio, S., Dell'Edera, O., Moscoloni, C. et al. Wind-driven and buoyancy effects for modeling natural ventilation in buildings at urban scale. Energy Efficiency 17, 95 (2024). https://doi.org/10.1007/s12053-024-10266-1

[2] Taddeo, P., Ortiz, J., Salom, J., Segarra, E.L., Vicente, González, G., Ruiz, G.R., & Bandera, C.F. (2018). Comparison of experimental methodologies to estimate the air infiltration rate in a residential case study for calibration purposes.

[3] Montazeri, A., Usta, Y., Mutani, G. (2024). Urban building energy modeling: A comparative study of process-driven and data-driven models. Mathematical Modelling of Engineering Problems, Vol. 11, No. 10, pp. 2615-2624. https://doi.org/10.18280/mmep.111003

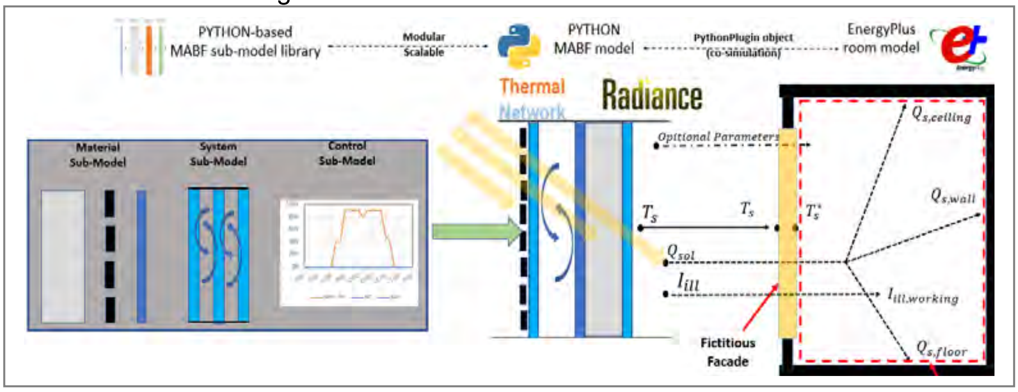
First name: Yangkong **LAST NAME**: ZHOU

Topic: Towards a tool for building performance simulation of Multi-functional and Adaptive Facade

Course year: 3rd **Tutor(s)**: Fabio FAVOINO

Highlights of the research activity

Achieving decarbonization from building sector demands innovative methodologies beyond traditional envelope approaches. This research emphasizes the development and evaluation of Multi-functional and Adaptive Façades (MAFs) that dynamically adjust thermo-optical properties to optimize indoor comfort, energy savings, and carbon emissions, with potential for power generation. Current challenges in assessing Advanced Building Envelopes(ABEs) performance at the building level include limitations in Building Performance Simulation (BPS) tools, knowledge gaps in developing physical numerical models, and difficulties in co-simulation data exchange.



To address these, a modular, scalable, and open-source Advanced Building Envelope (ABE) sub-model library is proposed, enabling customizable multi-physical domain simulations. The thesis outlines three key phases: 1) thermal co-simulation workflow, 2) coupled optical-thermal co-simulation workflow, and 3) sub-model modularization and assembly.

In the thermal domain, Micro-Fluidic Glazing (MFG) serves as a case study. A thermal Capacitance-Resistance (RC) model, validated against ISO 15099:2003 and experimental data, was integrated with EnergyPlus via a Python-based co-simulation framework. Building-level performance was assessed under various control strategies and configurations, demonstrating significant energy-saving potential.

For optical-thermal coupling, a framework linking EnergyPlus with Radiance was developed to evaluate advanced materials like translucent silica aerogel, characterized by ultra-lightweight, high insulation, and complex radiative properties. The multi-flux approach modeled its unique optical behavior, with ongoing validation and performance evaluation. These workflows establish robust methodologies for holistic ABE performance assessment.

External collaborations

- Polytech'Lab, UPR UCA 7498, Université Cote d'Azur Sophia Antipolis, France
- ETH Zurich Rämistrasse 101 8092 Zurich Switzerland
- China Academy of Building Research (CABR), Beijing, China

Academic context

[1] Zhou, Y., Gennaro, G., Fantucci, S., Ibrahim, M., Franquet, E., & Favoino, F. (2023). Building performance simulation of Advanced Building Envelope (ABE): towards a python-based open-source library to support co-simulation for design and operations. In Proceedings of Building Simulation 2023: 18th Conference of IBPSA (pp. 1215-1223). Shanghai, China. International Building Performance Simulation Association. DOI: 10.26868/25222708.2023.1628.
[2] Y. Zhou, M. Baracani, F. Favoino, S. Fantucci, M. Ibrahim, E. Franquet & V. Serra, "Numerical Modelling and Performance Assessment of MicroFluidic Glazing(MFG)", SDEWES, Dubrovnik, Croatia, 2023

First name: Khaoula **LAST NAME**: FRIJI

Topic: Application of advanced Numerical and Experimental based design approach for the optimization of the thermal performance of architectural integrated Solar Air Heating Façade Systems

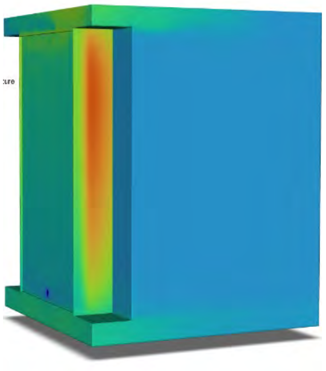
Course year: 1st **Tutor(s)**: Stefano FANTUCCI - Abdallah BOUABIDI

Highlights of the research activity

Advanced Solar Air Heating Façade (SAHF) is a passive solar heating technology designed to improve the energy efficiency of buildings.This system integrates a Trombe wall configuration or similar solar façade concepts to enhance heat transfer and storage.

In the first year of the PhD, the research focused on the study and optimization of Trombe wall systems used for heating buildings with solar energy.

The current phase of the PhD is dedicated to developing a simulation model of a fan-assisted solar façade and validating this numerical model using the experimental results through CFD simulations in ANSYS Fluent software. By integrating the experimental data with advanced numerical techniques, this research aims to deepen the understanding of the Trombe wall system's thermal performance and optimize its design for enhanced efficiency in sustainable building applications. Morover, preliminary analysis for evaluating different design alternatives, for a better architectural integration, will be experimentally evaluated in the lab by means of double climatic chamber apparatus (BET-cell) and in a full scale SAHF.



External collaborations

- M2EM Research Unit, university of Gabès, Tunisia.
- Laboratory of Building Construction & Building Physics (LBCP), Aristotle University of Thessaloniki.

Academic context

[1] F. Isaia, S. Fantucci, V. Serra, and V. Longo, “The effect of airflow rate control on the performance of a fan-assisted solar air heating façade,” IOP Conf. Ser.: Mater. Sci. Eng., vol. 609, no. 3, p. 032008, Sep. 2019.

[2] K. Friji, O. Ghriss, A. Bouabidi, Y. Aryanfar, H. G. Castellanos, and A. Keçebaş, “Optimizing Trombe Wall performances: The impact of L-shaped fins on solar heating efficiency and building thermal comfort,” International Journal of Heat and Fluid Flow, vol. 110, p. 109658, Dec. 2024.

First name: Ginevra **LAST NAME**: LI CASTRI

Topic: Energy Fexibility Potential Of Advanced Facades

Course year: 1st **Tutor(s)**: Fabio FAVOINO, Marco PERINO

Highlights of the research activity

Advanced facade technologies represent a solution to improve the energy flexibility of buildings, as they could provide a balanced behaviour across different building performance domains. The present work aims to propose a methodology to assess the degree of flexibility that these components can give to the building depending on the design and control strategy. The first year study prioritises two innovative technologies: dynamic glazing systems and double skin facades integrated with air-to-PCM latent heat exchangers.

The first focuses on spectrally selective dual-band electrochromic (DB-EC) windows, which can modulate solar radiation in both the visible and NIR and outperform conventional electrochromic glazing in terms of energy savings and occupant comfort. Simulation studies in five European climates showed that DB-EC windows, especially with model-based controls, can reduce annual energy consumption by up to 27% and improve visual comfort by 32%. This research also provided insights into the integration of experimental optical data into simulation workflows and highlighted the role of dynamic glazing in building energy flexibility.

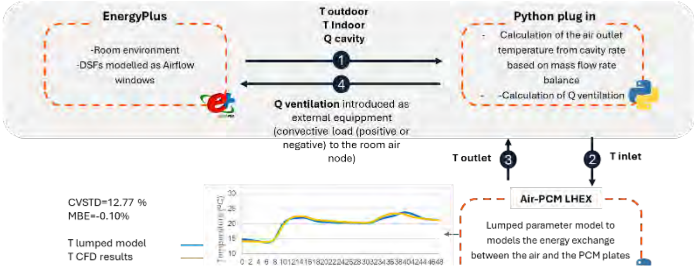


Figure 1 Co-simulation workflow

The second focus is on a novel double-skin façade with an air-to-PCM latent heat exchanger, developed under the Horizon 2020 'iclimabuilt' project. This component was evaluated through both simulation and experimental studies. A co-simulation workflow involving BEM software and a dedicated mathematical model was developed to simulate the PCM-Air HEX, optimised design variables such as glazing properties and PCM melting temperatures, showing that the façade improves energy performance in temperate climates when integrated with low g-value and U-value glazing. Experimentally, the prototype was characterized using extensive instrumentation in real-life conditions in an outdoor testing facility. The system demonstrated its ability to adjust ventilation strategies seasonally, reducing HVAC loads through energy storage and pre-heating or cooling of air, although it cannot fully maintain comfort conditions independently.

In the broader context, the research explores energy flexibility as a means of adapting buildings to dynamic grid requirements. By assessing advanced façade technologies, it seeks to enhance the adaptability of buildings to future energy needs, bridging the gap between energy efficiency and grid responsiveness. This first PhD year work lays the foundation for optimizing façade designs and operations to meet the multi-objectives aims.

External collaborations

- Leitat Technological center
- Horizon 2020 project Iclimabuilt
- MiSE-ENEA PTR 2022-2024, “Edifici ad alta efficienza per la transizione energetica: Rivestimenti superficiali e coating multifunzionali integrati nell’involucro opaco e trasparente per edifici salubri ed energeticamente efficienti”

Academic context

[1] Li Castri G., Baracani M., Favoino F., Serra V., Perino M. “Energy performance assessment of an innovative double-skin façade with Air-PCM heat exchanger”. Multiphysics and Multiscale Building Physics - Proceedings of the 9th International Building Physics Conference (IBPC 2024)

[2] Riganti M, Li Castri G, Serra V, Manca M, Favoino F. Energy saving potential of advanced dual-band electrochromic smart windows for office integration. Energy Build 2025;327:115084. https://doi.org/10.1016/j.enbuild.2024.115084.

[3] Gehbauer C, Lee ES, Wang T. An evaluation of the demand response potential of integrated dynamic window and HVAC systems. Energy Build 2023;298:113481.

First name: Martina **LAST NAME**: MAGGIULLI

Topic: Assessing the impact of AI-based intelligent services for enhancing the smartness of next generation grid-interactive buildings

Course year: 1st year **Tutor(s)**: Alfonso CAPOZZOLI, Cristian POZZA (Eurac)

Highlights of the research activity

The primary objective of the PhD activity is to develop a novel methodological framework for assessing the impact of data-driven intelligent services in buildings. In the first year of my PhD, I conducted an in-depth analysis of the current AI-based solutions used in building energy management. I also carried out a literature review of existing data-driven approaches to quantify the effects of implementing smart technologies and AI-based control strategies in buildings, with a particular focus on the emerging field of data-driven M&V. This employs real-time data from building operations and predictive models with the objective of enhancing energy savings assessments. A further research activity conducted during 2024 is the development of an innovative framework for the impact assessment of AI-driven services in integrated energy systems, as part of the Horizon Europe BuildON project. The main goal is the development of an evaluation framework designed to assess the impacts of various smart services and strategies deployed in different real-life buildings. Furthermore, in close connection with the aforementioned research, I focus on the development of a data-driven methodology for the European Smart Readiness Indicator (SRI). This indicator is a sort of qualitative KPI which evaluates the building's capability to use Information and Communication Technologies (ICTs) to adapt its operations to occupants' needs and the demands of the energy grid, always enhancing the overall building performance. The aim of my research in this field is to enhance the implementation of the SRI by addressing the challenges that have emerged from the existing literature and the current testing phase of this indicator. Specifically, I investigate the establishment of a data-driven methodology, using the monitoring data directly from buildings' operational phase, providing a precise evaluation of the actual level of smartness of the buildings, offering insight into the overall performance of the building stocks and identifying areas for improvement.

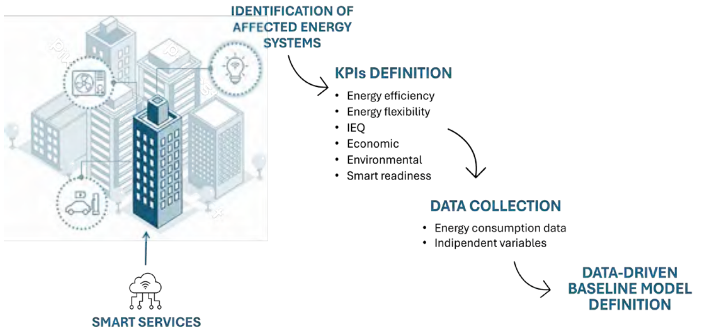


Figure 1. Scheme of the data-driven methodology developed to assess the impacts of smart control strategies in real-life buildings.

External collaborations

- GBC Italia.

Academic context

[1] Markoska, E.; Jakica, N.; Lazarova-Molnarc, S. and Kragh, M. K., "Assessment of Building Intelligence Requirements for Real Time Performance Testing in Smart Buildings," 2019 4th International Conference on Smart and Sustainable Technologies (SpliTech), Split, Croatia, 2019, pp. 1-6, doi:10.23919/SpliTech.2019.8783002.
[2] Märzinger, T.; Österreicher, D. Supporting the Smart Readiness Indicator—A Methodology to Integrate A Quantitative Assessment of the Load Shifting Potential of Smart Buildings. Energies 2019, 12, 1955. https://doi.org/10.3390/en12101955.
[3] Maggiulli, M., Piscitelli, M. S., & Capozzoli, A. (2024). A Data-Driven Approach to Evaluate the Smart Readiness Indicator for the Functionality "Respond to Users' Needs". In Sustainability in Energy and Buildings 2023 (pp. 589-599). Singapore: Springer Nature Singapore.

First name: Ahad **LAST NAME**: MONTAZERI

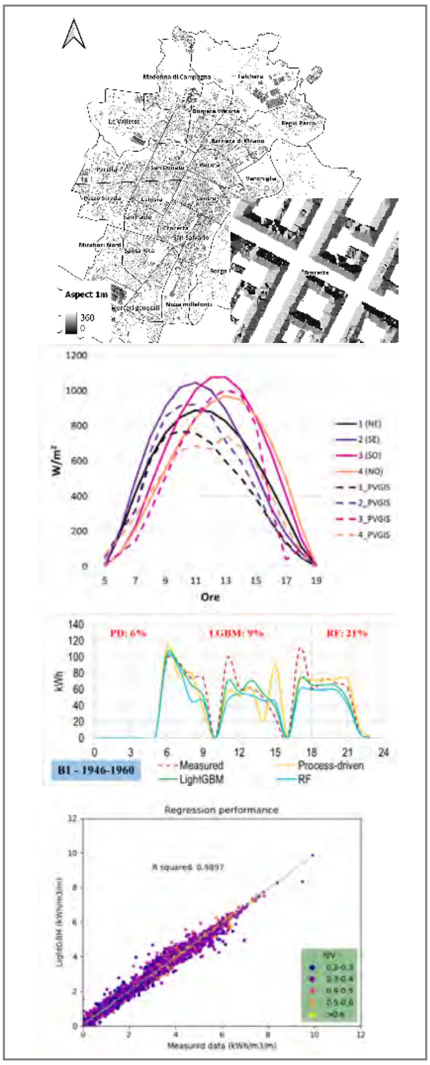
Topic: Modeling post-carbon cities and renewable energy communities

Course year: 1st **Tutor(s)**: Guglielmina MUTANI, Cristina Bertani

Highlights of the research activity

Integrating renewable energy sources (RES) into urban environments presents significant challenges in urban context. To address this, buildings must transition into active energy contributors or "prosumers," generating energy within certain limitations. Achieving this goal requires a comprehensive understanding of energy consumption patterns and production potential across larger scales, such as neighborhoods, or entire urban areas, to enable buildings to play an integral role in energy-sharing networks [1]. Urban Building Energy Modeling (UBEM) offers a robust framework for simulating and evaluating the energy efficiency of buildings on a broader scale. Using a bottom-up methodology, UBEM models the energy consumption and/or production of individual buildings and aggregates these findings to derive energy indices at the urban scale [2].

Focusing on placed-based approaches, my primary research aims have been to develop Process-driven and Data-driven UBEMs for detailed analyses of end-user energy consumption patterns. This research followed two parallel paths: first, exploring the application and potential of machine learning algorithms for predicting energy consumption, and second, advancing engineering models for building energy consumption predictions through hourly dynamic modeling. I enhanced the predictive performance of these models by integrating urban parameters that improve accuracy and reliability. In addition, I contributed to a study evaluating the rooftop potential for solar power generation across the city of Turin. This analysis involved a detailed assessment of rooftop availability, including identifying roof surface areas and orientations while accounting for constraints such as cultural restrictions, obstacles, or pre-existing solar installations. To streamline this process, I developed an image detection model capable of analyzing satellite images and orthophotos to identify and exclude rooftop disturbances. This method shows significant promise for optimizing the use of available rooftop space for solar energy production. The analysis remains under development, aiming to improve the model's performance in identifying rooftop obstacles. Further advancements include detailed modeling of rooftop surfaces by orientation and simulating solar radiation, the efficiency of solar thermal collectors (STCs), and the performance indices of photovoltaic (PV) panels for each roof configuration. By enhancing the reliability of such analyses in larger scales, the attempt is to support stakeholders in making informed decisions, ultimately facilitating more efficient and strategic energy planning.



External collaborations

- Gruppo Iren,Torino, IT
- Citta di Torino - Dipartimento Ambiente e Transizione ecologica
- Idiap research institute

Academic context

[1] Todeschi, V., Boghetti, R., Kämpf, J. H., & Mutani, G. (2021). Evaluation of Urban-scale building energy-use models and tools—Application for the city of Fribourg, Switzerland. Sustainability, 13(4), 1595

[2] Mutani, G., & Todeschi, V. (2020). Building energy modeling at neighborhood scale. Energy Efficiency, 13(7), 1353-1386.

First name: Marco **LAST NAME**: PAOLINI

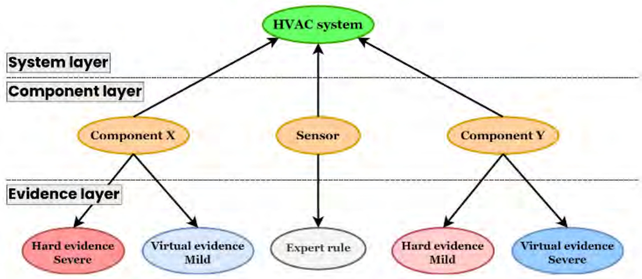
Topic: AI-based energy management and information systems for enhancing energy performance in grid-interactive efficient buildings

Course year: 1st **Tutor(s)**: Alfonso CAPOZZOLI, Marco Savino PISCITELLI

Highlights of the research activity

Energy Management and Information Systems (EMIS) offer valuable opportunities for building owners and facility managers to optimize energy use in buildings and their associated energy systems by leveraging data collected through monitoring infrastructures. By utilizing advanced data analytics and machine learning algorithms, EMIS solutions can transform raw monitoring data into meaningful insights, leading to more efficient energy management. In 2024, my research has focused on developing novel Fault Detection and Diagnosis (FDD) frameworks that can combine knowledge-based and data-driven strategies to accurately identify faults in building HVAC systems. Among various techniques, Bayesian Networks (BN) have proven particularly effective for FDD in HVAC systems. These networks model complex dependencies and uncertainties, providing a probabilistic graphical representation of relationships among HVAC system variables. In this context, the methods proposed in [1] include a Conditional Gaussian Network (CGN) and a Tree Augmented Naïve bayes classifier (TAN). A sensitivity analysis is conducted to identify the optimal number of input variables, aiming to achieve the best balance between model complexity and fault diagnosis performance. Moreover, a cost-sensitive approach is implemented for both Bayesian Network models to minimize the False Alarm Rate (FAR). The performance and effectiveness of these models are analyzed and compared to a baseline machine learning algorithm (Random Forest) demonstrating their potential to improve FDD techniques in building energy systems. Notably, the CGN-based models achieved the highest accuracy, and the cost-sensitive approach significantly reduced false alarms, achieving FAR values below 5% across all analyzed scenarios. Based on these results, my research has further explored hybrid FDD strategies to improve both interpretability and portability. A key innovation of the proposed framework is its independence from faulty labeled data, which are often scarce or unavailable in real-world applications. Moreover, the variables selected for analysis are intended to be as widely available as possible, while also minimizing the number of required sensors, avoiding excessive complexity. Additionally, the strategy addresses the challenges posed by interdependencies among system components and the presence of multiple operational modes, with a dedicated BN constructed for each mode of the building HVAC system.

Structure of hybrid Bayesian Network



External collaborations

- Università degli Studi della Campania Luigi Vanvitelli

Academic context

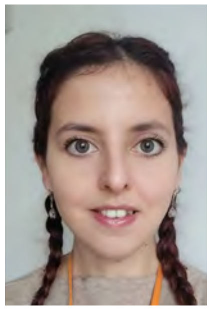
[1] Paolini, M., et al.: Experimental performance evaluation of cost-sensitive Bayesian Networks for fault detection and diagnosis in HVAC systems, Sustainability in Energy and Buildings 2024.
[2] Chen, Y., et al.: Using discrete Bayesian networks for diagnosing and isolating cross-level faults in HVAC systems. Appl. Energy, 327 (2022).
[3] Chen, Z. et al.: A review of data-driven fault detection and diagnostics for building HVAC systems. Appl. Energy, 339 (2023).

Industrial energy systems, technologies and materials for the energy transition

First name: Piera **LAST NAME**: DI PRIMA

Topic: Lithium-ion battery: calendar, cycle and fast charge aging

Course year: 3rd **Tutor(s)**: Massimo SANTARELLI, Silvia BODOARDO, Julia AMICI



Highlights of the research activity

This research focuses on understanding and modeling the degradation of lithium-ion batteries, with particular attention to LGM50LT cells. Calendar aging tests were conducted to assess anode and cathode degradation under varying state-of-charge levels and temperatures, while cycle aging tests, performed under subzero temperatures, focused on capturing lithium plating and its implications for battery performance. In addition to these studies, fast charging experiments were carried out at 25°C to explore the impact of high C-rate cycling on degradation. The findings from these experimental efforts informed the advancement of a simple modeling framework to a pseudo-four-dimensional (P4D) model, addressing the complex internal "jellyroll" structure of cylindrical cells. Building on experimental data collected from aging study, the P4D model was further refined to integrate multiple degradation mechanisms and their interactions. This was achieved by incorporating electrochemical kinetics dependent on the concentration of undesired species generated during degradation processes. The upgraded model, validated against experimental results, provides a highly accurate representation of battery aging, enabling the detailed investigation of individual and interacting degradation processes without the need for post-mortem analysis. Furthermore, the model serves as a predictive tool to estimate battery performance and lifetime under a variety of operating conditions, offering insights that are critical for the optimization of lithium-ion battery design and usage strategies. Additionally, a research period at the University of Ljubljana facilitated the application of the P4D model for impedance spectroscopy simulation, providing detailed insights into internal resistance and electrochemical dynamics. This comprehensive approach, combining experimental insights and advanced modeling, represents a step forward in understanding and mitigating the degradation of lithium-ion batteries, especially under demanding conditions such as fast charging.

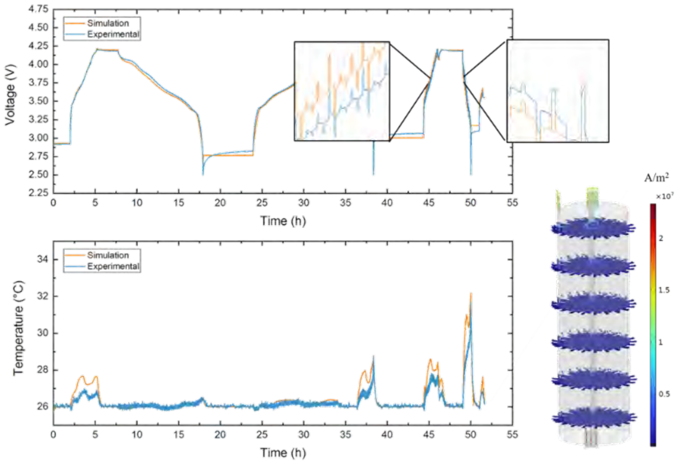


Figure 1 Model validation across various current regimes and current distribution within the jellyroll during charging.

External collaborations

- University of Ljubljana

Academic context

[1] Zülke, Alana, et al. "High-Energy Nickel-Cobalt-Aluminium Oxide (NCA) Cells on Idle: Anode- versus Cathode-Driven Side Reactions." Batteries & Supercaps, vol. 4, no. 6, 1 June 2021, pp. 934-47, doi:10.1002/batt.202100046.
[2] O'Kane, Simon E. J., et al. "Lithium-ion battery degradation: how to model it." Phys. Chem. Chem. Phys., vol. 24, no. 13, 30 Mar. 2022, pp. 7909-22, doi:10.1039/D2CP00417H.
[3] Di Prima, Piera, et al. "Understanding calendar aging degradation in cylindrical lithium-ion cell: A novel pseudo-4-dimensional electrochemical-thermal model." Appl. Energy, vol. 377, 1 Jan. 2025, p. 124640, doi:10.1016/j.apenergy.2024.124640.

First name: Simone **LAST NAME**: EIRAUDO

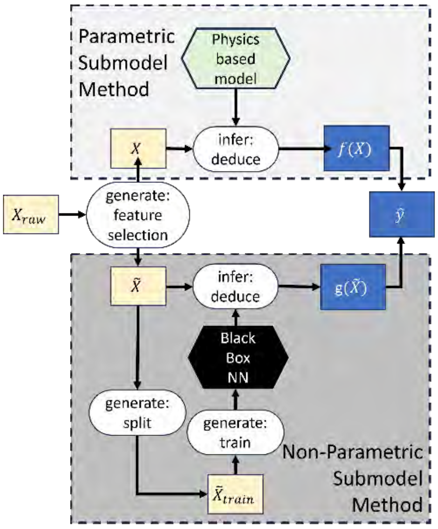
Topic: Artificial Intelligence for Energy Efficiency

Course year: 3rd **Tutor(s)**: 1st Andrea LANZINI, 2nd Lorenzo BOTTACCIOLI

Highlights of the research activity

Energy efficiency-oriented measures, including retrofit actions, optimal control of the buildings HVAC system reduction of abnormal events, and benchmarking of building stock, require deep understanding of the buildings' behavior, the physics underlying heat exchange with the environment and the other factor which affect buildings consumption. To this purpose, non-intrusive data-driven analysis, extracting useful information by the measurements collected by smart meters, is a fundamental research activity.Our research activity focuses on the application of advanced data analysis techniques, in particular Machine Learning algorithms, to be tested on a real-world case study, namely Data Centers. Our main research goals are:

- Identification of homogeneous groups of buildings and benchmarking
- Non-Intrusive Load Monitoring and anomaly detection
- Non-Intrusive Load Disaggregation
- Analysis of the buildings' thermal behavior
- Estimation of the benefits associated to retrofit actions.



A Semi-Parametric Regression Model

To these purposes, hourly electrical energy consumption data from about 2000 buildings were employed. During the previous years we focused on data pre-processing, buildings' benchmarking, and on the State-of Art techniques for energy audit of buildings. In addition to this, we designed specific Machine Learning-based tools, capable of providing reference thermal behavior and to estimate typical parameters of the buildings, such as the equivalent thermal resistance of the envelope, the cooling regimes intervals and the performance of the colling systems. Besides, the use of control charts, in particular, the so-called CuSum, enhanced detection of changes in operative conditions of the buildings and other deviation from reference behavior. During the last year, we worked on the integration of the previously employed tools in a unique framework. To this extent, we proposed the adoption of Semi-Parametric regression models, which can bring together the benefits of the parametric SoA energy audit tools, with the ones of the advanced forecasting algorithms, such as Neural Networks. The resulting ensemble approach features high load forecasting accuracy, can estimate buildings' typical parameters and is suitable to dive into the analysis of the impact of the input variables on buildings' consumption.

External collaborations

- Tim S.p.A.
- Departamento de Ciencias de la Computación e IA – Universidad de Granada

Academic context

[1] Afshari, A., & Friedrich, L. A. (2017). Inverse modeling of the urban energy system using hourly electricity demand and weather measurements, Part 1: Black-box model. Energy and Buildings, 157, 126-138.
[2] Miller, C., Nagy, Z., & Schlueter, A. (2018). A review of unsupervised statistical learning and visual analytics techniques applied to performance analysis of non-residential buildings. Renewable and Sustainable Energy Reviews, 81, 1365-1377.
[3] Garimella, S. V., Yeh, L. T., & Persoons, T. (2012). Thermal management challenges in telecommunication systems and data centers. IEEE Transactions on Components, Packaging and Manufacturing Technology, 2(8), 1307-1316.use font Arial 10)

First name: Djalila **LAST NAME**: GAD (née BEN-BOUCHTA)

Topic: A multi-disciplinary approach to energy service delivery to enable productive use of energy for female entrepreneurs in Africa

Course year: 3rd **Tutor(s)**: Pierluigi LEONE, Stefano CORGNATI

Highlights of the research activity

In alignment with several global initiatives, such as the UN SDG's focus on sustainable development, the European Green Deal's commitment to reducing greenhouse gas emissions and the Africa-Europe partnership to create sustainable prosperity, this research addresses energy access challenges faced by women entrepreneurs in Africa. By advancing inclusive energy transitions and exploring decarbonisation opportunities in small-scale industries, it contributes to shared global sustainability goals.

Filling critical gaps in the gender-energy nexus, this study examines productive energy use in the food and textile sectors across seven African countries: Egypt, Ghana, Kenya, Malawi, Nigeria, Tanzania, and Tunisia. Following the assessment of gendered productive use from 65 participating enterprises, the third year of research emphasised completing detailed energy audits and deepening the analysis of energy access from an additional 40 enterprises. A compilation of equipment, power ratings, energy carriers, and temperature requirements for the productive use sector was developed, crucial data for creating demand profiles that are typically not available. Using the World Bank's multi-tier framework (MTF), 40 women-owned enterprises were evaluated to assess energy access levels for both electric and non-electric energy carriers (see Figure 1). The analysis revealed sector-specific differences in energy access, with key challenges including reliability issues for electric supply (see Figure 2), affordability concerns for both electric and non-electric energy carriers, and significant health risks associated with the use of fossil fuels. Selected case studies explored the role of sustainable energy technologies – such as combined heat and power (CHP), heat pumps, solar PV, and biogas – in meeting energy needs and decarbonising small-scale industries.

Figure 1. Total energy access tier score obtained by industry sector (left graphic) and type of energy carrier (right graphic)

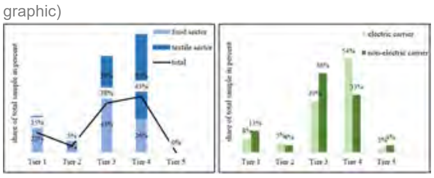
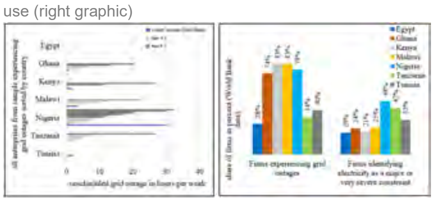


Figure 2. Grid outages across the sample in hours per week compared to national averages (left graphic) and national perceptions on grid outages and their impact on productive use (right graphic)



Looking ahead, findings will be integrated into actionable policy and financing recommendations, with feedback from entrepreneurs refining the practicality of proposed solutions. These steps will ensure the final thesis, on track for completion by June 2025, delivers impactful strategies for equitable energy transitions and sustainable development.

External collaborations

- ENI

Academic context

[1] Barua B.; Ferroukhi, R.; García-Baños, C.; Nagpal, D.; Renner, M. (2019): Renewable Energy: A Gender Perspective. Retrieved from IRENA Website: https://www.irena.org/publications/2019/Jan/Renewable-Energy-A-Gender-Perspective.

[2] Pueyo, A.; Maestre, M. (2019): "Linking Energy Access, Gender and Poverty: A Review of the Literature on Productive Uses of Energy". In: Energy Research and Social Science. Amsterdam, the Netherlands: Elsevier. Vol. 53. Issue July 2019. pp. 170-181. Doi: https://doi.org/10.1016/j.erss.2019.02.019.

[3] Bawakyillenuo, S.; Carreras, M.; Pueyo, A. (2020): "Energy Use and Enterprise Performance in Ghana: How Does Gender Matter?" In: The European Journal of Development Research. London, United Kingdom: Palgrave Macmillan. Vol. 32. Issue 4. pp. 1249-1287.

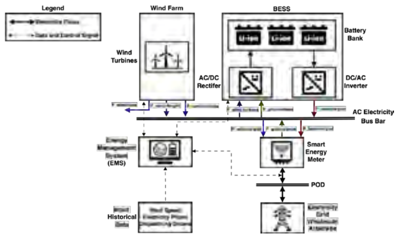
First name: Alberto **LAST NAME**: GRIMALDI

Topic: Optimal energy management and techno-economic analyses of utility-scale battery energy storage systems implementing price-taker optimization techniques

Course year: 3rd **Tutor**: Andrea LANZINI

Highlights of the research activity

During my PhD, I conducted comprehensive research on optimal energy management and techno-economic analyses of battery energy storage systems (BESS) integrated with renewable power plants. In the first year, my work focused on a detailed analysis of a utility-scale Li-ion BESS managed by Edison S.p.A., utilizing operational data to develop a data-driven empirical model. This research culminated in a publication in the *Elsevier Journal of Energy Storage* (https://doi.org/10.1016/j.est.2023.107232). In the second year, I advanced to optimization-based approaches, developing linear, mixed-integer linear, and mixed-integer non-linear programming techniques applied to BESS and PV-BESS energy systems. These research studies, developed during my mobility period at the University of California, Irvine (UCI), led to a collaborative journal article (https://doi.org/10.1016/j.est.2024.112380), and a collaborative conference proceeding presented at the 2024 IEEE PES General Meeting (https://doi.org/10.1109/PESGM51994.2024. These works demonstrated the economic potential of BESS and PV-BESS systems under real-world market conditions (i.e., CAISO electricity market), and highlighted the importance of incorporating critical factors (e.g., battery degradation and dynamic efficiency) into optimization frameworks in achieving realistic profitability results.
In my third year, I further refined these models, focusing on integrating BESS with an existent wind farm for wholesale energy arbitrage. I developed an optimization framework to determine the optimal battery size and dispatch strategy, incorporating a cycle-counting degradation model to evaluate battery ageing impacts. Using historical data from the Italian electricity market, I analyzed the economic viability of the wind farm-BESS system, finding that battery cost reductions below 325 €/kWh are necessary for financial feasibility. Key design, energy, and economic indicators were evaluated based on the optimization results. Sensitivity analyses were performed, focusing on the most relevant KPIs, such as battery cost, efficiency, and curtailed wind energy. This work, completed in collaboration with Edison S.p.A., is under review in the *Elsevier Journal of Energy Storage*. Additionally, I supervised a Master's Thesis projetc exploring similar topics (https://webthesis.biblio.polito.it/secure/31989/1/tesi.pdf).
My future research activity will explore multi-services optimization for BESS. I plan to develop forecasting models, such as Convolutional Neural Networks (CNNs) models, to simulate energy storage operations under varying market conditions. Furthermore, I aim to extend my work to hybrid energy storage systems, integrating Li-ion batteries with long-duration solutions like hydrogen-based storage. These next steps will form the core of my postdoctoral research at Argonne National Laboratory.



Wind Farm-BESS Layout

External collaborations

- Samueli School of Engineering, University of California Irvine (UCI), Irvine, California, USA.
- Research, Development & Technological Innovation, Edison S.p.A., Energy Center, Turin, Italy.

Academic context

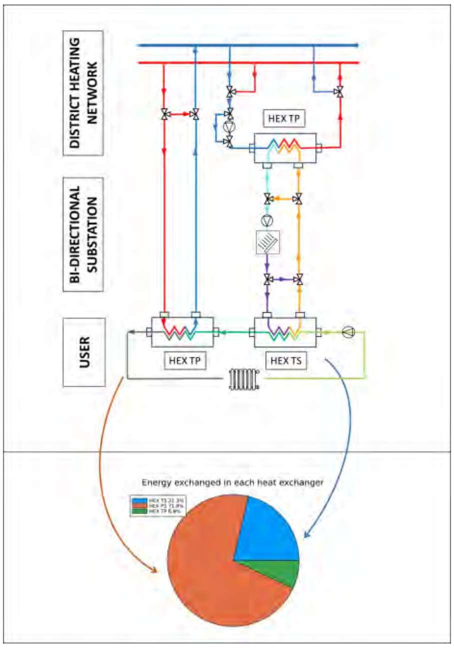
[1] A. Grimaldi, F. D. Minuto, J. Brouwer, and A. Lanzini, *"Profitability of energy arbitrage net profit for grid-scale battery energy storage considering dynamic efficiency and degradation using a linear, mixed-integer linear, and mixed-integer non-linear optimization approach"*, Journal of Energy Storage, 95, 112380, 2024. https://doi.org/10.1016/j.est.2024.112380
[2] F. Wankmüller, P.R. Thimmapuram, K.G. Gallagher, A. Botterud, *"Impact of battery degradation on energy arbitrage revenue of grid-level energy storage"*, Journal of Energy Storage, 10, 56–66, 2017.
[3] D. M. Rosewater, D. A. Copp, T. A. Nguyen, R. H. Byrne, and S. Santoso, *"Battery Energy Storage Models for Optimal Control"*, IEEE Access, 7, 178357–178391, 2019.

First name: Giulia **LAST NAME**: MANCO’

Topic: Advanced management for resilient and sustainable multi-energy systems **Course year**: 3st **Tutor(s)**: Vittorio VERDA, Elisa GUELPA

Highlights of the research activity

In the context of Multi-Energy Systems (MES) operation optimisation several challenges remain to be addressed: a) the characterisation of uncertainties affecting these systems; b) the operation of the district heating networks which are rapidly changing due to flexibility measures, prosumers integration, and operation at different temperature levels; c) the need for experimental validation to confirm the accuracy of the mathematical models and the competitiveness of the proposed MES strategy with respect to existing management strategies. My research aims to fill these gaps by developing a reliable optimisation model for the management of multi-energy systems, ranging from individual buildings to district level systems such as distributed generation systems. Particular emphasis is placed on modelling the district heating network and its integration with other system components (solar thermal, water heat pumps, thermal storage system). For my research, I can rely on a laboratory-scale system installed at the Energy Centre in Turin, which allows the validation of the mathematical models for individual components. Since the system was completed, we have been conducting various tests to compare the results with our digital twin developed in previous years. In parallel, over the past year, my research has focused on analysing various thermal prosumer district heating connections and how the type of configuration can influence the network operation. This analysis has led to the development of a simulation tool to model the behaviour of different heat exchangers needed in the so-called “bidirectional substation”. Additionally, an optimization tool has been developed to define the optimal design and operation of a solar thermal prosumer in the network. This tool determines the area of solar thermal collectors to be installed, the operating temperature of the solar thermal system, and the size of a potential heat pump to raise the thermal level of the water exiting of the solar system. The design decisions are driven by operational factors, particularly regarding sales to the network, which can occur in two modes: selling to the supply line or to the return line, depending on the temperature level achieved by the technologies. Given the importance of this topic, the research team decided to build a new test bed to thoroughly study the behavior of a thermal prosumer, so I am currently working on its design.



Bi-directional substation and some results from the simulation tool for the winter period.

External collaborations

- YANMAR R&D Europe S.r.L.
- IREN S.p.A

Academic context

[1] Guelpa E., Bachi A., Verda V., Chetco M., Lund H. Towards future infrastructures for sustainable multi-energy systems: A review. Energy 2019, Vol 184, Pages 2-21.
[2] Pipiciello M.- Trentin F., Soppelsa A., Menegon D., Fedrizzi R., Ricci M., Di Pietra B., Sdringola P., The bidirectional substation for district heating users: experimental performance assessment with operational profiles of prosumer loads and distributed generation, Energy and Buildings 2024, Vol.305, Pages 113872.
[3] Manco’ G., Tesio U., Guelpa E., Verda V., A review on multi energy systems modelling and optimization Applied Thermal Engineering 2023. Volume 236, Part E, Pages 121871.

First name: Francesco **LAST NAME**: ORSINI

Topic: Chemical looping applied to synthetic fuels production via solar thermochemical routes

Course year: 3rd **Tutor(s)**: Massimo SANTARELLI, Domenico FERRERO

Highlights of the research activity

The research activity covered both experimental activity and modeling. On the experimental side, the investigation on $Sr_2FeMo_{0.6}Ni_{0.4}O_6$ (SFMN) double perovskite in the Reverse Water-Gas Shift Chemical Looping (RWGS-CL) process were deepened with further experimental tests, suggesting how reversible metal nanoparticles exsolution – achievable at high temperatures in reducing atmosphere – can be addressed tuning some of the operational parameters. However, these results are still in the phase of preliminary analysis and verification and will be integrated with detailed microscopy characterizations conducted in collaboration with University of Udine and National Institute of Materials Physics (Măgurele, Romania). Fig.1 shows the pristine sample with smooth surface (metals embedded in the lattice), and the reduced sample with exsolved nanoparticles on the surface.

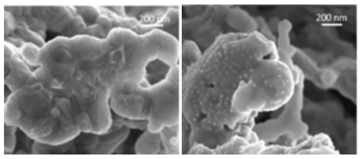


Fig.1. SFMN as pristine (left); after 2 h at 2.5% H2/Ar at 850 °C (right).

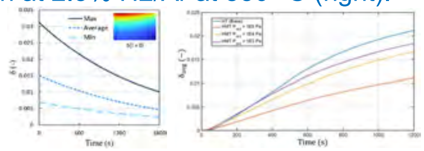


Fig.2. δ(t) evolution in the porous domain – ox. model (left); impact of total pressure – red. model (right).

On the modeling side, multiphysics modeling of solar reactors for solar thermochemical fuel production was addressed, mostly in collaboration with Massachusetts Institute of technology (MIT). Thermochemical Water Splitting (TCS) was simulated. To meet the literature gap identified by a comprehensive overview, a detailed modeling methodology for the oxidation step was developed, validated against third models, and tested in sample studies. The novel approach features (i) easiness of coupling to other physics in multiphysics modeling, (ii) inclusion of detailed morphology-calibrated kinetics, and (iii) wide versatility and applicability. The complete multiphysics model (currently addressing dual-scale porosity ceria structures as the active material) includes: fluid flow in the free-flow and porous domains; reactive species transport; heat transfer in and out of the porous medium (including local thermal non-equilibrium resolved in the porous domain); radiative heat transfer; gas-phase water splitting equilibrium; redox thermodynamics to impose the equilibrium limit to nonstoichiometry; and oxidation kinetics based on the novel method developed. Fig.2 (left) shows how the nonstoichiometry is decreasing in time in the porous ceria domain in a sample simulation, with the inset showing the initial δ distribution taken from a parallel multiphysics reduction model. The development of a multiphysics reduction model was indeed the second milestone of the activity. Specifically, a previous reduction model developed at MIT, including accurate heat transfer (HT) modeling, was expanded and detailed integrating heat and mass transfer (HMT) physics and implementing sophisticated porous morphology correlations and redox thermodynamics models taking into account the full dependence of equilibrium nonstoichiometry on T and pO_2, that is of utmost importance in the reduction step. Models were successfully cross validated. Fig.2 (right) shows the impact of total pressure (red: 1 atm, yellow: 0.1 atm, violet: 0.01 atm) on average nonstoichiometry evolution during a sample reduction simulation, against HT alone (blue profile).

External collaborations

- University of Udine
- Massachusetts Institute of Technology

Academic context

[1] Orsini et al., «Exsolution-enhanced reverse water-gas shift chemical looping activity of Sr2FeMo0.6Ni0.4O6-δ double perovskite», Chem Eng Journal 2023. DOI: 10.1016/j.cej.2023.146083.
[2] A. Lidor, T. Fend, M. Roeb, and C. Sattler, “High performance solar receiver–reactor for hydrogen generation,” Renewable Energy, vol. 179, pp. 1217–1232, Dec. 2021, DOI: 10.1016/j.renene.2021.07.089.

First name: Roberto **LAST NAME**: PAGLINI

Topic: Analytics for methane emissions detection and quantification from the

Natural Gas Distribution Network

Course year: 3rd **Tutor(s)**: A. Lanzini, F.D. Minuto, R. Borchiellini

Highlights of the research activity

In Italy, in cooperation with Italgas Reti, the High Flow Sampling (HFS) experimental campaign started in 2023 was implemented into standard leak detection and repair practices, enabling the gathered emission rate data from a few hundreds of detected leaks across Italy. The analysis of these data enables the investigation of direct-measurement-based source-level leak rate estimates for natural gas service lines to support the existing site-level leak detection surveys carried out by the Natural Gas Distribition System Operator (DSO) on national scale by means of a commercial system. The investigation of the leakage phenomena in the Italian DSO network has been further developed though the integration of the site-level monitoring on national scale with leak rapair data from blue collar personnell. The resulting dataset has been used to derive the main failure modes of the Italian natural gas distribution network that result in lekage from pipes and equipment. Finally, methane controlled release experiments have been carried out in a test facility owned by Italgas Reti to assess the quantification accuracy of the High Flow Sampling analyzer as well as the responses of the site-level commercial system used by the DSO to controlled emissions in from an heterogeneous set of above-ground and underground sources.

Left: atmospheric methane peaks detected with a mobile system are merged with wind direction data to triangulate a gas emission source in an industrial plant in France.

Right: a laser-based high flow sampling analyzer is used to measure methane leak rates from natural gas pipelines in Italy.

In the Netherlands and in France, the research focuse shifted from the source-level quantification to the site-level one. There, additional controlled release experiments have been carried out in cooperation with Utrecht University and Total Energie inside a real industrial site. Atmospheric methane changes resulting from (single-blinded) controlled emissions have been investigated by driving a vehicle with different commercial methane analyzers on board as well as a GPS system and an anemometer. Sensors' data are used to localize methane peaks, triangulate the emission source and estimate the downwind distance of the detected peaks. The collaboration with different institutions participating with different analyzers allows to adress the effect that analyzers' characteristics (e.g., sampling frequency, pump speed) have on the model; thus, on the final emission rate estimates.

External collaborations

- ITALGAS RETI
- UTRECHT UNIVERSITY
- UN ENVIRONMENTAL PROGRAMME (OGMP 2.0)

Academic context

[1] Maazallahi, Hossein, et al. "Methane mapping, emission quantification, and attribution in two European cities: Utrecht (NL) and Hamburg (DE)." *Atmospheric Chemistry and Physics* 20.23 (2020): 14717-14740.
[2] Lamb, Brian K., et al. "Direct measurements show decreasing methane emissions from natural gas local distribution systems in the United States." *Environmental Science & Technology* 49.8 (2015): 5161-5169.

First name: Elena **LAST NAME**: ROZZI

Topic: Decarbonization of the gas sector: green fuels and carbon emissions mitigation

Course year: 3rd **Tutor(s)**: Andrea LANZINI, Massimo SANTARELLI

Highlights of the research activity

To address the urgent need to mitigate methane emissions, a greenhouse gas with 80 times the global warming potential of CO_2 over 20 years, our research emphasizes transitioning from estimates to direct measurements of methane emissions. Collaborating with Italy's largest gas distribution grid operator, we align our efforts with the European Green Deal's ambitious goal of climate neutrality by 2050. Our work encompasses monitoring, reporting, and mitigating gas emissions across the gas distribution infrastructure, integrating innovative methodologies and technologies to achieve precise emission assessments.

Fig. Map of the leak probability of the gas distribution grid.

A cornerstone of our research involved quantifying methane emissions across Italy's national gas distribution network using an advanced mobile measurement method. This approach enabled comprehensive surveys, facilitating a detailed analysis of the network's emission landscape. By correlating leak events with specific pipeline characteristics, we developed a robust framework for targeted mitigation strategies.

Our top-down vehicle-based surveys captured high-resolution georeferenced data, complemented by bottom-up measurements of specific sources to ensure a balanced and thorough emissions assessment. To further refine the emission estimates, we employed a data-driven approach to prioritize monitoring and maintenance activities. This analysis involved the application of spatial clustering techniques and detailed statistical assessments of both underground mainlines and above-ground pipelines using Python and QGIS software.Multivariate linear models, Bayesian Poisson regression models, and advanced machine learning algorithms were implemented to enhance predictive capabilities and improve the accuracy of activity and emission factor predictions. These models accounted for infrastructure characteristics, such as age, material, nominal operating pressure, and corrosion protection, along with exogenous factors like hydrogeological risk, proximity to the sea, traffic, and railways.These approaches not only provided valuable insights for predicting leaks but also informed the development of preventive strategies tailored to the network's unique characteristics. Our work not only contributes to accurate reporting and compliance with frameworks such as the OGMP 2.0 but also offers actionable insights for reducing emissions, advancing the EU’s decarbonization goals, and establishing a benchmark for future methane reduction initiatives worldwide.

External collaborations

- Italgas Reti

Academic context

[1] Weller, Z. D.; Hamburg, S. P.; von Fischer, J. C. A National Estimate of Methane Leakage from Pipeline Mains in Natural Gas Local Distribution Systems. *Environ Sci Technol* **2020**, *54* (14), 8958–8967. https://doi.org/10.1021/acs.est.0c00437

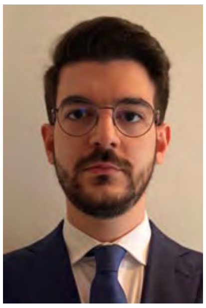
[2] GERG. *Methane Emission Estimation Method for the Gas Distribution Grid (MEEM) - Requirements for a Benefit-Effort Optimized Method, Potential for Improvements and Need for Further Research*; 2018.

[3] Climate and Clean Energy Coalition. *Mineral Methane Initiative OGMP2.0 Framework*; 2020.

First name: Davide **LAST NAME**: TRAPANI

Topic: Design, modelling and optimization of power-to-hydrogen systems for the decarbonization of industrial processes

Course year: 3rd **Tutor(s)**: M. SANTARELLI



Highlights of the research activity

Green hydrogen is widely recognized as a promising strategy to effectively curb CO_2 emissions in hard-to-abate industries, but some techno-economic challenges have still to be solved. The PhD research activity thus focuses on the modelling and cost-optimal design of power-to-hydrogen (P-t-H) systems with the goal of identifying the most viable and cost-effective configuration for various industrial processes. During the third year of the PhD, the previously developed optimization tool was further improved by including additional features. The techno-economic modelling of alkaline and proton exchange membrane (PEM) electrolyzers was refined with real data from MW-range systems and the zero-dimensional electrochemical models of anion exchange membrane (AEM) and solid oxide (SO) electrolyzers were implemented. Hydrogen production from steam methane reforming (SMR) was incorporated into the model and the hydrogen production cost was estimated based on a well-established correlation available in literature, which was properly modified to include also the cost of CO_2 emissions. Moreover, a database of historical natural gas prices for non-household consumers and values from the European Emission Trading System (EU ETS) market was created and integrated into the cost-optimal design tool. Hydrogen handling and transport were also modelled considering pressurized tube trailers at 200, 350 and 540 bar and liquid hydrogen. Modelling the SMR production process and the hydrogen transport allows for an in-depth evaluation of the cost-competitiveness of P-t-H plants. Specifically, when investigating the decarbonization of an industrial site relying on merchant hydrogen, it enables the determination of a breakeven distance for the cost-parity between fossil-based and renewable hydrogen.

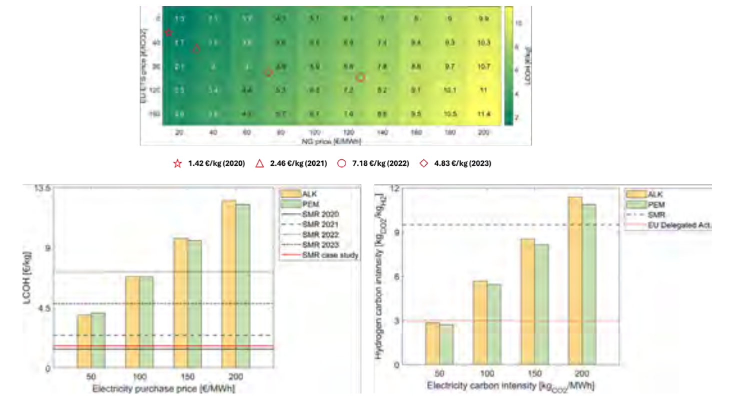


Figure 1. Cost and emission assessment of an oil refinery.

The updated version of the optimal design tool was then applied to investigate the cost-effectiveness of installing a P-t-H system in a real oil refinery located in Augusta (Italy). A grid-connected configuration was investigated and a sensitivity analysis on the electricity purchase price (50-200 €/MWh) was conducted. Finally, a cost and emission comparison with the SMR scenario was carried out, as shown in Figure 1.

External collaborations

- Environment Park S.p.A., Turin (Italy)
- SINTEF, Trondheim (Norway)
- Enel Green Power, Milan (Italy)

Academic context

[1] I. Moradpoor et al., "Green hydrogen production for oil refining – Finnish case," Renewable and Sustainable Energy Reviews, vol. 175, Apr. 2023, doi: 10.1016/j.rser.2023.113159.
[2] R. Dufo-López et al., "Optimisation of size and control strategy in utility-scale green hydrogen production systems," Int J Hydrogen Energy, 2023, doi: 10.1016/j.ijhydene.2023.08.273.
[3] G. Matute et al., "Techno-economic model and feasibility assessment of green hydrogen projects based on electrolysis supplied by photovoltaic PPAs," Int J Hydrogen Energy, vol. 48, no. 13, pp. 5053–5068, Feb. 2023, doi: 10.1016/j.ijhydene.2022.11.035.

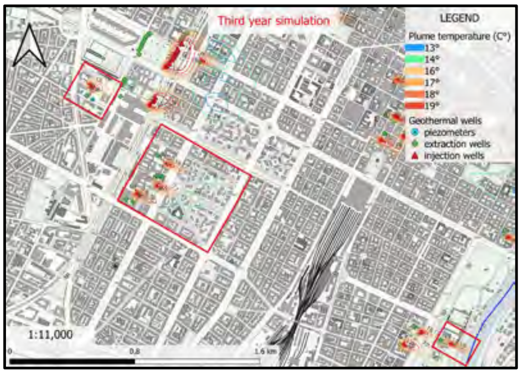
First name: Alessandro **LAST NAME**: BERTA

Topic: Geothermal Energy Low Enthalpy in urban contest

Course year: 2nd **Tutor(s)**: Glenda TADDIA, Vittorio VERDA

Highlights of the research activity

To adequately address the escalating challenges posed by climate change, it is essential to implement a substantial transformation in energy systems, particularly within the heating and cooling sector. This sector continues to be a significant contributor to greenhouse gas emissions, necessitating a transition towards renewable energy solutions in order to achieve global net-zero targets by 2050. In order for Italy to achieve the climate goals set out by the EU for 2030, the proportion of renewable energy used for heating must be increased from 20% to 34%. In this context, low-enthalpy geothermal energy emerges as a crucial element, particularly in urban settings, where geothermal heat pumps provide sustainable and efficient solutions for heating and cooling buildings. Low-enthalpy geothermal systems employ the utilisation of moderate heat from shallow subsurface layers, typically within 200 metres, which is then transferred via heat pumps in order to reduce carbon emissions. My research is centred on the integration of these systems into district heating networks, with a particular focus on advanced numerical simulations. In order to model the performance of geothermal energy systems under a variety of operational scenarios, I utilise both finite element and finite difference methods. This encompasses an analysis of the thermal efficiency and environmental impact of open-loop and closed-loop systems. Open-loop systems extract and reinject groundwater from shallow aquifers, whereas closed-loop systems circulate a heat transfer fluid through sealed underground loops, either horizontally or vertically. In addition to geothermal heat pumps, my work addresses the variability of renewable energy sources like solar. This necessitates the development of effective energy storage solutions for maintaining grid stability and ensuring energy availability. The objective of my research is to explore the potential of underground thermal energy storage technologies, with a particular focus on Aquifer Thermal Energy Storage and Borehole Thermal Energy Storage, as a means of storing excess thermal energy for utilisation during periods of high demand. These systems offer a particularly advantageous solution in densely urbanised areas, where space for traditional energy infrastructure is limited. A series of numerical simulations is employed to evaluate the long-term sustainability, efficiency, and environmental impact of new low-enthalpy geothermal and thermal storage systems. The incorporation of geological, hydrological, and thermal data into the models allows for the optimisation of system design and the formulation of strategies for large-scale deployment.



Simulation of geothermal plants in Torino city

External collaborations

- Iren S.p.A.
- Norwegian University of Science and Technology (NTNU)

Academic context

[1] A. Berta, M. Gizzi, G. Taddia, S. Lo Russo, The role of standards and regulations in the open-loop GWHPs development in Italy: The case study of the Lombardy and Piedmont regions, Renew Energy 223 (2024) 120016. https://doi.org/10.1016/j.renene.2024.120016
[2] M. Gizzi, A. Berta, F. Vagnon, G. Taddia, Groundwater heat pumps diffusion in the Turin city urban area: modelling for the thermally affected zone analysis of an open-loop geothermal system, https://doi.org/10.4408/IJEGE.2024-01.S-19
[3] A. Berta, G. Taddia, Exploring Urban Sustainability: The Role of Geology and Hydrogeology in Numerical Aquifer Modelling for Open-Loop Geothermal Energy Development, the Case of Torino (Italy). https://doi.org/10.3390/GEOSCIENCES14070180

First name: Matteo **LAST NAME**: CALO’

Topic: Hydrogels for adsorption-based desalination

Course year: 2nd **Tutors**: Eliodoro CHIAVAZZO, Matteo FASANO, Vincenzo Maria GENTILE

Highlights of the research activity

Many industrial and domestic applications require an effective capture of water molecules in the vapor phase, with aims ranging from preserving machinery integrity to clean water production, from heat storage to providing a proper level of dehumidification or humidification. In this context, adsorption-based machines represent a viable solution, with most of the current commercial implementation using silica-gels or zeolites as active material. Sorption Technologies Srl is interested in understanding whether polymeric hydrogels can be a suitable alternative adsorbent material for one of their most recent industrial applications: water desalination. Considering the high water uptake shown in experimental campaigns and the numerical models developed during the 1st PhD year, the candidate selected the composition *NaAlg1Psi10* as possible suitable sorbent for the application [1].
Given the availability of resources in company spaces in Germany, the candidate worked abroad on designing and producing a testing rig and then on assembling an adsorption-based machine in Sorption Technologies’ workshop in Mönchengladbach. The first prototype was functional in June 2024: the candidate played the role of designer, tester, and data analyst. A second prototype (for the Horizon Europe EU project ZHENIT) is currently under production, implementing some improvements such as an easier system to replace the salty water in the input and the clean water in the output. These prototypes, at the moment, implement silica-gel as an adsorbent. Some preliminary stress tests on a smaller prototype are necessary to replace it with the chosen hydrogel composition. To do so, a third smaller company prototype at the Clean Water Center (CWC) in PoliTO was adapted and prepared for testing by the candidate. An experimental setup like in [1] was built for producing 900 grams of dry calcium alginate for the necessary future activities. The plan for the last PhD year is to replace the material in the small prototype and perform a full experimental campaign to prove the feasibility of the use of this hydrogel composition for desalination.

Figure: (a) Prototype for adsorption-based desalination at CWC; (b) hydrogel spheres after gelification; (c) Final product: 900g of NaAlg1Psi10 spheres, after processing and drying.

External collaborations

- Sorption Technologies Srl

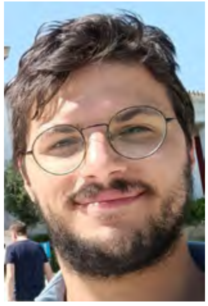
Academic context

[1] V. Gentile, M. Calò, M. Bozlar, M. Simonetti, F. Meggers, “Water Vapor Mass Transfer in Alginate-Graphite Bio-based Hydrogel for Atmospheric Water Harvesting”, International Journal of Heat and Mass Transfer (2024), https://doi.org/10.1016/j.ijheatmasstransfer.2023.124794.
[2] Y. Zhang, D. Palamara, V. Palomba, L. Calabrese, A. Frazzica, “Performance analysis of a lab-scale adsorption desalination system using silica gel/LiCl composite”, Desalination (2023), https://doi.org/10.1016/j.desal.2022.116278.
[3] V. Gentile, M. Bozlar, M. Calò, M. Simonetti, F. Meggers, “Alginate Biopolymeric Coated Heat Exchanger for Atmospheric Water Harvesting”. ACS ES&T WATER, 2024. DOI: https://dx.doi.org/10.1021/acsestwater.3c00847.

First name: Alberto **LAST NAME**: FERRARESE

Topic: Offshore renewable energy generation for H2 production in long-term models of Europe

Course year: 2nd **Tutor(s)**:Massimo SANTARELLI, Giuliana MATTIAZZO



Highlights of the research activity

The main activities of this year were 2:

1) Definition of an Exclusion parameters Taxonomy and of “Exclusion scenarios” for offshore energetic applications.
2) H2 producibility and LCOH assessments, spatially solved over the eligible areas identified.

Exclusion parameters Taxonomy and Exclusion scenarios

This activity aimed to detect eligible areas to be used for green energy and H2 production. The taxonomy of “exclusion parameters” was necessary since there is not a unique nomenclature nor a clear definition of the set of parameters to be used for a specific kind of GIS-based energetic study. Assigning to each “study profile” (i.e., theoretical models of kind of studies) a set of classified exclusion parameters, has been possible to produce the “exclusion scenarios”. They can be used to identify and set the specific conditions required for the performance of the offshore, GIS-based, energy-oriented eligibility study desired, guaranteeing a correct comparison among studies. One of these exclusion scenarios has been used in my research to select the eligible areas of the northern Adriatic Sea, to generate input data for macro-scale energy models.

Model for spatially solved H2 producibility and LCOH assessment

The spatially solved LCOH and H2 producibility assessments are main goals of my PhD. The H2 production system had been designed with a PEM electrolyser (PEMEL) coupled with an offshore wind farm (OWF). The system cost and the H2 producibility have been designed considering an H2 centralized production by means of an H2 hub sited in the OWF field barycenter which also sets the values of physical inputs for the model. The produced H2 is supposed to be transported to the mainland thanks an underwater pipeline. Some spatially dependent parameters influence the model and the spatially solved LCOH assessment demonstrated its strong dependency from them. A sensitivity analysis on the LCOH with respect to the PEMEL size has been also performed, looking for an optimum as the best trade-off between PEMEL costs and H2 producibility. However, on the contrary of what happens for onshore sites, this optimum seems to be hidden from the high OWF installation costs.

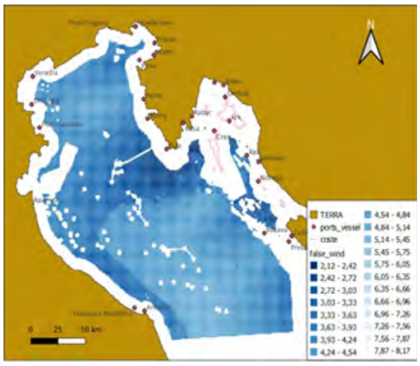


Figure 1 Spatially solved LCOH for the eligible areas of the northern Adriatic Sea

The future activities (e.g., identification of the best sites for production and displacement of offshore green H2) will be developed partially abroad, in collaboration with the Norwegian SINTEF research center.

External collaborations

- SINTEF

Academic context

[1] Rafael Martínez-Gordón et al., Benefits of an integrated power and hydrogen offshore grid in a net-zero North Sea energy system, Advances in Applied Energy, 2022, https://doi.org/10.1016/j.adapen.2022.100097
[2] Andy Moore et al., The role of floating offshore wind in a renewable focused electricity system for Great Britain in 2050, Energy Strategy Reviews, 2018, https://doi.org/10.1016/j.esr.2018.10.002
[3] Laura Castro-Santos et al., Planning of the installation of offshore renewable energies: A GIS approach of the Portuguese roadmap, Renewable Energy, 2019, https://doi.org/10.1016/j.renene.2018.09.031

First name: Pacifique **LAST NAME**: KOSHIKWINJA MATABISHI

Topic: Regional Energy modeling for green energy carrier production and utilization in Africa.

Course year: 2nd **Tutor(s)**: Pierluigi LEONE & Marco CAVANA

Highlights of the research activity

The primary objective of my Ph.D. research is to develop a customized regional energy model for the Southern African Development Community (SADC) region, incorporating the local socio-economic context. This model will enable the analysis of various pathways for green energy carriers' production and utilization in the African continent. It also aims to assess the role of productive energy uses in achieving clean energy access, focusing on electricity and clean fuels such as hydrogen, particularly for domestic industrial applications in Africa in line with the AU Agenda 2063 and the joint vision for 2030 between Africa and Europe towards energy transition.

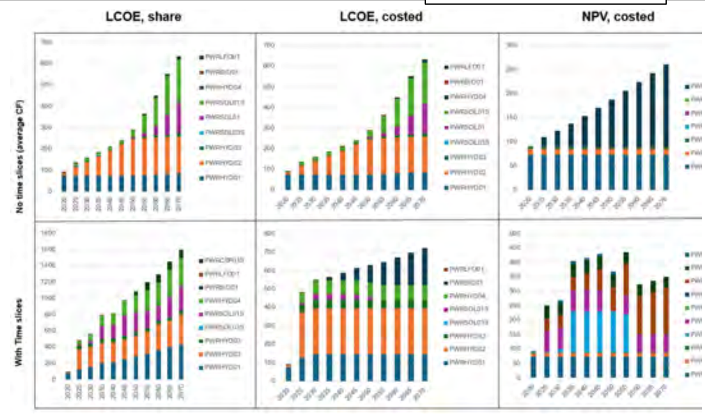


Figure 1. Capacity expansion (in PJ/yr) for selected agent decision metrics and powerplants dispatch methods.

The first year of the Ph.D. was mainly dedicated to a systematic literature review which led to both the analysis of the hydrogen value chain in Africa; and the identification and selection of energy system modeling tools to be used for future analysis. Among the preselected open source and open access energy modeling tools: OnSSET, OseMOSYS, MUSE, and TEMOA; MUSE was found to be more suitable for our study given its ability to model human behavior taking into consideration agent objectives and power, priorities, and budget. The tool is able to model under uncertainties the whole energy system; and simulate the most likely scenario in which the energy system will evolve, and therefore, highlight the most priority technologies to invest in, in the short, mid, and long term both on the supply and demand side. Relevant techno-economic data for energy technologies have also been collected and synthesized during the first year.

During the second year, the focus was given to the development of the regional energy model and the analysis of different scenarios. Based on the gathered data, we first perform a model comparison between an optimization modeling tool and agent-based tools using the power sector of DRC as a case study. This study contributes to the use and application of these modeling tools according to the policy question under investigation by drawing a parallel between OseMOSYS and MUSE, respectively an optimization and agent-based energy system modeling too. A model of the power sector of the DRC was developed in both tools and different scenarios were analyzed to capture the particularities of these two tools.

The current ongoing research focuses on developing the MUSE-South-Africa model with a particular focus on hard-to-abate industrial and maritime sectors as potential off-takers of green hydrogen for their future decarbonization.

Academic context

[1] S. Giarola, J. Sachs, M. d'Avezac, A. Kell, A. Hawkes, "MUSE: An open-source agent-based integrated assessment modelling framework", Energy Strategy Reviews, vol. 44, p. 100964, November 2022, doi: 10.1016/J.ESR.2022.100964.

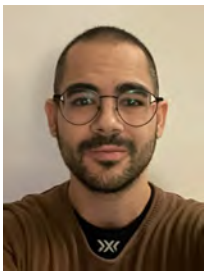
[2] P. M. Koshikwinja, M. Cavana, S. Sechi, R. Bochiellini, and P. Leone, "Review of the hydrogen supply chain and use in Africa," *Renew. Sustain. Energy Rev.*, vol. 208, p. 115004, Feb. 2025, doi: 10.1016/j.rser.2024.115004.

[3] P. M. Koshikwinja, M. Cavana, and P. Leone, "OseMOSYS vs MUSE, A case study of DRC power sector development," *In preparation.*

First name: Matteo Maria **LAST NAME**: PIREDDA

Topic: Lattice Boltzmann Method CFD techniques applied to multiphase flows

Course year: 2nd **Tutor(s)**: Pietro ASINARI, Matteo FASANO



Highlights of the research activity

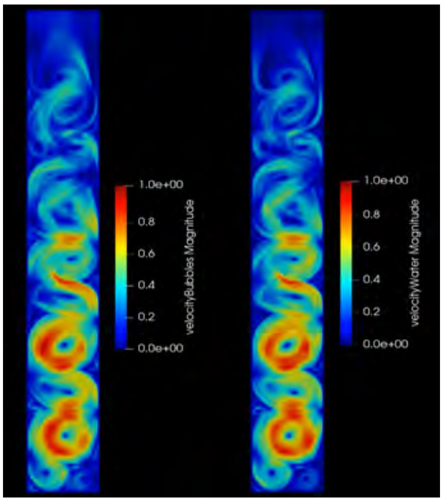


Figure 1 Example frame of a simulation of the model implemented

This research project, funded by ENI, focuses on advancing the Lattice Boltzmann Method (LBM) for simulating multiphase flows, such as those in bubble columns and stirred reactors. While traditional Computational Fluid Dynamics (CFD) methods are capable of modeling these systems, they are computationally demanding and unsuitable for the rapid timelines required in industrial settings. Meeting such demands typically requires extensive parallel computing resources. To face these problems, this research employs LBM, which offers enhanced efficiency for simulating complex flows on parallel architectures [1].
This second year of PhD started with a visiting period at the ENI research center. We conducted a preliminary study of bubble column devices and initiated a collaboration with the Lattice Boltzmann Research Group at the Karlsruhe Institute of Technology (KIT) through the OpenLB consortium. Some 3D turbulent cases were tested on ENI's HPC4 cluster to evaluate a new GPU parallelization configuration.
We arranged also a research visit to KIT for implementing a bubble column simulation referring to the study from Maniscalco et al. [2]. In Figure 1 some results of the implemented model are shown. Subsequently, a validation of the implemented case was conducted referring to the experimental results of Pfleger, who studied a bubble column with a rectangular base and a square sparger. Adapting the OpenLB implementation to match Pfleger's experimental setup revealed several code stability issues related to the pressure field, prompting a detailed debugging process. To address the outlined issues, a novel LBM framework for multiphase flows was derived based on Eulerian-Eulerian Navier-Stokes equations without any finite-difference correction and paying particular attention to the volume fraction transport and to ensure that the same pressure gradient governs the evolution of both phases. The findings, along with the developed model, are detailed in an arXiv paper [3] co-authored with my supervisor, prof. Pietro Asinari. This progress underscores the potential of LBM in advancing multiphase flow simulation for industrial applications on parallel computational architectures, particularly through collaboration with industry stakeholders.

External collaborations

- Eni S.p.a. (Homepage | Eni)
- KIT, Karlsruhe Institute of Technology (Lattice Boltzmann Research Group)

Academic context

[1] Sauro Succi, The Lattice Boltzmann Equation: For Complex States of Flowing Matter, Oxford University Press, 2018, ISBN: 0199592357, DOI:10.1093/oso/9780199592357.001.0001
[2] Francesco Maniscalco et al., Numerical simulation of bubble columns: LES turbulence model and interphase forces blending approach, Chemical Engineering Research and Design, 2021, DOI:10.1016/j.cherd.2021.06.024
[3] Matteo Maria Piredda and Pietro Asinari, Lattice Boltzmann framework for multiphase flows by Eulerian-Eulerian Navier-Stokes equations, 2024, DOI:10.48550/arXiv.2409.10399

First name: Gianmarco **LAST NAME**: PRESO

Topic: Advanced modeling for district heating based on renewable energy sources

Course year: 2nd **Tutor(s)**: Vittorio VERDA, Elisa GUELPA

Highlights of the research activity

District heating is a well established technology, since the first network date back to the end of the 19th century. One of the biggest opportunities we have, is to try to integrate renewable energy sources (RES) such as solar thermal or heat pumps driven by electricity from RES, and waste heat coming from datacenter, wastewater ecc.. in the high temperature network. This is a very difficult task, because to do this it's mandatory to decrease the temperature to operate the systems with a high efficiency. The decrease of the temperature, for sure, will bring to an increase of the mass flow rate and so of the pumping cost. One of the main topic of my PhD, is to make this transistion as efficient as possible. During the second year I've been for 6 months at the HAWK University in Göttingen, Germany as a visiting researcher. In this period, I've tried to study the transition of the network located in the north campus of the University of Göttingen. The main objective was to analyze the main criticalities that the network might present whenever the supply temperature is reduced. The analysis on the supply temperature has been done after long studies on the decreasing of the heat demand after a refurbishment of the buildings served from the network. A scenario analysis has been performed and all the scenario is different from the others on the basis of the supply temperature and of the location of the refurbished buildings. It's possible to see how the pumping cost is strongly dependent on the supply temperature from the Figure 1. On the left you can see the pumping cost at the current conditions, on the right you can see the pumping cost in the case the supply temperature is reduced. Furthermore, the location of the refurbished building plays a key role in the analysis of the pumping cost. The renovation of the farthest building from the supply point is clearly the most convenient situation. I've also analyzed with a model-based approach the heat losses in the network, and came out that the position of the refurbished building is not so important as it is in the fluid-dynamic analysis.

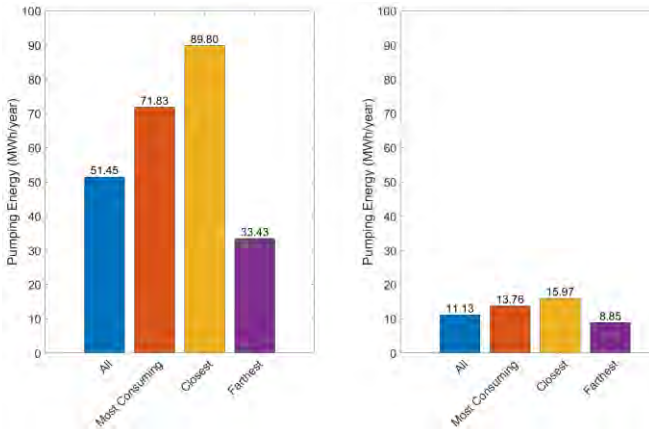


Figure 1 - Pumping cost for each analyzed scenario

In the period spent in Turin, I kept on with the modeling of the district heating network. In this year I focused my work on the validation of the fluid dynamic model on experimental data supplied by Iren S.p.A. All these data needed a huge work of pre-processing and I've done it using data analytics procedure in Python. The validation has been completed in the last month. The next step is to complete the model, going in the direction of the optimization of the pressure present in the network, which has to be minimized.

External collaborations

- Iren S.p.A.
- HAWK University

Academic context

[1] Preso, G.; Romanov, D.; Holler S.; Guelpa, E.; Verda, V.; Scenario analysis for efficient transition of a district heating network – case study in Göttingen. i*n Book of Abstracts: 10th International Conference on Smart Energy Systems, September 10-11, **2024**, Aalborg, Denmark.*

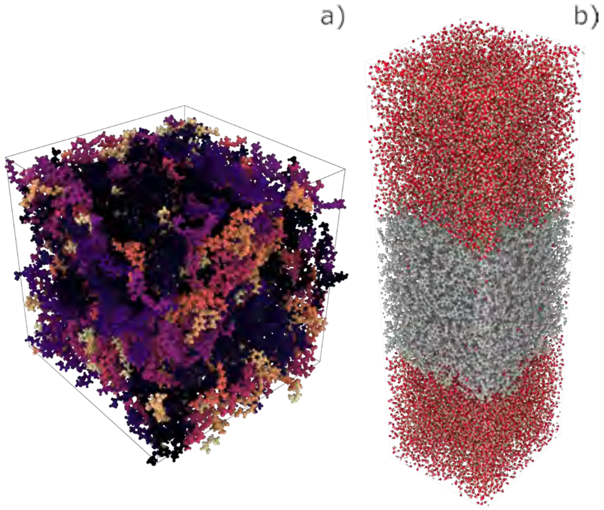
First name: Marina **LAST NAME**: PROVENZANO

Topic: Multi-scale modeling of thermochemical processes for efficient recycling of polymer composite materials

Course year: 2nd **Tutor(s)**: Matteo FASANO, Matteo MORCIANO

Highlights of the research activity

During the second year of my Ph.D. program, the main focus of my research was on employing molecular dynamics methodologies to investigate material properties and physicochemical phenomena relevant in the context of thermochemical recycling processes applied to polymer composites, such as supercritical water solvolysis. Carbon fiber-reinforced polymers are currently used in a wide range of applications, and an atomistic analysis of the formation and degradation mechanisms of these materials can provide useful insights to improve understanding and enhance the energy efficiency of the processes they are involved in, thereby reducing their environmental impact. The research activity began with an analysis of the key materials related to supercritical water solvolysis: after using various classical molecular dynamics models to evaluate the properties of water under high-pressure and high-temperature conditions, we focused on modeling thermosetting polymer networks with different degrees of cross-linking, using DGEBA-DETA epoxy resin as a case study. By means of a pseudo-reactive algorithm, we simulated the polymerization reaction underlying the formation of this resin, where the original epoxy rings disappear and the terminal carbons of the resin molecules bond to the nitrogen atoms of a curing agent, thus creating a cross-linked structure. We then studied the thermomechanical properties of these thermosetting polymers at varying cross-linking degrees using nonequilibrium molecular dynamics approaches. Thermal conductivity was assessed using the Müller-Plathe algorithm, which induces a thermal gradient within the simulation box, while the elastic coefficients of the resin were calculated by slowly deforming the system and evaluating its mechanical response. The polymer structures thus created were then used to study the infiltration of supercritical water within the resin under varying pressure and temperature conditions. This ongoing activity aims to understand how polymer-solvent interface interactions contribute to material degradation and how different thermodynamic parameters influence this process. The next goals of this research involve modeling polymer composites reinforced with carbon structures and coupling these materials with supercritical water to investigate the heat and mass transfer phenomena occurring at the interfaces.



a) Epoxy resin after the cross-linking process.
b) Coupling of epoxy resin and water to simulate supercritical water infiltration.

External collaborations

- Technical University of Dresden, Institute of Lightweight Engineering and Polymer Technology (ILK)
- Leipzig University of Applied Sciences (HTWK Leipzig)
- National Technical University of Athens (NTUA), R-NanoLab

Academic context

[1] Nejad, S. M.; Srivastava, R.; et al. *Int. J. Therm. Sci.* **2021**, *159*, 106588.
[2] Karalis, K.; Ludwig, C.; et al. *Sci. Rep.* **2019**, *9* (1), 15731.
[3] Li, G.; Hu, P.; et al. *Comput. Theor. Chem.* **2021**, *1200*, 113240.

First name: Nodira**LAST NAME**: ABDIVAKHIDOVA

Topic: Modelling for planning and operational optimization of gas networks for sustainable and green supply in Uzbekistan

Course year: 2nd **Tutor(s)**: Pierluigi LEONE, 2nd Uktam SALOMOV, 3rd Marco CAVANA

Highlights of the research activity

Uzbekistan plays a key role in the gas infrastructure sector in Central Asia.
This research focuses on studying the gas system of Uzbekistan, analyzing it from both technical and energy perspectives, and exploring potential ways to improve environmental sustainability in the energy sector by introducing renewable gases into the gas system.
For studying the effect of renewable gas in the network it was used the modelling and simulation tools.
A real case study on a city of 200,000 inhabitans that experiences gas supply difficulties was selected. Using the SIMPLE applied to real data, gas pressures and flow were calculated and areas witout gas access to gas were identified real data, areas without access to gas were identified,
In winter the increased demand for heating results in only 30% of the population being supplied with natural gas according to the simulation (Figure 1). By increasing the pressure at the medium pressure stations, 57% of the population could be supplied with gas, although this still leaves almost half the population without reliable access. Another solution is to use biomethane. Biomethane was injected into the critical medium pressure node(single injection), but due to pressure restrictions (3 bar), the network could only be saturated with gas to 94%.
A more effective solution was the simultaneous introduction of biomethane into two points. This allowed to reduce the total amount of injected biomethane for fully covering the network with gas (Figure 2).

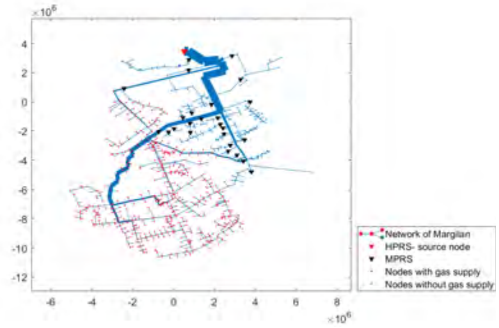


Figure 1. Simulation of gas network at Tamb=-14oC, PHPRS=1 bar, PLPRS=0.05 bar, consumption in a single household = 10m3/day

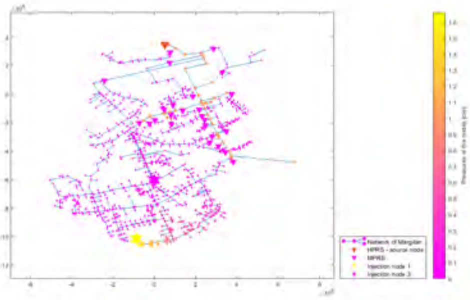


Figure 2. Gas network simulation with 2 injection points G(node 1)=0.27 kg/s and G (node 3)=0.1 kg/s

Future research will focus on analysing hydrogen injection into the proposed gas network, taking into account its possible applications in this area. The next stage of the work will include calculating the most cost-effective solution for decommissioning and reconstudction of the gas transportation system across Uzbekistan.

External collaborations

- Turin Polytechnic University in Tashkent
- Fergana Polytechnic Institute

Academic context

[1] S. Pellegrino, A. Lanzini, and P. Leone, “Greening the gas network – The need for modelling the distributed injection of alternative fuels,” *Renew. Sustain. Energy Rev.*, vol. 70, no. November 2016, pp. 266–286, 2017, doi: 10.1016/j.rser.2016.11.243.

[2] M. Cavana and P. Leone, “Biogas blending into the gas grid of a small municipality for the decarbonization of the heating sector,” *Biomass and Bioenergy*, vol. 127, no. February, p. 105295, 2019, doi: 10.1016/j.biombioe.2019.105295.

First name: Nada **LAST NAME**: ALGHAMDI

Topic: Construction and metrological validation of digital models (digital twins) for materials and energy storage devices.

Course year: 1st **Tutor(s)**: Eliodoro Chiavazzo, Pietro Asinari, Paolo De Angelis, Matteo Fasano.

Highlights of the research activity

Li-ion batteries play an important role in the advancement of sustainable energy technologies. Central to their performance, stability, and safety is the solid-electrolyte interphase (SEI), a passivation layer that forms at the interface between the electrode and electrolyte [1]. Despite its critical importance, the structure and function of the SEI remain poorly understood due to its complex and multi-scale nature.

Our research focuses on developing and validating machine learning based force fields to accurately predict transport and reactive phenomena within the SEI. Specifically, we are using MACE-MP-0 [2], a state-of-the-art machine learning force field potential for molecular dynamics (MD) simulations. This tool holds the potential to offer the precision of *ab-initio* methods while maintaining computational efficiency. At the same time, it can also increase its accuracy if accurate DFT data is available beforehand. We start our analysis with lithium fluoride (LiF). LiF is important due to its beneficial properties in the passivation layer [1]. We are employing MACE to model the diffusion of lithium interstitials in LiF and investigating LiF aggregation processes, key to understanding the formation and evolution of the SEI. To validate our findings, we are comparing MACE results with those obtained using ReaxFF and DeepMD.

Our initial results with MACE are promising, as shown in Figure.1 below, we construct two LiF clusters using the newly developed SEI Builder, an SEI geometry generator [3]. Then we deform the simulation box until we reach experimental density. We observe the formation of a polycrystalline structure where grain boundaries can be observed while the bulk structure of the initial clusters is preserved. These early findings are encouraging, further tweaks and refinements to the approach are currently underway. Once we have validated our approach with LiF, our long-term goal is to extend these simulations to more SEI components, incorporating other key SEI components such as lithium oxide (Li_2O) and lithium carbonate (Li_2CO_3) for a more comprehensive atomistic model of the inorganic SEI structure

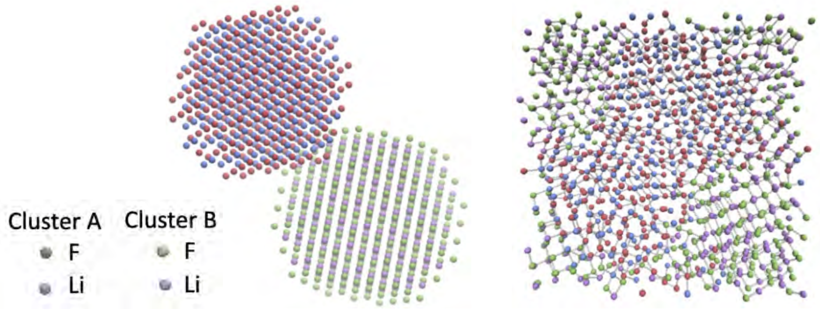


Figure 1: Simulation of LiF cluster aggregation using MACE. The process begins with the construction of two LiF monocrystals using the SEI generator [3], followed by box deformation until the experimental density is reached. The resulting polycrystalline structure demonstrates preserved bulk order.

External collaborations

- The National Metrology Institute of Italy (INRIM)

Academic context

[1] De Angelis, P, et al (2024). *Scientific Reports*, *14*(1), 978
[2] I. Batatia, et al, arXiv:2401.00096, (2024).
[3] P. De Angelis, et al, SEI Builder, Version 0.1.0 (2024) Source code https://big-map.github.io/big-map-registry/apps/SEI-Builder.html

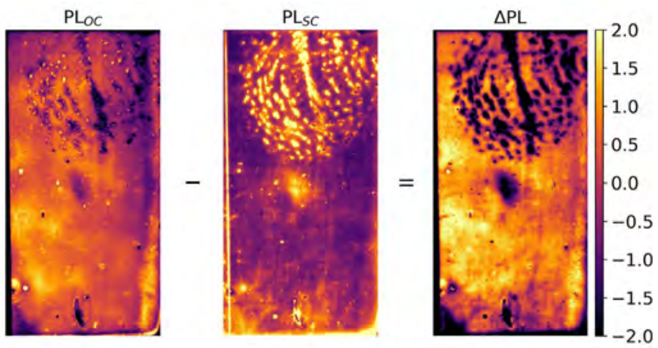
First name: Giulio **LAST NAME**: BARLETTA

Topic: Use of artificial intelligence techniques for the optimization of innovative solar cells production

Course year: 1st **Tutor(s)**: Eliodoro CHIAVAZZO, Pietro ASINARI, Aldo DI CARLO (ISM-CNR, Università di Roma Tor Vergata)

Highlights of the research activity

During the first year of Ph.D., my research has been focused on the development and use of state-of-the-art artificial intelligence (AI) algorithms to discover new perovskite materials with high potential for photovoltaic (PV) application, and to predict the in-situ lifespan of perovskite solar cells (PSCs).
The first part of my activity led to the development of two ML-mathematical methods to discover possible groups or combinations of primitive variables in physical phenomena, regardless of data origin, being it numerical or experimental. Those methods can be later applied to the data collected during the PSCs experiments. The first approach is based on regression models, whereas the second on classification models.
The second part of my research dealt with the preliminary investigation of machine vision and deep learning methods to be used for in-situ characterization and lifetime prediction of operating PSCs, along with the engineering of the experimental setup, in collaboration with experienced researchers from CHOSE. In this first phase of the activity, a pilot setup was built to investigate the possibility of using non-invasive characterization techniques (electro- and photoluminescence imaging) to correlate the excitation response of the PSC with its state-of-health, thus obtaining both a model to predict the cell's remaining lifetime and a deeper insight into the degradation mechanisms of perovskites. The results from the preliminary study encouraged me to follow on with an extensive and exhaustive analysis of multiple cells with a more accurate setup, which is currently under development. The next steps would be to finalize the experimental setup, build a data acquisition, storage and transmission protocol, and develop algorithms and codes for the pre-processing, ML-assisted analysis, and post-processing of the visual data.



Normalized PL (in open-circuit (OC) or short-circuit (SC) conditions) images obtained with the same perovskite solar cell, along with the calculated difference

Finally, I have collaborated with other researchers from my group (multi-Scale ModeLing Laboratory) to develop a novel protocol for AI-assisted screening of large materials databases (namely the GNoME database by Google DeepMind) to search for novel, untested materials with high potential for energy applications. In particular, my efforts were focused towards the identification of candidate perovskites for PV cells, and the prediction of selected physical properties relevant to the application considered. This effort led to the identification of 4,259 possible perovskites with high potential for use in PV applications.

External collaborations

- Center for Hybrid and Organic Solar Energy (CHOSE), Università di Roma Tor Vergata

Academic context

[1] De Angelis, Paolo, et al. "Energy-GNoME: A Living Database of Selected Materials for Energy Applications". *arXiv preprint arXiv:2411.10125* (2024).
[2] Ji, K., Lin, W., Sun, Y. et al. "Self-supervised deep learning for tracking degradation of perovskite light-emitting diodes with multispectral imaging". Nat Mach Intell 5, 1225–1235 (2023).
[3] Juan-Pablo Correa-Baena et al. "Promises and challenges of perovskite solar cells". Science 358, 739-744 (2017).

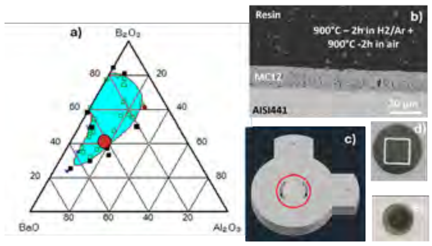
First name: Francesco **LAST NAME**: DA PRATO

Topic: Proton ceramic cells (PCC) stacks for ultrapure hydrogen production

Course year: 1st **Tutor(s)**: Massimo SANTARELLI, Federico SMEACETTO

Highlights of the research activity

This research activity focuses on scaling up the proton-conducting electrolysis ceramic cells (PCECs) technology, with the objective of designing, assembling, and testing a single repeating unit (SRU), followed by the development of short stacks. Since March 2024, experimental work has concentrated on the selection and evaluation of components and materials for the SRU. This has included the design, fabrication, and preliminary testing of interconnects, protective ceramic coatings, and glass-based sealants for PCEC integration. A thermo-electrochemical multiscale model was used to design interconnects for a button-cell format SRU, enabling predictions of performance and key parameter distributions (current density, chemical species, temperature) to optimize interconnect geometry and shape. Various coatings were developed and deposited for interconnect protection to mitigate the potential accelerated oxidation of interconnects under PCEC operating conditions. This ensured mechanical integrity and good electrical conductivity even after prolonged exposure. Specifically, different Mn-Co spinel ceramic formulations were investigated, optimizing both deposition parameters and sintering processes to achieve dense and adherent coatings. In parallel, various glass-based sealants were developed and characterized. Glass systems with different main formers (Si-based and B-based) were studied, demonstrating chemical and thermomechanical compatibility with the materials selected for interconnects and PCEC membranes. Compatibility was verified after thermal joining treatments, long-term thermal aging in air and air + steam environments at 600°C, and extreme thermal cycling between room temperature and 600°C. For future SRU assembly, the robocasting extrusion technique was chosen to ensure controlled and homogeneous deposition of the glass sealants. A comprehensive study optimized the organic paste formulations used to disperse the glass powders. This ensured printability via robocasting, focusing on optimizing rheology, extrudability, and shape retention. Using these optimized formulations, interconnect, sealant, and cell samples were successfully joined, with glass sealant applied via robocasting. A future goal of this research is to achieve self-sufficiency in the manufacturing and processing of both button and real-size PCC cells.



a) Composition range of the selected seal glass systems; b) Mn-Co based protective coating deposited on AISI441 interconnect (IC); c) Design of SRU IC; c) Robocasting deposition of seal glass system; e) Button cell for SRU assembly

External collaborations

- SNAM hydrogen team of HyAccelerator
- Politecnico di Milano – Dipartimento di Energia
- University of California - Irvine

Academic context

[1] Anelli, S., Baggio, A., Ferrero, D., Schmider, D., Dailly, J., Santarelli, M., & Smeacetto, F. (2024). Characterization and testing of glass-ceramic sealants for protonic ceramic electrolysis cells applications. *Ceramics International*, *50*(10), 17520–17531. https://doi.org/10.1016/j.ceramint.2024.02.240

[2] E. Zanchi *et al.*, “Electrophoretic deposition of MnCo2O4 coating on solid oxide cell interconnects manufactured through powder metallurgy,” *Mater Des*, vol. 227, Mar. 2023, doi: 10.1016/j.matdes.2023.111768

[3] D. Ferrero *et al.*, “Modeling of a Single Repeating Unit for Protonic Ceramic Cell Applications,” *ECS Trans*, vol. 111, no. 6, pp. 1185–1194, May 2023, doi: 10.1149/11106.1185ecst.

First name: Antonio **LAST NAME**: DE PADOVA

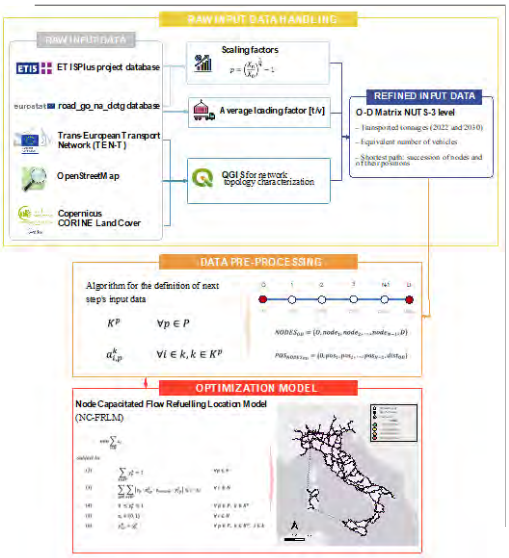
Topic: Techno-economic and environmental sustainability analysis of hydrogen transport and storage technologies for the production of e-fuels

Course year: 1st **Tutor(s)**: Andrea LANZINI, Francesco Demetrio MINUTO, Claudio CARBONE

Highlights of the research activity

The initial phase of the research focused on an extensive literature review to identify the current state of the art and potential research gaps that need to be addressed in the field of a sustainable hydrogen supply chain implementation in the current energy system. As part of this effort, a detailed database was developed, containing the key techno-economic data for the most widely used hydrogen-related processes, covering production, storage, transportation, and utilization. In particular, the focus was on low-emission hydrogen technologies and on the processes for the production of the most important e-fuels (e.g., e-methanol, e-ammonia, etc.). When possible, dynamic parameters were defined as well (such as ramp-up and ramp-down times, etc.), which are essential for accurately modeling the performances of the processes in a real-world energy system model.

To effectively assess the techno-economic and environmental impact of the integration of a hydrogen supply chain in the energy system, the hydrogen demand in different end-use sectors should be carefully assessed (e.g., e-fuels production, heavy-duty transport, industrial sector, etc.). The case study of the road freight transport system was first assessed in order to develop a methodology which could be used for other end-use sectors as well. Using a Geographic Information System (GIS) software, traffic volumes were mapped onto the italian territory and especially on the major routes that are part of the Trans-European Transport Network (TEN-T). This outcome provides a realistic estimation of current and future freight transportation demands and infrastructure requirements, based on the national policy objectives and forecasts. A Mixed-Integer Linear Programming (MILP) optimization model was developed to determine the optimal location of Hydrogen Refueling Stations (HRS) across the national territory, with the objective of minimizing the number of stations to be placed while ensuring that all the hydrogen vehicles on the territory can be refueled. These preliminary results could be used to characterize the forecasted hydrogen demand on a more refined temporal and spatial basis which is a key requirement to effectively assess the impact of the integration of hydrogen supply chain into the energy system - both from a techno-economic and an environmental point of view - as it is linked with some parameters which are strictly spatial-dependent (e.g., renewable electricity availability, etc.).



Optimization framework for locating Hydrogen Refueling Stations by using real-world georeferenced data.

External collaborations

- ENEA – Italian National Agency for New Technologies, Energy and Sustainable Economic Development

Academic context

[1] P. K. Rose, F. Neumann, Hydrogen refueling station networks for heavy-duty vehicles in future power systems, Tran. Res. Part D: Transport and Environment, 2020, https://doi.org/10.1016/j.trd.2020.102358.

[2] S. Öberg, M. Odenberger, F. Johnsson, The cost dynamics of hydrogen supply in future energy systems – A techno-economic study, Applied Energy, 2022, https://doi.org/10.1016/j.apenergy.2022.120233.

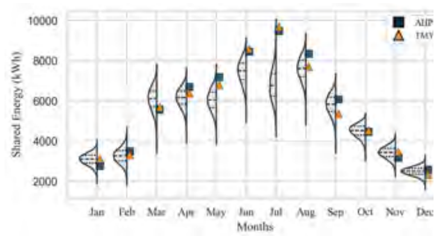
First name: Federico **LAST NAME**: DE BETTIN

Topic: A tool-set for the optimal design and coordination of a renewable energy community

Course year: 1st **Tutor(s)**: Andrea LANZINI, Francesco Demetrio MINUTO

Highlights of the research activity

My research focused on developing a stochastic and holistic simulation framework for Renewable Energy Communities (RECs), integrated into a scalable software application. A novel methodology was created to generate synthetic photovoltaic production profiles for Monte Carlo simulations, combining path integral and Fokker-Planck formalisms to model renewable energy systems under uncertainty. The software leverages PostgreSQL, MongoDB, and InfluxDB databases, Python microservices, and an Angular front-end. A key contribution of this framework is its ability to estimate uncertainties in solar energy production, self-consumption, and shared energy predictions over various time periods. Traditional methods were found to tend to be optimistically biased when estimating self-consumption and shared energy during months with excess production. Yearly relative uncertainties in shared energy for residential solar energy communities were found to be around 2% to 3%. Additionally, I implemented heuristic optimization algorithms, including Particle Swarm Optimization (PSO) and Genetic Algorithms (GA), to optimize the sizing of photovoltaic plants and lithium-ion batteries for residential and industrial applications. This framework enables optimization across the most probable, worst-case, and best-case scenarios, offering insights into risk-reward investment strategies for RECs. I also developed an electricity consumption datalake by merging open datasets with private data from DBA PRO. S.P.A., enhancing access to complex datasets for refining the simulation framework. This data is valuable for future research and applications. Furthermore, my work incorporates timeseries clustering, feature extraction for data mining and classification. Lastly, I explored the use of georeferenced datasets, such as the JRC Energy Atlas, to estimate energy consumption in specific load areas, with a focus on municipalities and primary substations.



Renewable Energy Community monthly shared energy probability distributions obtained by the stochastic simulation framework, compared with estimates made with the typical meteorological year and the average hourly production profile.

External collaborations

- DBA PRO. S.P.A. – Engineering and ICT company

Academic context

[1] Minuto F.D., Lanzini A. (2022). “Energy-sharing mechanisms for energy community members under different asset ownership schemes and user demand profiles”, Renewable and Sustainable Energy Reviews, 168, 112859, https://doi.org/10.1016/j.rser.2022.112859
[2] Andres Felipe Ramírez, Carlos Felipe Valencia, Sergio Cabrales, Carlos G. Ramírez (2021). ”Simulation of photo-voltaic power generation using copula autoregressive models for solar irradiance and air temperature time series”, Renewable Energy, 175, Pages 44-67, https://doi.org/10.1016/j.renene.2021.04.115
[3] European Commission, Joint Research Centre (JRC) (2023): EU energy atlas - demand 2019. European Commission, Joint Research Centre (JRC) [Dataset] PID: http://data.europa.eu/89h/76a6b550-253c-44a4-9a4c-d22079e7bf62

First name: Luisa **LAST NAME**: DI FRANCESCO

Topic: Modelling Safe Hydrogen Injection and Management for European Gas Network Resilience and Decarbonization

Course year: 1st **Tutor(s)**: 1st Pierluigi LEONE, 2nd Marco CAVANA

Highlights of the research activity

This doctoral research focuses on hydrogen infrastructure and its role in hydrogen integration within the energy system, supported by the European projects "SHIMMER" and “SH2AMROCK”. The key objectives are:

1. Review current hydrogen infrastructure projects and future demand/supply projections to identify research gaps.

2. Develop open-source tools for planning and operation of hydrogen-based gas networks.

3. Simulate case studies and extrapolate findings to a European scale to identify constraints for hydrogen integration, and evaluate technologies for gas quality tracking and mitigation for safe hydrogen integration.

Research Progress: In the area of fluid-dynamic gas network modelling, the research has enhanced a pre-existing transient gas network model for hydrogen blending. A key improvement is the integration of a hydrogen curtailment algorithm, which regulates hydrogen concentrations to stay within allowable limits, ensuring compliance with technical regulations and safeguarding sensitive users. To support broader accessibility and future development, the physical equations, coding structure and database architecture are used to develop an open-source gas network simulation tool.

Progress has also been made in simulating hydrogen integration in European gas networks through case studies. Relevant networks were identified in collaboration with SHIMMER partners, and operational data were gathered for simulation. Current efforts focus on transmission networks, including the Norwegian grid transporting hydrogen and natural gas from the North Sea to Germany and France, and the Italian infrastructure in Sicily, connecting North Africa to Europe. Another significant case study involves Germany's gas transmission network. This latter study explores the potential of power-to-gas technologies in a sector coupling framework, showing that up to 30% of curtailed renewable electricity could be harnessed for hydrogen production through injection into the gas grid.

Key Impact: The research advances open-source tools, provides actionable insights into hydrogen network integration, and supports optimal strategies for transporting hydrogen into European gas networks.

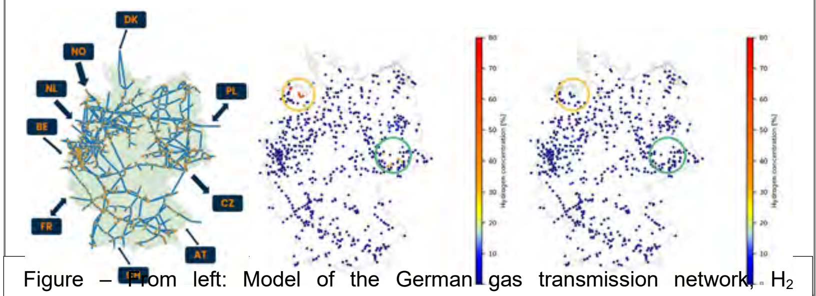


Figure – From left: Model of the German gas transmission network, H_2 concentration when full-injection from power-to-gas is allowed, H_2 concentration when H_2 is curtailed and stored to be compliant with technical constraints

External collaborations

- Forschungszentrum Jülich, Germany
- SINTEF, Norway
- TNO, The Netherlands

Academic context

[1] Cavana et al., Solar hydrogen from North Africa to Europe through greenstream: A simulation-based analysis of blending scenarios and production plant sizing, International Journal of Hydrogen Energy, Volume 46, Issue 43, 2021, Pages 22618-22637, ISSN 0360-3199, https://doi.org/10.1016/j.ijhydene.2021.04.065.
[2] Neumann et al., The Potential Role of a Hydrogen Network in Europe, Joule 7, 1793–1817 August 16, 2023 https://doi.org/10.1016/j.joule.2023.06.016.

First name: Maftuna **LAST NAME**: ESHKOBILOVA

Topic: Energy management and simulation of hybrid hydrogen heavy-duty trucks to minimize energy consumption

Course year: 2nd **Tutor(s)**: Massimo SANTARELLI

Highlights of the research activity

During the programm it is planned the modelling, simulation and energy management of a fuel cell hybrid heavy-duty truck. For this purpose, it is being used to apply a **longitudinal dynamic model**.

Moreover, the load requirement for the drive train should be identified based on driving cycle. To achieve high efficiency, low fuel consumption, low life cycle impact and meet the load requirement as efficiently and dynamically three different Energy Management Systems (EMSs) are planned to implement.

The simulation model is being developed in MATLAB/Simulink. According to the backward simulation technique, the inputs of the simulation model include the vehicle velocity, track geometry, and auxiliary system power requirement for the hydrogen trucks mode. The major output is the continuous hydrogen consumption. In a physical system, converters will be used to regulate power flows based on the energy management and control strategy created by the control unit.

The proposed PEMFC model plans to measure hydrogen consumption and recovered thermal energy while simultaneously taking into account the dynamics and efficiency of a fuel cell system.

$$\eta_{\mathrm{fc}}(PLR(t))=\begin{cases}0.2716, & \text{if } (PLR)< 0.05\\ 0.9033\cdot(PLR(t))^5-2.9996\cdot(PLR(t))^4 & \\ +3.6503\cdot(PLR(t))^3-2.0704\cdot(PLR(t))^2 & \text{if } (PLR)\geq 0.05.\\ +0.4623\cdot(PLR(t))+0.3747 & \end{cases}$$

$$\eta_{\mathrm{electrical}}=\frac{E_{\mathrm{fc,conv}}(T)}{M_{\mathrm{fc}}(T)\cdot LHV_{H_2}}$$

$$r_{\mathrm{te}}(PLR(t))=\begin{cases}0.6801, & \text{if } (PLR)< 0.05\\ 1.0785\cdot(PLR(t))^4-1.9739\cdot(PLR(t))^3 & \\ +1.5005\cdot(PLR(t))^2-0.2817\cdot(PLR(t)) & \text{if } (PLR)\geq 0.05.\\ +0.6838 & \end{cases}$$

$$E_{\mathrm{fc,conv}}(T)=\int_0^T P_{\mathrm{fc,conv}}(\tau)\,d\tau \ \ [\mathrm{Ws}]$$

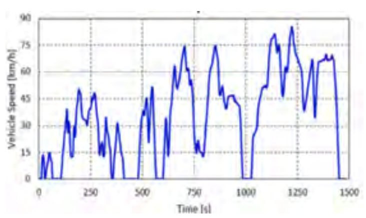


Figure 1: drive cycle

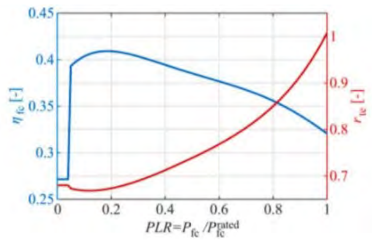


Figure 2: normalized efficiency

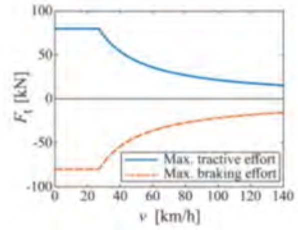


Figure 3: Max tractive and braking effort

External collaborations

- Turin polytechnic university in Tashkent
- Fergana polytechnic institute

Academic context

[1] Simulation and experimental research on energy management control strategy for fuel cell heavy-duty truck

[2] Energy management of heavy-duty fuel cell vehicles in real-world driving scenarios: Robust design of strategies to maximize the hydrogen economy and system lifetime

[3] Performance and energy-consumption evaluation of fuel-cell hybrid heavy-duty truck based on energy flow and thermal-management characteristics experiment under different driving conditions

First name: Laura **LAST NAME**: GENNARO

Topic: Multi-physics model and energy performance analysis of high pressure water electrolysis systems with anionic polymeric membrane technology

Course year: 1st **Tutors:** Massimo SANTARELLI, Domenico FERRERO, Giuseppe NIGLIACCIO

Highlights of the research activity

Hydrogen production from low temperature water electrolysis encompasses several technologies starting from the most mature Alkaline Electrolyzers (AELs) and Proton-Exchange Membrane Electrolyzers (PEMELs) from a technical and commercial point of view, up to emerging technology like Anion Exchange Membrane electrolyzer (AEMEL). Water electrolyzers that use an anion exchange membrane (AEM) are expected to be new devices for hydrogen (H2) production that achieve high performance at low capital cost. In this context the PhD research activity focuses on modelling, testing and design high pressure water electrolysys systems with anion exchange membrane technology, with the scope to create a test cell that can improve performance in terms of pressure and energy operation.

During the first year of the PhD, my research activity focused on analyzing the scientific literature regarding the state of art for Anion Exchange Membrane electrolyser, with a particular focus on high pressure electrolysis. Hydrogen produced by low-pressure electrolysis requires additional systems to pressurize the hydrogen to end-use pressure for storage and transportation, which increases costs and complexity of the balance of plant. Despite high-pressure electrolysis enables direct production of pressurized hydrogen, it suffers from technical bottlenecks such as gas-cross permeability, which not only reduces faradic efficiency but also constitutes a safety concern if the concentration of hydrogen in the hydrogen-oxygen mixture reaches the explosive limit of 4%. The research activity I am developing aims to individuate the main drawbacks on operating at high pressure and possible technical solutions in terms of materials and design. Next step will include the development of multiphysics model with the purpose of simulate the cell behaviour with different geometries, materials and operating conditions in order to estimate the impact of of each on the performance of the device.

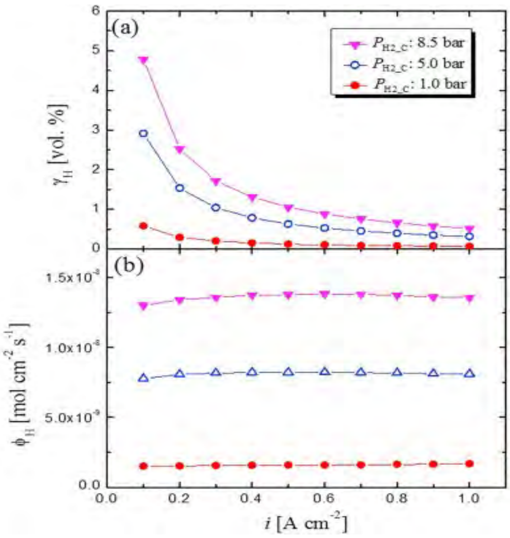


Figure. Volumetric H2 content in O2 in the anode compartment (a) and calculated net hydrogen permeated flux (b) versus current density under different H2 pressures in the cathode compartment.

External collaborations

- ENEA, Bologna (Italy)

Academic context

[1] S. Bin *et al.*, "High-pressure proton exchange membrane water electrolysis: Current status and challenges in hydrogen production," *Int J Hydrogen Energy*, vol. 67, pp. 390–405, May 2024, doi: 10.1016/J.IJHYDENE.2024.04.188.

[2] H. Ito, N. Kawaguchi, S. Someya, and T. Munakata, "Pressurized operation of anion exchange membrane water electrolysis," *Electrochim Acta*, vol. 297, pp. 188–196, Feb. 2019, doi: 10.1016/j.electacta.2018.11.077.

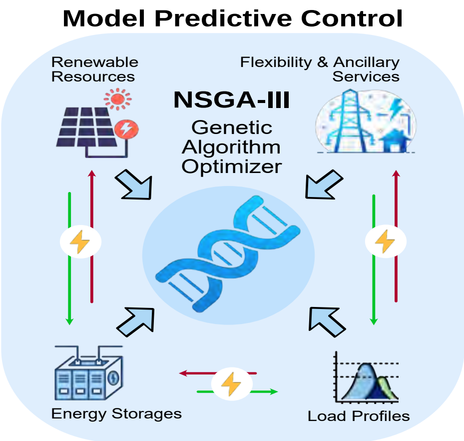
First name: Lorenzo **LAST NAME**: GIANNUZZO

Topic: The value of flexibility in aggregates of consumers/prosumers

Course year: 1st **Tutor(s)**: Andrea LANZINI, Francesco Demetrio MINUTO

Highlights of the research activity

In the initial phase of the research activities, an innovative methodology was developed to reconstruct the electrical load profiles of residential users in the context of data scarcity. This was achieved by combining advanced clustering techniques with classification algorithms, including Random Forest and XGBOOST. The primary objective was to facilitate the utilization of more sophisticated algorithms that are commonly employed to assess aggregates and their interactions with the electrical grid, such as demand response programs and flexibility services, which often necessitate high-resolution data that are not always readily available. In the second phase of the research period, the activities concentrated on developing a Non-Dominated Sorting Genetic Algorithm III (NSGA-III) within a Model Predictive Control (MPC) framework to optimize a complex energy system comprising Battery Energy Storage Systems (BESS), photovoltaic power plants, and both residential and commercial loads. The objective was to establish control rules for managing internal and external energy flows to maximize profits from self-consumption and energy sales, while considering the aging of the different technologies and the possibility of providing flexibility services through the smart usage of BESS, with the aim of improving the electrical grid management. The second phase of the research period also encompassed the production of a review article on the Key Performance Indicators (KPIs) used to assess the performance of Renewable Energy Communities (RECs), in collaboration with ENEA. This research work made a significant contribution to the field by exploring the various applications, uses, and objectives associated with the most commonly utilized KPIs, exposing the actors and activities that are often not considered. Additionally, it developed a comprehensive KPIs Reference List comprising 25 metrics, providing a valuable toolkit for assessing the performance of RECs across different operational domains. The final phase of the research project concentrated on the creation of an Agent-Based Model (ABM) to assess the efficacy of penalty mechanisms within P2P Local Energy Markets (LEMs). This involved an investigation into the impact of such mechanisms on market equilibrium and overall market stability. The initial findings from this research indicated that the selection of an appropriate penalty mechanism is really important, as certain mechanisms may result in either unfairness or instability, ultimately leading to market failure.



An MPC integrating the NSGA-III to manage a complex energy system.

External collaborations

- ENEA – Italian National Agency for New Technologies, Energy and Sustainable Economic Development;
- fabbricadigitale srl – ICT company.

Academic context

[1] Fang, N., Ma, S., Liao, X., Ding, H., & Yu, J. (2024). Optimized scheduling of Integrated Community Energy stations based on improved NSGA-III algorithm. Journal of Energy Storage, 99, 113362. https://doi.org/10.1016/j.est.2024.113362

[2] Zhou, Y., & Lund, P. D. (2023). Peer-to-peer energy sharing and trading of renewable energy in Smart Communities ─ trading pricing models, decision-making and agent-based collaboration. Renewable Energy, 207, 177–193. https://doi.org/10.1016/j.renene.2023.02.125

First name: Yosef Berhan **LAST NAME**: JEMBER

Topic: Hydrogen trains: adaptive algorithms for section consumption forecast

Course year: 1st **Tutor(s)**: Massimo SANTARELLI, Marta GANDIGLIO, Paolo MAROCCO

Highlights of the research activity

The research aims to develop a predictive machine learning algorithm for estimating the power demand of a hybrid hydrogen fuel cell train. Fuel cells exhibit high efficiency under steady operation but respond relatively slowly to rapid changes in power demand. Sudden fluctuations in power generation can adversely impact both fuel cell performance and battery longevity. Hence it requires the ability to forecast power demand throughout the train's journey, enabling advanced scheduling of power generation and distribution. Also it needs optimal allocation of energy between the fuel cell and battery systems. The initial phase involved building a simulation model of the traction system in MATLAB as in figure 1, integrating key components such as the proton exchange membrane fuel cell, battery system, power electronics converters, electric motor, mechanical transmission, and auxiliary unit. Also, boundary conditions, such as passenger load, and track gradient, were incorporated to ensure a realistic representation of operational scenarios.

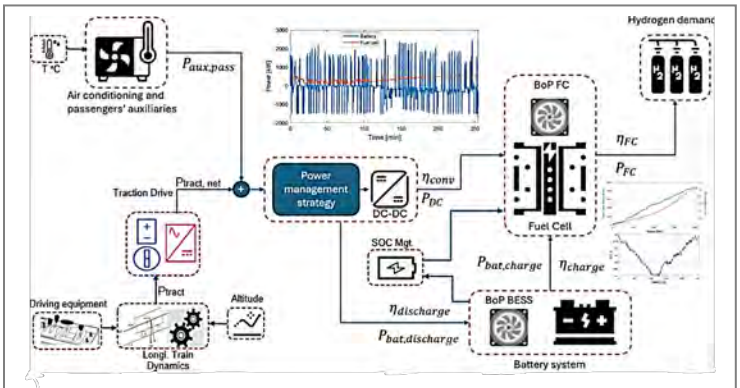


Figure 1: Block diagram of the hydrogen train traction

Outputs from the simulation include the power contributions of the fuel cell and battery, state of charge, and hydrogen consumption. It revealed the complementary roles of the fuel cell and battery in meeting varying power demands, with the fuel cell supplying steady-state power and the battery responding to peak loads and energy recovery during braking.
The simulation model will provide the data necessary to train the predictive algorithm. The next task will involve leveraging this data to develop a machine learning-based predictive framework that estimates the train’s power demand under dynamic conditions. This framework will integrate key operational parameters such as speed, track gradient, and temperature, alongside performance metrics from the fuel cell and battery systems, to forecast energy requirements and optimize power distribution. The predictive model will undergo validation using real-world operational data collected from a pilot hydrogen train line.

External collaborations

- ALSTOM FERROVIARIA S.P.A.

Academic context

[1] Kapetanović, Marko, et al. "Energy model of a fuel cell hybrid-electric regional train in passenger transport service and vehicle-to-grid applications." Journal of Rail Transport Planning & Management 28 (2023): 100415.
[2] Peng, Hujun, et al. "A comparison of various universally applicable power distribution strategies for fuel cell hybrid trains utilizing component modeling at different levels of detail: From simulation to test bench measurement." ETransportation 9 (2021): 100120.
[3] Murray-Smith, David. "Modelling and simulation of hybrid electric trains powered by hydrogen fuel cells and batteries for routes in the highlands of Scotland: preliminary results." (2020).

First name: Tommaso Filippo **LAST NAME**: LUPATELLI

Topic: Multiscale modeling for innovative battery cells, focused on Li-metal and Li-S chemistry.

Course year: 1st **Tutor(s)**: Massimo SANTARELLI, Silivia Bodoardo

Highlights of the research activity

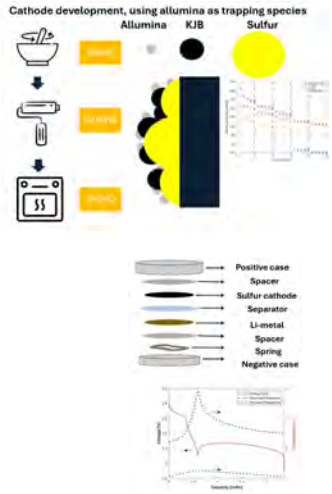


Figure. Sketch of the first year activity

The aim of this Ph.D is building multiscale model to understand and predict the behaviour of Lithium-sulfur (Li-S) batteries, and at the same time the development and characterization of new cathode materials. Li-S batteries have intricate reaction pathways involving multiple reduction steps, as the battery during charge and discharge cycles undergoes significant volumetric and chemical transformations, posing a challenge in isolating the contribution of each individual step. A 0D discharge model, incorporating five reduction mechanisms to simulate sulfur reduction. This was coupled with precipitation and dissolution reactions to account for the active surface area within the cathode and the overpotential during the conversion of intermediate products. The primary objective of this model was to explore the influence of Li-ion concentrations within the electrolyte and the resulting effect of viscosity on the overall ohmic drop. To characterize the model, PEIS (Potentiostatic Electrochemical Impedance Spectroscopy) was employed, allowing us to isolate each. Li-S cells exhibit several polysulfide species in the discharge process, which are challenging to measure experimentally due to the parallel nature of reactions. A modeling approach, combined with experimental data fitting, helps overcome the complexities and reduce the need for intricate experimental setups. A 1D model was built and to verify its robustness of the model, it was tested under varying scan rates. At lower scan rates, the two current peaks observed in cathodic mode align with the voltage plateaus characteristic of Li-S cells, corresponding to the reduction of long and short polysulfide chains, respectively. At higher scan rates, the insufficient active surface area for recovering reduction products emphatasizes the role of Li-S deposition during charging. For cathode development, a double-layer approach was implemented to mitigate polysulfide diffusion toward the anode. Three strategies are currently being tested: 1. KJB-Al2O3: A porous conductive carbon (KJB) and alumina layer is deposited on top of a sulfur-KJB electrode using a doctor blade technique, with adjustable thickness. 2. PEDOT-PSS-Al2O3: A conductive polymer (PEDOT-PSS) acts as a binder for alumina particles dispersed in ethanol, with a conductivity of approximately 1e3 S/cm. 3. Graphene: Commercial graphite is sonicated in NMP, followed by solvent evaporation under an ice bath to break down the planes and form highly conductive graphene. The dispersion is separated using centrifugation and spray-coated onto an S-KJB electrode. Furthermore to characterize the capacity retention of each cathode, a new protocol is underdevelopment, which consists of alternating galvanostatic and potentiostatic charge and discharge cycle, in order to determine the rate of capacity loss due to cycling.

External collaborations

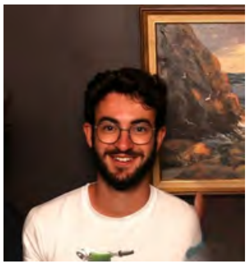
- Stellantis (Amsterdam, Netherland)
- CRF (Torino, Italy)

Academic context

[1] Teng Zhang, Monica Marinescu, Laura O'Neill, Mark Wildb and Gregory Offer, : Phys. Chem. Chem. Phys., 2015, 17, 22581

[2] Natalia A. Cañas, Kei Hirose, Brigitta Pascucci, Norbert Wagner, K. Andreas Friedrich, Renate Hiesgen,, Electrochimica Acta, Volume 97, 2013

First name: Alessandro **LAST NAME**: MAGNINO



Topic: Techno-economic and environmental analysis of the role of low-carbon fuels in the design of future energy systems

Course year: 1st **Tutor(s)**: Marta GANDIGLIO, Paolo MAROCCO, Massimo SANTARELLI

Highlights of the research activity

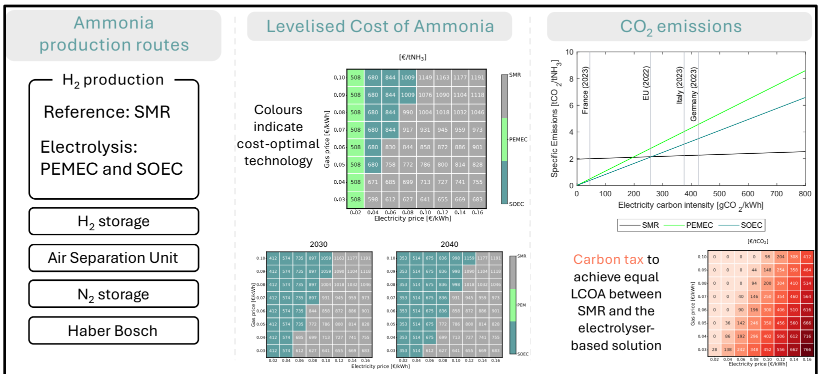


Fig.: List of main components of the plant, main outcomes regarding costs, and main outcomes regarding CO_2 emissions

Low-carbon fuels and chemicals are crucial for decarbonising hard-to-abate sectors, representing an important alternative to electrification and offering advantages over pure hydrogen due to simpler handling and storage. Decarbonising ammonia (NH_3) production - a highly polluting chemical due to its reliance on fossil resources - is a vital challenge. Given NH_3's growing importance, it became the focus of my first PhD year.

After an extensive literature review, I developed models for key components of an NH_3 production plant, incorporating various hydrogen production pathways. These included Solid Oxide Electrolysis Cells (SOECs), Proton Exchange Membrane Electrolysers (PEMECs), Steam Methane Reformers (SMRs), Cryogenic Air Separation Units, and Haber-Bosch reactors. For electrolyser systems, I created two models: one detailing the electrochemical performance of the stack (producing polarisation curves) and another analysing the balance of plant, including auxiliary components. These models enabled precise evaluations of the plant's electrical and thermal consumption and identified opportunities for heat integration to reduce operational costs. Notably, coupling SOECs with the exothermic Haber-Bosch process significantly reduced SOECs' thermal needs, enhancing their economic viability.

Building on this component-level modelling, I conducted a cost and CO_2 emissions comparison of three plant layouts featuring different hydrogen production systems: SMR, PEMEC, and SOEC. This comparative analysis, presented in the article *"Economic Viability and CO_2 Emissions of Hydrogen Production for Ammonia Synthesis: A Comparative Analysis Across Europe"* (under review at *Advances in Applied Energy*), yielded key insights: 1) Electrolysers are not yet cost-competitive with SMRs due to higher capital costs and electricity prices. Current carbon pricing is insufficient for parity in most European contexts, 2) Future scenarios for 2030 and 2040 suggest SOECs will achieve cost competitiveness with SMRs as technology and costs improve, while PEMECs will likely remain constrained by lower efficiency, 3) Emissions analysis revealed electrolysers can surpass SMRs in CO_2 emissions if electricity carbon intensity exceeds 200 gCO$_2$/kWh for PEMECs or 260 gCO$_2$/kWh for SOECs, limiting the feasibility of grid electricity in many European regions.

This work highlights the need for low-cost renewable electricity to unlock the potential of electrolyser-based ammonia production.

External collaborations

- AMPS Project
- ETH - Zurich

Academic context

[1] Magnino et al., "Economic Viability and Co2 Emissions of Hydrogen Production for Ammonia Synthesis: A Comparative Analysis Across Europe", under review, https://doi.org/10.2139/SSRN.4940087

[2] Campion et al., "Techno-economic assessment of green ammonia production with different wind and solar potentials", Renew Sustain Energy Rev 2023;173:113057. https://doi.org/10.1016/J.RSER.2022.113057

[3] Gabrielli et al. "Net-zero emissions chemical industry in a world of limited resources", One Earth 2023;6:682–704. https://doi.org/10.1016/j.oneear.2023.05.006

First name: Roberto Raffaele **LAST NAME**: MEO

Topic: Sustainable water treatment technologies based on solar thermal energy: From multi-scale modelling to lab-scale prototyping

Course year: 2nd **Tutor(s)**: Prof. Matteo FASANO, Prof. Eliodoro CHIAVAZZO, Dr. Matteo MORCIANO

Highlights of the research activity

My research focuses on advancing membrane distillation (MD) and passive solar desalination systems, critical technologies for achieving energy-efficient and sustainable water desalination. Through a detailed review of existing studies, I identified key challenges, including the need to optimize energy consumption in MD systems, particularly by integrating low-grade heat sources such as solar energy, and addressing salt accumulation in passive desalination systems, which compromises long-term performance.

To address these issues, I investigated the integration of solar heat into MD systems, evaluating over 1,000 configurations to improve heat and mass transfer. This approach significantly increased vapor flux and reduced temperature polarization, making the process more efficient. Additionally, I focused on enhancing the Marangoni effect in passive systems, using advanced fluid dynamics and salt removal techniques to develop models that mitigate salt accumulation and ensure reliable performance in off-grid scenarios.

The results of this work demonstrate significant progress. Solar-driven MD systems achieved a remarkable productivity increase, with over 200% improvement at low flow rates, highlighting their viability for energy-efficient desalination in remote and off-grid locations. In passive desalination, the optimization of the Marangoni effect enhanced mass transfer by up to three orders of magnitude compared to simple diffusion. The semi-empirical model developed offers accurate predictions for system optimization. Rapid nighttime brine discharge was achieved, reducing salinity to seawater levels within just two hours, an unprecedented result in the field.

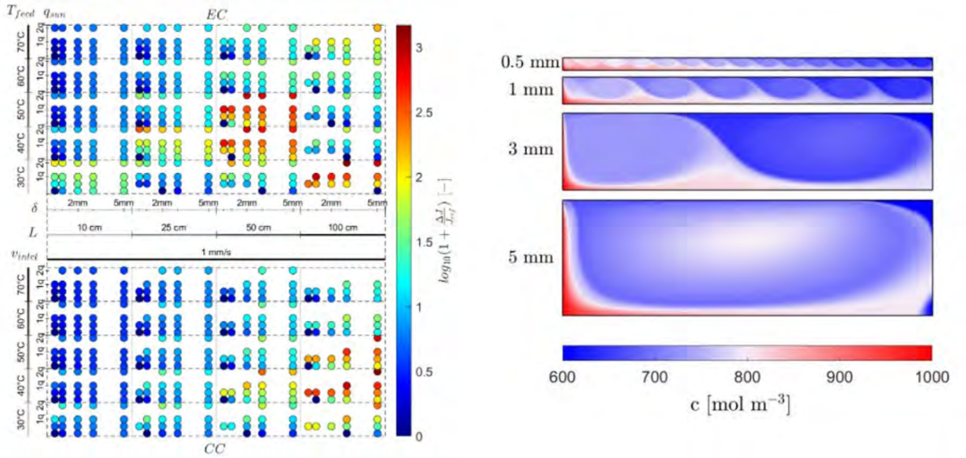


Figure 1 On the left graph on productivity as a function of input parameters in MD module enhanched by solar radiation. On the right, steady-state concentration surface plots, including the Marangoni effect.

External collaborations

- Consiglio Nazionale delle Ricerche (CNR-ITM)
- Centro de Investigaciones (CIEMAT)
- Amapex (AMX)

Academic context

[1] Stincone, G., Meo, R. R., Chiavazzo, E., Asinari, P., Fasano, M., & Morciano, M. (2024). Optimizing the Marangoni effect towards enhanced salt rejection in thermal passive desalination. *Desalination, 583*, 117673.
[2] Shalaby, S. M., et al. "Membrane distillation driven by solar energy: a review." Journal of Cleaner Production 366 (2022): 132949.
[3] Chiavazzo, E., Morciano, M., Viglino, F., Fasano, M., & Asinari, P. (2018). Passive solar high-yield seawater desalination by modular and low-cost distillation. *Nature Sustainability, 1*(12), 763–772

First name: Alessio **LAST NAME**: MONDELLO

Topic: Innovative processes and materials for long-term thermal energy storage

Course year: 1st **Tutor(s)**: Eliodoro CHIAVAZZO, Matteo PAVESE, Luca LAVAGNA.

Highlights of the research activity

In this first year of Ph.D., the primary focus of my research has been the investigation of innovative processes and materials suitable for long-term low-temperature thermal energy storage (TES), mainly focusing on salt hydrates and cement-based salt-inside porous matrix (CSPM) materials. My research focuses on developing newly cost-effective, high energy density salt-matrix combinations, primarily cement-based, for domestic heating applications. AI-driven sequential learning will guide material screening, optimization, and experimental validation. Promising materials will be characterized for properties and energy performance. Building on my research scholarship, I reviewed literature on key CSPM materials and cement-based TES technologies to deepen my understanding of synthesis techniques, identify challenges in state-of-the-art materials, and explore the mechanisms behind water sorption processes. In the meantime, I also began a campaign of synthesis on various composites and materials, starting with those that had already been synthesized and then expanding to new combinations. For the former, my efforts were directed at resolving well-known issues in the synthesis process to establish a reliable and repeatable protocol. For the latter, I focused on adapting this protocol to ensure a consistent synthesis method across all materials, that is fundamental at a later stage to obtain a consistent dataset for the AI data treatment. These activities resulted in the production of various CSPM samples, such as Portland Cement (PC) combined with $MgSO_4$, $Al_2(SO_4)_3$, $CaCl_2$, $MgCl_2$ and $SrBr_2$, which have been tested in a dynamic vapour sorption (DVS) instrument to obtain their water adsorption isotherms. They will also be tested soon to evaluate other key properties, including water uptake, energy density, kinetics data and stored energy per cost unit. Regarding the material properties, some tests were already carried out like SEM imaging on some composites, suggesting that the synthesis using a saturated solution of certain salts hinders the formation of the typical cementitious matrix structure, making it necessary to identify the maximum concentration for each salt that still allows the formation of an acceptable cement matrix during synthesis. In parallel with the production of the composite samples, I conducted a characterization analysis of the pure hydrated salts using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). For each salt, I obtained data on the enthalpy of the dehydration reactions, the number of water molecules released at each dehydration step, the onset temperature at which each dehydration step begins and additional information related to salt degradation.

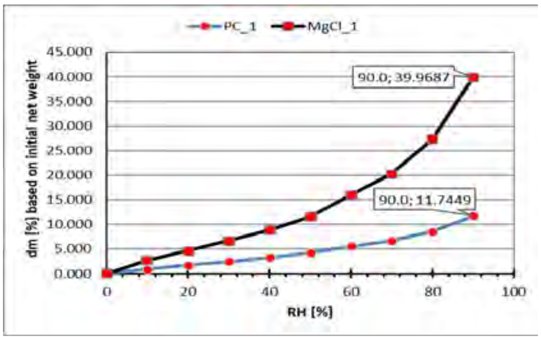


Figure 1. Water adsorption isotherms of PC and a $MgCl_2$-PC composite. *RH%* is the relative humidity percentage while *dm* is the weight percentage difference based on the dry initial weight.

External collaborations

- Politecnico di Milano – Dipartimento di Energia
- CNR – Istituto di Chimica dei Composti Organometallici (ICCOM)
- Università degli Studi di Messina – Dipartimento di Ingegneria

Academic context

[1] Salustro, S., et al. (2024). Thermal characterization and cost analysis of cement-based composite materials for thermochemical energy storage. *Journal of Energy Storage, 93*. https://doi.org/10.1016/j.est.2024.112308
[2] Lavagna, L., et al. (2020). Cementitious composite materials for thermal energy storage applications: A preliminary characterization and theoretical analysis. *Scientific Reports, 10*(1), 12833. https://doi.org/10.1038/s41598-020-69502-0
[3] Donkers, P., et al. (2017). A review of salt hydrates for seasonal heat storage in domestic applications. *Applied Energy, 199*, 45–68. Elsevier Ltd. https://doi.org/10.1016/j.apenergy.2017.04.080

First name: Andrea **LAST NAME**: Moranti

Topic: Proton conductive ceramic cells for FC/EL and for compression / separation (N_2, cracking NH_3, H_2/H_2O)

Course year: 1st **Tutor(s)**: Massimo SANTARELLI, Federico SMEACETTO, Matteo TESTI

Highlights of the research activity

The research focuses on the development of multiphysics models for proton conductor ceramic cells (PCCs), with an emphasis on assessing the electrochemical properties of barium-based zirconates and cerates (BCZY). A particular focus is placed on the transport of multiple defects, such as protons and oxygen vacancies, and the evaluation of the performance worsening caused by electronic leakage.
The study incorporates material characterization by manufacturing BCZY/BCZYYb pellets for Electrochemical Impedance Spectroscopy (EIS) under controlled atmospheres. This approach is designed to analyze both equilibrium and Distribution Relaxation Times (DRT). Using COMSOL, 1D, 2D, and 3D models were developed to simulate membranes and single repeat units (SRUs), integrating thermal-fluid-dynamic and electrochemical phenomena. These models evaluate planar, bottom and tubular configurations, analyzing temperature distributions and defect transport in co-flow and cross-flow geometries.
Advanced modeling applications include the simulation of catalytic reactions for co-ionic cells, such as Fischer-Tropsch to Olefins (FTO) and Methanol to Olefins (MTO) pathways, as part of the ECOLEFINS project. Additionally, ammonia decomposition for hydrogen purification and transient gas-perovskite interactions, incorporating multiple defect effects, are explored.
Finally structural analyses investigate thermal expansion and stress within SRUs, focusing on the behavior of glass sealants in collaboration with the DISAT department.
The research culminates in the implementation of planar 5x5 cm² SRUs and bottom cell configurations, with ongoing work on tubular designs. This integrated approach advances understanding of PCCs through material and structural analysis, and exploration of practical configurations for industrial applications

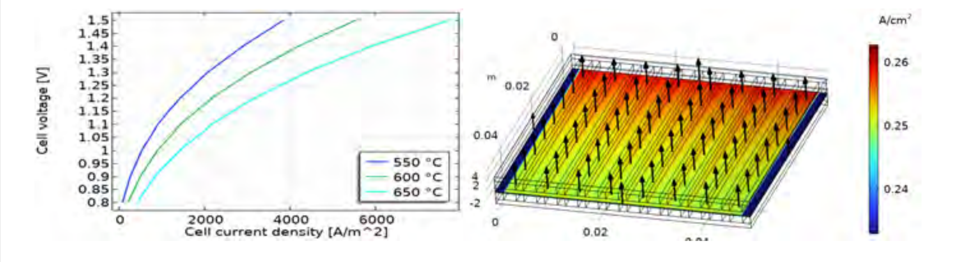


Figure 1: Polarization curve (top) and hydrogen ion fluxes (bottom) for planar

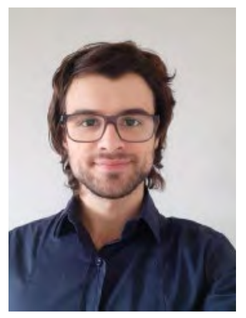
External collaborations

- Fondazione Bruno Kessler
- Colorado School of Mines

Academic context

[1] H. Zhu et al., “Defect Incorporation and Transport within Dense BaZr0.8Y0.2O3 − δ (BZY20) Proton-Conducting Membranes,” J Electrochem Soc, vol. 165, no. 9, p. F581, May 2018, DOI: 10.1149/2.0161809jes
[2] J.-H. Zhang et al., “Mathematical modeling of a proton-conducting solid oxide fuel cell with current leakage,” J Power Sources, vol. 400, pp. 333–340, 2018, DOI: 10.1016/j.jpowsour.2018.08.038

First name: Stefan **LAST NAME**: MOROSANU



Topic: Enhancing the energy efficiency of solar-water purification technology for green hydrogen production

Course year: 1st **Tutor(s)**: Matteo FASANO, Matteo MORCIANO

Highlights of the research activity

My PhD research focuses on developing and testing a water desalination prototype to be coupled with a green hydrogen production system. This system integrates photovoltaic (PV) panels, a water desalination unit, and an electrolyzer. The desalination module is based on thermal membrane distillation (MD). Waste heat from PV panels powers the process, and a multistage version is under development to enhance efficiency by reusing the latent heat of condensation between stages. The first characterization test involved the use of bulk preheating of feedwater; the prototype achieved a productivity of 0.8–1.2 L/(m²h) at feed temperatures of 61–68°C, respectively, and mass flow rates of 96 mL/min. In Figure 1 on the right side, the performance under a wider range of operating conditions. The second experimental characterization campaign instead involved the use of waste heat or (artificial) solar energy in place of bulk heating of feedwater. In this condition, the device was able to produce 0.18-0.24 L/(m²h) in case of a mass flow rate between 6-30 mL/min. Future work involves developing a thermo-fluid dynamics model and validating it against experimental results. The validated model will be used to explore interesting and promising operating configurations. Two publications have been planned in the near future: the first will provide a literature review on the coupling of desalination technologies with green hydrogen production technologies, while the second will illustrate the experimental and numerical results obtained.

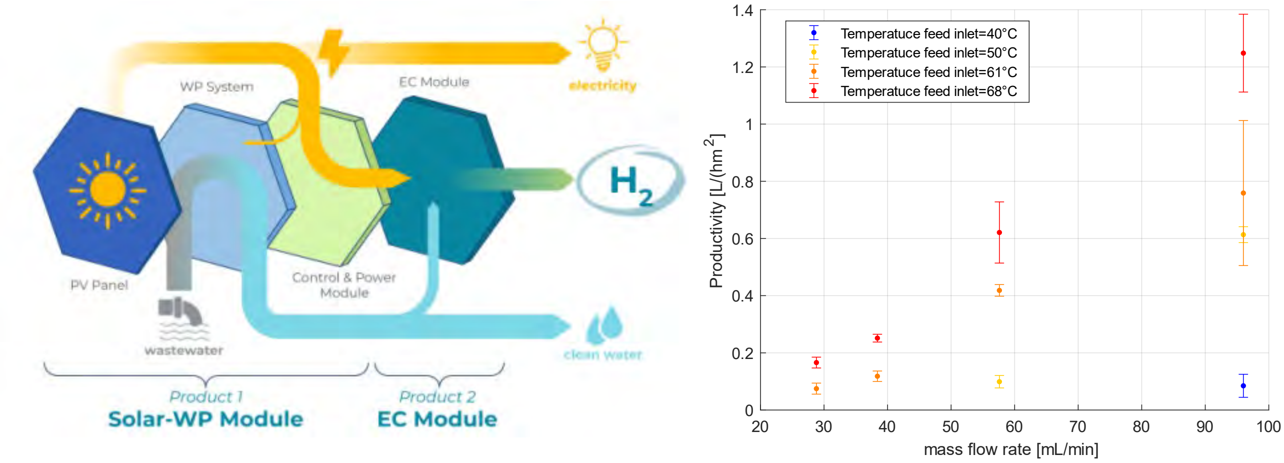


Figure 1: On the left-hand side, a schematic of the coupling between the various envisioned systems, i.e. the water purification system, the PV panel and the electrolyzer, is shown. On the right side experimental results are shown when pre-heated water is used. The X-axis represents the mass flow rate, while the Y-axis shows productivity values, measured as liters of freshwater produced per hour and normalized to the membrane area. The color corresponds to the feedwater inlet temperature.

External collaborations

- Green Independence s.r.l
- Athena s.p.a
- Memetis GmbH

Academic context

[1] Antonetto et al. "Synergistic freshwater and electricity production using passive membrane distillation and waste heat recovered from camouflaged photovoltaic modules." *J. of Cleaner Production* 318 (2021): 128464.

First name: Lucia **LAST NAME**: PERA

Topic: Detailed in-operando analysis of SOFC operating with bio-syngas: evaluation of the simultaneous impacts of organic and inorganic contaminants

Course year: 1st **Tutor(s)**: Massimo SANTARELLI, Marta GANDIGLIO, Paolo MAROCCO

Highlights of the research activity

The aim of this work is to comprehensively explore trace contaminants in biogas and understand their influence on SOFCs. This research focuses on understanding the impact of biogas contaminants on SOFC performance, a critical step as biogas offers a renewable, hydrogen-compatible fuel source for these cells. This study begins combining a comprehensive literature review with on-site analyses at biogas plants, identifying key contaminants and their threshold effects on SOFCs. Contaminants such as sulfur compounds, siloxanes, halocarbons, and aromatic compounds are identified and categorized based on their source: landfill gas, agricultural gas, gas from the organic fraction of municipal solid waste (OFMSW), and gas from wastewater treatment plants (WWTP). The study highlights significant variability in contaminant concentrations across different sources, with hydrogen sulfide (H_2S) being the most prevalent. These findings underscore the importance of accurate contaminant measurements for advanced technologies like SOFCs.
Experimental activities focused on assessing the effects of biogas contaminants on SOFC performance have involved electrochemical characterization of SOFC samples exposed to simulated syngas containing representative contaminants. Long-term tests monitor cell performance under constant conditions, analyzing the impact of selected impurities at concentrations below and above theoretical thresholds. Real-time measurements include continuous monitoring of cell voltage and periodic electrochemical impedance spectroscopy (EIS) to evaluate process evolution. Advanced analytical techniques, such as Distribution of Relaxation Times (DRT) analysis, are employed to gain deeper insights into the electrochemical processes and identify degradation mechanisms associated with specific contaminants.
Parallel to the experimental work, a theoretical model is being developed to simulate the observed degradation processes and predict SOFC performance under various operating conditions. This model, supported by experimental data, aims to provide a framework for understanding and mitigating the impact of biogas contaminants on fuel cell technologies.
The research highlights the critical need for targeted contaminant management in biogas applications to ensure the reliability and efficiency of advanced energy conversion systems such as SOFCs.

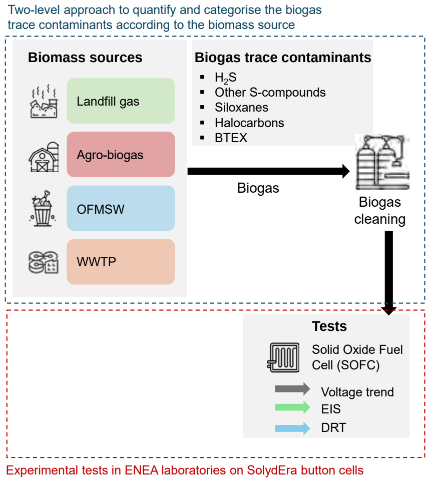


Figure. Sketch of the first year activity

External collaborations

- ENEA Casaccia (Rome, Italy)
- Consorzio Monviso Agroenergia (CMA)
- École Polytechnique Fédérale de Lausanne (EPFL)

Academic context

[1] L. Pera *et al.,* “Trace contaminants in biogas: Biomass sources, variability and implications for technology applications,” Dec. 01, 2024, *Elsevier Ltd*. doi: 10.1016/j.jece.2024.114478.
[2] A. Lanzini *et al.*, “Dealing with fuel contaminants in biogas-fed solid oxide fuel cell (SOFC) and molten carbonate fuel cell (MCFC) plants: Degradation of catalytic and electro-catalytic active surfaces and related gas purification methods,” 2017, *Elsevier Ltd*. doi: 10.1016/j.pecs.2017.04.002.
[3] M. Gandiglio, *et al*., “Results from an industrial size biogas-fed SOFC plant (the DEMOSOFC project),” *Int J Hydrogen Energy*, vol. 45, no. 8, pp. 5449–5464, Feb. 2020, doi: 10.1016/j.ijhydene.2019.08.022.

First name: Gabriele **LAST NAME**: PEYRANI

Topic: Techno-economic analysis of hydrogen regional trains

Course year: 1st **Tutor(s)**: Massimo SANTARELLI, Marta GANDIGLIO, Paolo MAROCCO, Pierpaolo CHERCHI (Alstom)

Highlights of the research activity

The global railway sector faces growing pressure to adopt more sustainable and low-emission technologies, particularly for non-electrified routes. While electric traction through overhead lines is often preferred, its implementation is limited by high infrastructure costs and technical challenges in remote or complex terrains. Battery-electric trains, despite their high roundtrip efficiency, are similarly constrained by limited driving range and increased weight due to energy storage requirements. In this context, integrating fuel cell and battery systems emerges as a promising alternative for decarbonizing rail transport.

My research presents a comprehensive methodology to calculate energy requirements, optimizing energy management strategies, reduce hydrogen consumption and minimize the aging of the fuel cell-batteries powertrain. In the end, a Total Cost of Ownership (TCO) analysis has been conducted to compare the economic viability of hybrid fuel cell systems with conventional (diesel and electric) and innovative (battery-electric) solutions. The methodology was applied to a 103 km railway line in Italy (Brescia-Iseo-Edolo), currently served by diesel trains but set to transition to 14 Hydrogen Multiple Units (HMUs).

This case study provides an ideal scenario for analyzing the potential benefits of hydrogen-based propulsion. Results indicate that fuel cell trains can reduce primary energy consumption by up to 40% compared to diesel alternatives, while maintaining comparable operational performance. Although diesel trains currently exhibit a slightly lower TCO (3-6% less), rising diesel prices and declining hydrogen costs are expected to make hydrogen trains always more competitive in future. These findings highlight the transformative potential of hydrogen technology in advancing rail decarbonization. The developed framework serves as a valuable tool for guiding decision-making, optimizing system design, and supporting the adoption of low-carbon solutions in regional rail transport.

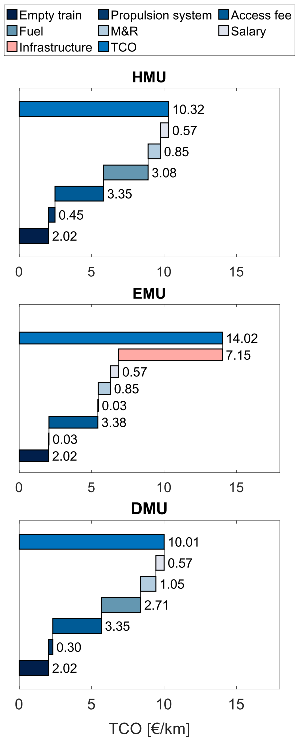


Figure 10: TCO results of hydrogen, diesel and electric trains for the Brescia-Edolo line.

External collaborations

- Alstom
- Università di Bologna
- Università di Genova
-

Academic context

[1] Zenith, F., Isaac, R., Hoffrichter, A., Thomassen, M. S., & Møller-Holst, S. (2020). Techno-economic analysis of freight railway electrification by overhead line, hydrogen and batteries: Case studies in Norway and USA. *Proceedings of the Institution of Mechanical Engineers, Part F: Journal of Rail and Rapid Transit*, *234*(7), 791–802. https://doi.org/10.1177/0954409719867495.
[2] Fedele, E., Iannuzzi, D., & del Pizzo, A. (2021). Onboard energy storage in rail transport: Review of real applications and techno-economic assessments. *IET Electrical Systems in Transportation*, *11*(4), 279–309. https://doi.org/10.1049/ELS2.12026.

First name: Vincenzo **LAST NAME**: ROMANO

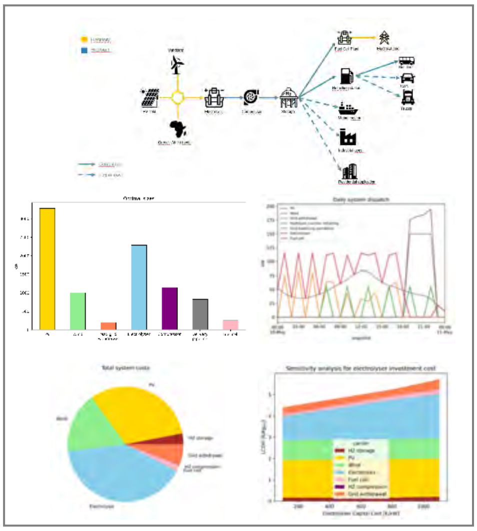
Topic: Modelling of hydrogen valleys, including experiments in H_2 tunnel

Course year: 1st **Tutor(s)**: Massimo SANTARELLI, Marta GANDIGLIO, Paolo MAROCCO

Highlights of the research activity

My research activity, which began in March 2024, spans three EU-funded projects: HYDRA, CRAVE-H2, and IMAGHyNE. This year's work has primarily focused on the first two projects, divided into the following key areas:

- **Hydrogen Market Policies and Supply Chain Analysis:** Conducted as part of the HYDRA project, this segment involved an extensive study of hydrogen market policies and supply chains on both global and regional scales. The analysis included key hydrogen-based products such as ammonia, methanol, and refinery products. The primary objective was to establish a comprehensive policy framework and compile a robust market dataset. These findings, besides being essential for calibrating an agent-based model developed within the project, provide a broader framework situating hydrogen valleys within the wider hydrogen economy.



Scheme of the CRAVE-H2 valley and key results from the preliminary optimization study

- **Optimization Model Development for Hydrogen Valleys:** As part of the CRAVE-H2 project, the focus has been on developing an optimization model designed to serve as a digital twin of a hydrogen valley, with the initial case study being based on the facility currently under construction in Crete island. This model, ran on a yearly horizon with hourly timesteps, is able to perform both optimal capacity planning and optimal dispatching having fixed components' size under a cost minimization perspective. The initial focus is on addressing two primary demands: refuelling a fleet of fuel cell-powered touristic buses and providing grid stabilization services through a stationary fuel cell, leveraging the benefits of seasonal hydrogen storage. A constant hydrogen demand, simulating an industrial end-user, is also added to increase electrolyser's utilisation. The next phase of analysis will expand the model to include hydrogen supply for the marine and industrial sectors. Moreover, future advances in the model will see it become a flexible tool suitable for application in a variety of contexts.
  This preliminary study will serve as a starting point for a broader analysis to explore different methodologies and modelling choices, to depict a complete framework of what kind of specific analysis might best represent the main characteristics of hydrogen valleys.

These activities form the foundation for advancing knowledge and tools in hydrogen systems modelling and their integration into future energy systems.

Academic context

[1] M. Bampaou and K. D. Panopoulos, "An overview of hydrogen valleys: Current status, challenges and their role in increased renewable energy penetration," Renewable and Sustainable Energy Reviews, vol. 207, p. 114923, Jan. 2025, doi: 10.1016/J.RSER.2024.114923.
[2] S. Rosén, L. Göransson, M. Taljegård, and M. Lehtveer, "Modeling of a 'Hydrogen Valley' to investigate the impact of a regional pipeline for hydrogen supply," Front Energy Res, vol. 12, 2024, doi: 10.3389/fenrg.2024.1420224.
[3] S. Esquivel-Elizondo, A. Hormaza Mejia, T. Sun, E. Shrestha, S. P. Hamburg, and I. B. Ocko, "Wide range in estimates of hydrogen emissions from infrastructure," 2023, Frontiers Media SA. doi: 10.3389/fenrg.2023.1207208.

First name: Giampiero **LAST NAME**: SACCHI

Topic: Upscaling and techno-economic optimization of upgrading technologies and biogas methanation

Course year: 1st **Tutor(s)**: Andrea LANZINI, Marta GANDIGLIO

Highlights of the research activity

In its first year, the project conducted a thorough literature review to assess the state of biogas upgrading technologies and emerging trends. Collaborative meetings with partners have facilitated knowledge sharing and enhanced understanding of the five pilot technologies' technical and operational requirements. Preliminary process flowsheets of all Pilots have been assessed using Aspen+ software, laying the groundwork for the first deliverable due in January 2025. Ex-situ Thermochemical Methanation (ETM) uses the Sabatier reaction in fixed-bed reactors to reduce CO_2 to methane. While well-studied with pure CO_2, its application to biogas methanation is still at the demonstration stage. Ex-situ Biological Methanation (EBM) separates CO_2 from biogas and converts it to methane in a mesophilic biological reactor using hydrogen. In-situ Biological Methanation (IBM) introduces hydrogen directly into an anaerobic digester, favoring hydrogenotrophic methanogenesis over acetoclastic processes. This method produces biogas enriched to ~80% CH_4, requiring further treatment for grid injection. Ex-situ Syngas Biomethanation (ESB) upgrades syngas from biomass gasification. CO is converted to methane biologically, with external hydrogen enabling >95% CH_4 purity. ElectroMethanoGenesis (EMG) involves two reactors: one improves anaerobic digestion through electrochemical processes, and the other uses a proton exchange membrane to combine CO_2 and protons, forming methane. These technologies aim to maximize biomethane yield while aligning with sustainability and renewable energy goals. Present advancements will be presented at the 33rd European Biomass Conference and Exhibition (EUBCE) in June 2025, accompanied with a preliminary Life Cycle Assessment (LCA) to compare the environmental impacts of these technologies, with emphasis on their carbon footprints, ensuring compliance with renewable energy directives. The goal is to harmonize biological and non-biological contributions into a unified biomethane stream. Future efforts will focus on refining these processes and preparing for pilot demonstrations. Through this project, the Biomethaverse team aspires to deliver scalable, sustainable solutions for biomethane production, advancing renewable energy innovation.

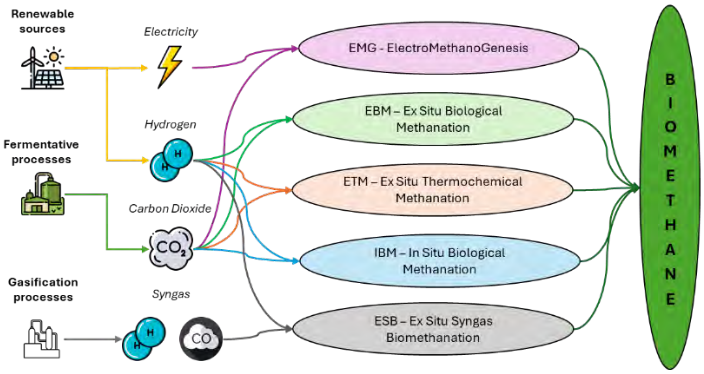


Figure 1 - Overview of the 5 innovative pathways for Biomethane production through CO2 recovery

External collaborations

- ENEA – Italian National Agency for New Technologies, Energy and the Environment
- EBA – European Biogas Association
- University of Aberdeen

Academic context

[1] M. Tommasi, S. N. Degerli, G. Ramis, and I. Rossetti, “Advancements in CO2 methanation: A comprehensive review of catalysis, reactor design and process optimization,” *Chem. Eng. Res. Des.*, vol. 201, no. December 2023, pp. 457–482, 2024. https://doi.org/10.1016/j.cherd.2023.11.060

[2] T. J. Ao, C. G. Liu, Z. Y. Sun, X. Q. Zhao, Y. Q. Tang, and F. W. Bai, “Anaerobic digestion integrated with microbial electrolysis cell to enhance biogas production and upgrading in situ,” *Biotechnol. Adv.*, vol. 73, no. May, p. 108372, 2024. https://doi.org/10.1016/j.biotechadv.2024.108372

[3] T. Antukh, I. Lee, S. Joo, and H. Kim, “Hydrogenotrophs-Based Biological Biogas Upgrading Technologies,” *Front. Bioeng. Biotechnol.*, vol. 10, no. April, pp. 1–14, Apr. 2022. https://doi.org/10.3389/fbioe.2022.833482

First name: Anis Ahmad **LAST NAME**: SHER

Topic: Analysis, modelling, experimental tests and design of solutions for H_2 on-board storage and upstream production/distribution

Course year: 1st **Tutor(s)**: Massimo SANTARELLI, Domenico FERRERO, Marta GANDIGLIO

Highlights of the research activity

We have determined the state of the art of four main pathways of on-board hydrogen storage, which are compressed gas, liquid/cryo-compressed, LOHC and other liquids, solid adsorption structures). Now we are further analyzing these pathways on the basis of Key Performance Indicators (KPIs) and have done most of the review. Here is presented some data, collected from literature.

In Physical based, Liquid and cryo-compressed performance is better in terms of gravimetric and volumetric densities. On the basis of energy consumption and overall cost, the compressed gaseous hydrogen is performing well.

In material based, metal hydrides, both densities are large, but it is possible theoretically. High energy consumes in dehydrogenation process in LOHC. In most metal hydrides the KPIs are achievable but the problem is low hydrogen release rate, and need high release temperature. From the chart, it is clear, that Liquid and cryo-compressed system cost is low, but overall cost is high due to conversion along with vent losses in liquid. Moreover, it also needs extra components (heat exchanger) to use as a fuel and causes complications in the system.

In heavy duty vehicle gravimetric and volumetric is more dominating, but in light duty vehicles (LDV) the above complications effect the vehicle cost. We will further analyze these pathways in the next year and will then model and experimentally investigate them for determining the best solution.

Figure 1. Fig. Comparison of technical and economic KPIs

Hydrogen can be produced by number of ways. We have adopted electrolysis and determined State-of-the-art of the 2 main electrolysis pathways: low Temperature (Proton Exchange Membrane, Anion Exchange Membrane) and high Temperature (Solid Oxide Fuel Cell) electrolysis technologies. Now we will validate the models (through lab experiments) of the 2 electrolysis pathways, and then will design best solution of the H2 production.

At the end we will do analysis, through modeling and lab experiments, of the conversion need for H_2 distribution.

External collaborations

- Stellantis
- IVECO

Academic context

[1] P. Dogliani, et al, “Multi-option analytical modeling of levelized costs across various hydrogen supply chain nodes,” Int. J. Hydrogen Energy

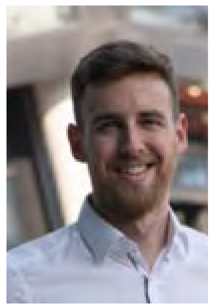
[2] R. K. Ahluwalia, et al, “Liquid hydrogen storage system for heavy duty trucks: Capacity, dormancy, refueling, and discharge,” Int. J. Hydrogen Energy

[3] IEA (2024), Global Hydrogen Review 2024, IEA, Paris https://www.iea.org/reports/global-hydrogen-review-2024

First name: Marcel **LAST NAME**: STOLTE

Topic: “Technical and economic assessment of Long-Duration Energy Storage (LDES) options for the energy markets”

Course year: 1st **Tutor(s)**: Francesco MINUTO, Silvia CASAGRANDE, Andrea LANZINI



Highlights of the research activity

The growing need for long-duration energy storage (LDES) to support renewable integration highlights hydrogen as one of the viable options for storage durations exceeding the capabilities of Li-ion batteries. This was the research focus during the first year of my PhD. In particular, I concentrated on the optimal sizing of green hydrogen production systems, integrating renewable energy sources. The work included hybrid storage systems, combining compressed hydrogen storage and battery energy storage systems (BESS) to achieve optimal system designs. Particle swarm optimization (PSO) was employed to determine the ideal plant configurations.
Two scientific papers were produced (one published, the other in late stages of peer review), both of which explore the technical and economic dimensions of hydrogen production. The first article considers the variability of renewable resources across different geographic locations, electricity prices, and demand profiles, investigating their effect on the levelized cost of hydrogen (LCOH) and greenhouse gas (GHG) emissions (Figure 1). The second article analyzes the impact of incentives and land availability in an Italian case study.

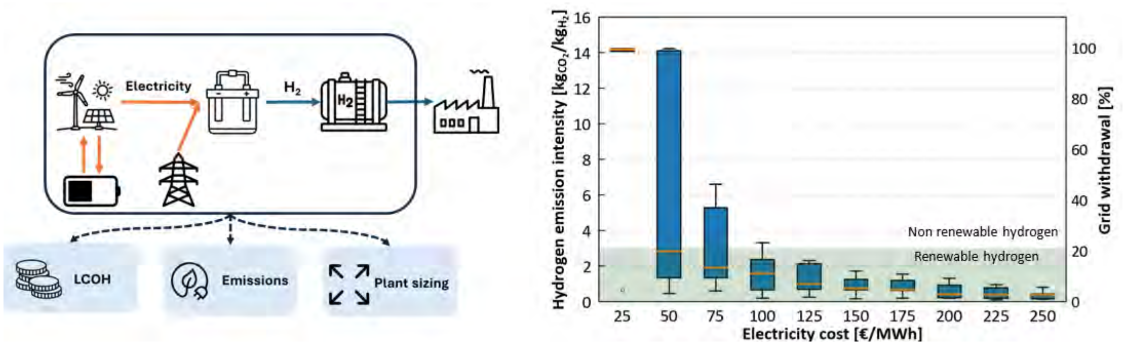


Figure 1: On the **left**: System layout that was optimized using Particle Swarm Optimization. On the **right**: GHG emission intensity of the produced hydrogen for different grid electricity prices considering the average European electricity grid emission factor. Each bar incorporates the emission intensity for different locations.

The results identify the high LCOH, typically ranging from 6 to 8 EUR/kg, as a significant barrier to the widespread adoption of hydrogen. The cost gap to fossil fuels underscores the need for incentives, which, in the Italian case study, reduced the LCOH by 70%, but still fell short of achieving cost parity with natural gas. To further decrease LCOH, selecting sites with high renewable energy potential is essential. Moreover, incentives promoted the installation of larger dedicated renewable energy systems and storage solutions, reducing GHG emissions by up to 85% and minimizing grid withdrawal.

External collaborations

- Edison S.p.A.
- EDF Australia

Academic context

[1] M. Stolte, F. D. Minuto, and A. Lanzini, ‘Optimizing green hydrogen production from wind and solar for hard-to-abate industrial sectors across multiple sites in Europe’, Int. J. Hydrog. Energy, vol. 79, pp. 1201–1214, Aug. 2024, doi: 10.1016/j.ijhydene.2024.07.106.

First name: Jamshid **LAST NAME**: YAKHSHILIKOV

Topic: Hydrogen utilization path for transport sector of Uzbekistan

Course year: 2nd **Tutor(s)**: 1st Pierluigi LEONE, 2nd Massimo SANTARELLI, 3rd Marco CAVANA.

Highlights of the research activity

During the first year of research, the focus was primarily on conducting an in-depth and comprehensive review of the transport and energy sectors in Uzbekistan. The overarching goal of this review was to analyze the current state of the transport sector, with particular emphasis on identifying viable pathways for the integration of hydrogen-based solutions that could contribute to the country's sustainability goals.

The analysis began with a detailed assessment of both the rail and road fleets, which included an examination of vehicle types, fuel consumption patterns, the level of railroad electrification as well as location of logistic hubs. Furthermore, emphasis was placed on understanding the broader energy policy landscape in Uzbekistan, revealing a significant gap in the institutional and policy frameworks necessary to foster the development of hydrogen infrastructure and technologies.

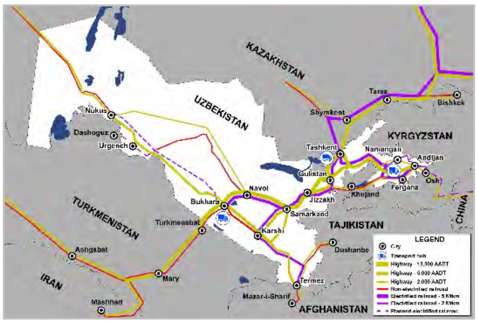


Figure 1. International highways, railroads, and logistic hubs in Uzbekistan (Yakhshilikov et al.)

Several challenges were uncovered during the review, including the high initial capital investment required for the establishment of hydrogen infrastructure. Additionally, the need for enhanced regional cooperation was highlighted, as many hydrogen-related projects will require cross-border collaboration to facilitate their implementation in the region.

The study also explored the feasibility of various hydrogen production methods, with a particular focus on green hydrogen derived from renewable energy sources such as solar and wind power, as well as hydrogen produced from natural gas with carbon capture technology. These methods were analyzed in the context of Uzbekistan's energy resources and infrastructure, taking into account the country's current energy mix and future potential for green energy development. A review of global hydrogen technologies, including H2-ICE, H2CNG, and FCEVs, was conducted to assess their applicability and potential impact on Uzbekistan's transport sector.

The results of this thorough analysis were subsequently published in a review paper, which presents a detailed overview of the opportunities and challenges associated with hydrogen utilization in Uzbekistan's transport sector. The collected data from this review will form the foundation for the next stage of research, which focuses on the development of a bottom-up energy-transport model. This model will be instrumental in creating detailed scenarios for a sustainable transition of Uzbekistan's transport sector, with an emphasis on integrating hydrogen solutions into the broader energy and mobility landscape. The outcomes of this work are expected to provide valuable insights and recommendations for policymakers, enabling evidence-based decision-making to foster the adoption of hydrogen technologies and promote sustainable development in the transport sector.

External collaborations

- Turin Polytechnic University in Tashkent
- The Ministry of Innovation Development of the Republic of Uzbekistan
- JSC UzAutosanoat

Academic context

[1] Yakhshilikov, J.; Cavana, M.; Leone, P. A Review of the Energy System and Transport Sector in Uzbekistan in View of Future Hydrogen Uptake. Energies 2024, 17, 3987. https://doi.org/10.3390/en17163987

Sustainable nuclear energy

First name: Alex **LAST NAME**: AIMETTA

Topic: Multiphysics modelling of fusion machines liquid-breeder blankets

Course year: 3rd **Tutor(s)**: Sandra DULLA, Antonio FROIO

Highlights of the research activity

During the 3rd year of PhD, my research activity has been focused on advanced nuclear engineering aspects studied and assimilated during the first two years of PhD: multiphysics modelling and uncertainty propagation. Concerning uncertainty propagation aspects, I have been involved in a collaboration between Politecnico di Torino, ENEA Casaccia, Argonne National Laboratory and Ben-Gurion University, for the study of sensitivity and uncertainty due to nuclear data in the TAPIRO reactor, located in Casaccia. The analysis has been carried out using the Serpent code, both using intrusive techniques (e.g., Generalized Perturbation Theory) and non-intrusive methods (e.g., Unscented Transform). The analysis has shown that ^{235}U and ^{63}Cu are the main contributors to the uncertainty of k_{eff}, β_{eff}, and Λ_{eff}.

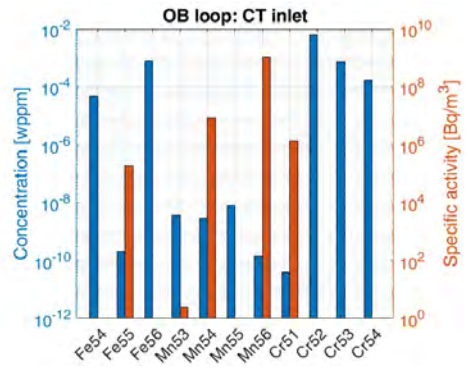


Fig. Concentrations and specific activities of dispersed material in WCLL EU DEMO.

Uncertainties come from modelling choices too, like the selection of the energy grid to be used in deterministic neutronics codes. Generally, this choice is based on expert judgement, but this approach is clearly not the most appropriate one in the case of next generation reactors, where the expertise is quite limited. A more rigorous approach consists of using Genetic Algorithms (GA) to find the optimal energy grid. Here, the GA developed by Dr. Mattia Massone (ENEA) has been employed to find out the optimal energy grid to be used in the FRENETIC code, developed at PoliTo, for the modelling of the ALFRED (LFR) reactor. The results bring out that the optimal grids have a total amount of groups about 10, of which one group in the thermal region and three groups in the fast region [2]. The expertise developed during this work is currently being exploited to find the optimal grid to be used in the nemoFoam multiphysics tool [1], for the ARC fusion reactor.
Finally, I have been involved in a collaboration for the assessment of the generation and the transport of the activated corrosion products (ACPs) in the Water-Cooled Lithium-Lead (WCLL) breeding blanket designed for the EU DEMO fusion reactor, in the framework of the EUROfusion Consortium. The assessment of ACPs is particularly important from the safety point of view. For this reason, a module for the simplified modelling of activation and decay of ACPs according to the Bateman equations have been implemented in the system-level GETTHEM code [3], developed at PoliTo. The results obtained so far are still preliminary but promising, showing the importance, in terms of activity, of isotopes like ^{54}Mn and ^{56}Mn, as shown in the figure.

External collaborations

- ENEA
- Tokamak Energy
- Argonne National Laboratory

Academic context

[1] M. Caravello, A. Aimetta, N. Abrate, S. Dulla; A. Froio; (2024); An OpenFOAM solver for multiphysics modeling of fusion reactor design: The nemoFoam code. In: NUCLEAR MATERIALS AND ENERGY, vol. 40.
[2] N. Abrate, A. Aimetta, M. Massone, S. Dulla, P. Ravetto; (2024); A genetic-driven optimisation of the energy grid structure for nodal full-core calculations in lead-cooled fast reactors; In: NUCLEAR SCIENCE AND ENGINEERING, under submission.
[3] F. Lisanti, A. Aimetta, P. Arena, R. Bonifetto, M. Ferraris, A. Froio; (2024); Multiphysics modelling of the Activated Corrosion Products generation and transport in the WCLL PbLi loop with GETTHEM, SOFT 2024 Conference, Dublin, Ireland, September 22-27, 2024.

First name: Pietro **LAST NAME**: CIOLI PUVIANI

Topic: Multiscale approach for the thermal-hydraulic analysis of heavy liquid metal pool systems

Course year: 3rd **Tutor(s)**: Roberto Zanino

Highlights of the research activity

My research focuses on Heavy Liquid Metal (HLM) technologies, particularly the GEN-IV Lead-cooled Fast Reactor (LFR), in collaboration with ENEA Brasimone. ENEA, a key player in advancing LFR technologies, supports R&D for demonstrator reactors, like ALFRED and LFR-AS-200, in cooperation with industrial partners such as Ansaldo Nucleare and *new*cleo.

During the third year of my PhD, I further developed a thermal-hydraulic simulation tool combining CFD (ANSYS CFX) and system codes (RELAP5) via coupling. This method bridges STH codes' efficiency in global reactor behavior modeling with CFD's detailed 3D flow analysis, achieving comprehensive and computationally viable simulations. The tool gives the possibility to select between explicit and semi-implicit time-advancing schemes and among different spatial domain approaches (decomposition and overlapping).

Validation exercises involved simulating the NACIE-UP LBE loop, yielding a good agreement with experimental data. The results of this activity have been presented as ENEA contribution for a dedicated IAEA Coordinated Research Project. Further applications included the validation against TALL-3D loop experimental results. The coupled tool effectively replicated forced-to-natural circulation transitions, highlighting its superiority over standalone RELAP5 in capturing complex 3D phenomena (Figure 1). Stability analysis showed the superiority of semi-implicit and overlapping approaches, though stable configurations were achieved with all the available options within the tool. The ATHENA pool type facility, under the ALFRED R&D project, also represented a suitable test bench with conditions representative of LFRs. Among the different cases, the most relevant numerical test simulates a LOFS accident, exploring with the CFD code the heat transfer in the Core Simulator, including the inter-wrapper flow regions. Results demonstrated discrepancies with respect to STH standalone results in temperature profiles, showcasing the potential of CFD potential to refine system-scale analyses.

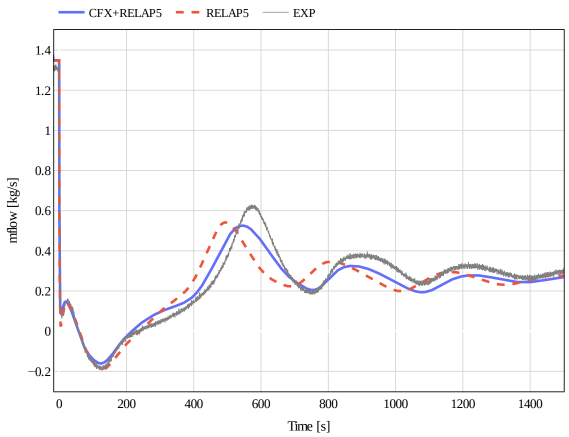


Figure 1 – Comparison between experiment, RELAP5 and coupled simulation of the mass flow rate in the TALL3D facility.

External collaborations

- ENEA
- Ansaldo Nucleare
- *new*cleo

Academic context

[1] P. Cioli Puviani et al., Development of a thermal mass flow meter for heavy liquid metal applications, Nuclear Engineering and Design, Volume 427, 113427, ISSN 0029-5493, 2024. https://doi.org/10.1016/j.nucengdes.2024.113427.

[2] P. Cioli Puviani et al., CFD – STH code coupling for the thermal-hydraulic analysis of NACIE-UP experimental facility, 20th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-20), 20-25 August 2023.

[3] P. Cioli Puviani et al., Coupled CFD-STH modelling of the ATHENA lead-cooled pool-type facility, 14th International Topical Meeting on NUTHOS-14 Vancouver, BC, Canada, August 25 – 28, 2024.

First name: Gianvito **LAST NAME**: COLUCCI

Topic: Development of new sustainability paradigms for bottom-up energy system modeling

Course year: 3rd **Tutor(s)**: Laura SAVOLDI, Valeria DI COSMO

Highlights of the research activity

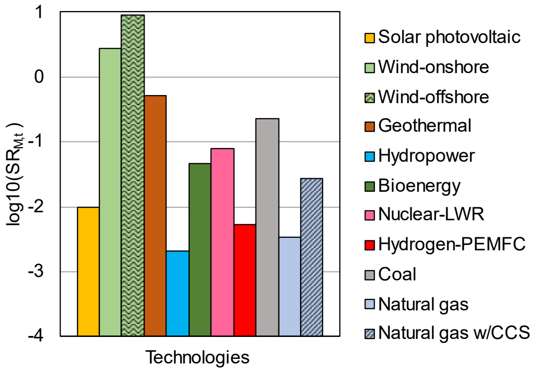


Figure 1. Supply risk ($\mathrm{SR}_{\mathrm{M,t}}$) magnitude of power sector technologies.

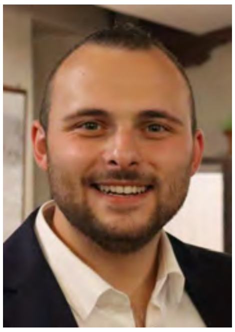
My PhD project within the MAHTEP Group aims to expand the current paradigm of the bottom-up energy system optimization models (ESOMs) behind the traditional macro-economic schemes. The development and maintenance of several energy system models carried out during the first two years of the project served as a basis for the integration of critical raw materials (CRMs) aspects in such models, to enhance their capability in providing policy-relevant insights on CRMs for the energy transition. In particular, three approaches were developed and tested in the TEMOA-Italy open-source model. The first approach concerned the development of CRMs supply disruption scenarios by applying devoted constraints to the supply of CRMs. The latter were integrated as a new commodity type in the TEMOA framework. Also, CRMs requirement by power, storage, hydrogen, and transport technologies can be tracked. These scenarios were studied in a paper that is currently under review for publication in *Materials Today Energy*. The second approach involved the development of metrics to assess the supply risk (SRs) associated with the requirement of CRMs (see Figure 1). In particular, SR indicators encompassed the concentration, political stability, and import reliance along the supply chains of CRMs. They were included in more comprehensive metrics measuring the sustainability (paper published in *Energy Reports*) and security (paper under review in *Materials Today Energy*) of energy systems, which were applied ex-post to decarbonization energy scenarios. The third approach encompassed the first-of-a-kind ex-ante evaluation of the SR associated with the energy transition by developing material and energy SR objective functions. A combined assessment of these two risks aims to provide insights about possible trade-offs from the transition from fossil fuels to clean energy technologies: this shift might decrease the fossil fuels import dependency, but it is going to increase a lot the requirement of CRMs. A journal paper concerning the Italian case study is under review for publication in *Applied Energy*.

External collaborations

- Università di Torino
- Ruhr University Bochum
- EUROfusion

Academic context

[1] G. Colucci et al., “A dynamic accounting method for CO2 emissions to assess the penetration of low-carbon fuels: application to the TEMOA-Italy energy system optimization model”, Applied Energy, 2023.
[2] D. Mosso et al., “How much do carbon emission reduction strategies comply with a sustainable development of the power sector?”, Energy Reports, 2024.
[3] M. Nicoli et al., “Enabling Coherence between Energy Policies and SDGs through Open Energy Models: the TEMOA-Italy Example,” in “Aligning the Energy Transition with the Sustainable Development Goals: Key Insights from Energy System Modeling”, Springer, 2024.



First name: Marco **LAST NAME**: DE BASTIANI

Topic: Development of an integrated platform for the multi-physics modeling of superconducting magnets for nuclear fusion reactors

Course year: 3rd **Tutor(s)**: Prof. Roberto ZANINO

Highlights of the research activity

This year my research has been mainly devoted to the finalization of the development of the last model to be added to the Multiphysics platform for superconducting modeling which will be the final outcome of my PhD. This model is dedicated to the thermo-mechanical modeling of superconducting magnets or cables.
A key innovation of this model lies in its integration with the 4C or H4C thermal-hydraulic codes. This integration enables the use of detailed temperature distributions, calculated by validated state-of-the-art codes, as input for the mechanical solver. This approach allows for a more accurate consideration of local temperature gradients, beyond mere overall temperature changes.
From a software perspective, the thermo-mechanical model is controlled by a Python API. This API initially retrieves results from the thermal-hydraulic simulation, processes them, and subsequently feeds them into the ANSYS APDL-based mechanical model, managed by the PyMAPDL Python package. Additionally, the API handles mesh generation, load and boundary condition definition, problem solution, and post-processing, all while leveraging parallel computing for enhanced computational efficiency. The developed model can be applied both at coil and cable level. Indeed, the first application has been the DTT TF coil cooldown analysis [M. De Bastiani et al., SOFT 2024], while then has been applied to assess the mechanical effect of quench induced temperature in HTS cables [M. De Bastiani et al., IEEE TAS, 2024].

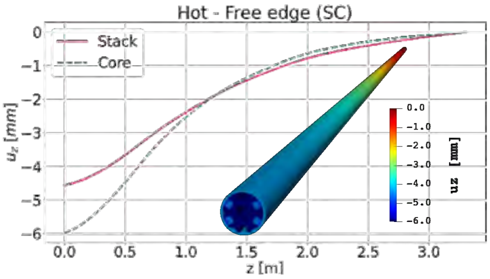


Figure 1. Axial displacement along stacks and core of a slotted core HTS cable during quench. Displacement map is shown as well.

DTT TF cooldown analysis showed that controlled cooldown does not produce excessive stress in the coil, while localized temperature differences may delaminate the insulation layers.
On the contrary, in HTS cable quench it is shown that high hot spot temperature, and thus strong gradients, may induce strong axial strain on the HTS tape, possibly overcoming the permanent critical current degradation strain threshold. Displacement induced by quench temperature increase in a slotted core conductor is shown in Figure 1. Validation of the model against experimental data is foreseen in the next future.
In parallel to the thermo-mechanical analysis, other modeling activities have been carried out, mainly in support of DTT design activities. Coupled electrical, electromagnetic and thermal-hydraulic analysis has been carried out to evaluate the consequences of a quench in the DTT TF coil in cold test facility configuration. Moreover, detailed electrical and thermal-hydraulic analyses has been carried out to assess the impact of using varistors fast discharge units instead of classical resistive ones for TF coil discharge.

External collaborations

- DTT S.c.a.r.l.
- ENEA
- EUROfusion

Academic context

[1] L. Savoldi Richard, F. Casella, B. Fiori and R. Zanino, "The 4C code for the cryogenic circuit conductor and coil modeling in ITER", *Cryogenics*, vol. 50 (3), pp. 167-176, 2010
[2] R. Bonifetto, M. De Bastiani, R. Zanino and A. Zappatore, "3D-FOX – a 3D transient electromagnetic code for eddy currents computation in superconducting magnet structures: DTT TF fast current discharge analysis", *IEEE Access*, 2022
[3] M. De Bastiani, R. Bonifetto, A. Froio, R. Zanino, A. Zappatore, "Self-Consistent Electrical and Thermal-Hydraulic Model of Faults in Superconducting Magnets: EU DEMO TF Short Circuit During a Fast Discharge", IEEE TAS, 2024

First name: Gabriele **LAST NAME**: FERRERO

Topic: Innovative thermo-nuclear fusion

Course year: 3rd **Tutor(s)**: Massimo ZUCCHETTI, Raffaella TESTONI

Highlights of the research activity

The activities during the PhD involved the analysis of the phenomena with Multiphysics connections which are relevant in an ARC-class reactor molten salt Liquid immersion blanket. Fluid dynamics, heat transfer, and tritium transport analysis have been carried out for the liquid immersion blanket and the divertors, together with the electromagnetic responsive force of the vacuum vessel in response to a plasma disruption due to the induced currents.

The activities in the third year contributed to:

- The analysis on Vacuum Vessel electromagnetic eigenmodes, which are responsible for the temporal evolution of the vertical position of a tokamak plasma during displacements and disruption events. The analysis has been carried out for isotropic and anisotropic systems with COMSOL and OpenFusionToolkit, in collaboration with PSFC and Columbia University.
- The development, verification, validation, and comparison of Tritium transport codes, to simulate diffusion, trapping, and other relevant mechanisms which may impact Tritium transport and inventory estimation for fusion reactors. Reliable Tritium transport codes represent a fundamental tool to use in conjunction with experimental campaigns to evaluate Tritium transport properties, which are crucial for breeding blanket design. Activities with the open-source Tritium transport code *festim* team have been conducted during the period spent at MIT PSFC, resulting in the publication of "Delaporte-Mathurin, Rémi, et al. "FESTIM: An open-source code for hydrogen transport simulations." *International Journal of Hydrogen Energy* 63 (2024): 786-802."
- The development of the open-source code TRIOMA, for the analysis of Tritium transport and inventory estimation for the outer fuel cycle of fusion reactors. TRIOMA employs analytical solutions for the systems in analysis to have a 0D but detailed formulation, which results in fast computation times. The tool is well-suited for preliminary design, parametric screening, sensitivity analysis and feasibility studies. The code is verified against COMSOL models, and includes tests and documentation. This activity has been presented as a poster presentation G. Ferrero et al. "Sensitivity analysis and uncertainty quantification for Tritium transport in molten salt components for ARC-class reactors" at the SOFT 2024 conference in Dublin.

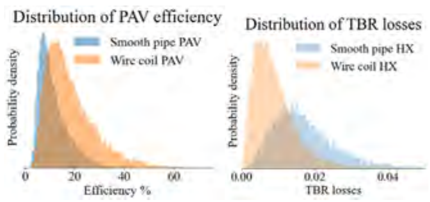


Figure 1: Tritium extraction efficiency and Tritium losses resulting from Uncertainty quantification of the Outer fuel cycle

External collaborations

- ENI
- MIT – Plasma Science and Fusion Center
- ENEA

Academic context

[1] B. N. Sorbom *et al.*, "ARC: A compact, high-field, fusion nuclear science facility and demonstration power plant with demountable magnets," *Fusion Eng. Des.*, vol. 100, pp. 378–405, 2015, doi: 10.1016/j.fusengdes.2015.07.008

[2] A. Q. Kuang *et al.*, "Conceptual design study for heat exhaust management in the ARC fusion pilot plant," *Fusion Eng. Des.*, vol. 137, pp. 221–242, 2018.

[3] S. E. Ferry, K. B. Woller, E. E. Peterson, C. Sorensen, and D. G. Whyte, "The LIBRA Experiment: Investigating Robust Tritium Accountancy in Molten FLiBe Exposed to a D-T Fusion Neutron Spectrum," *Fusion Sci. Technol.*, pp. 1–23, Jun. 2022, doi: 10.1080/15361055.2022.2078136

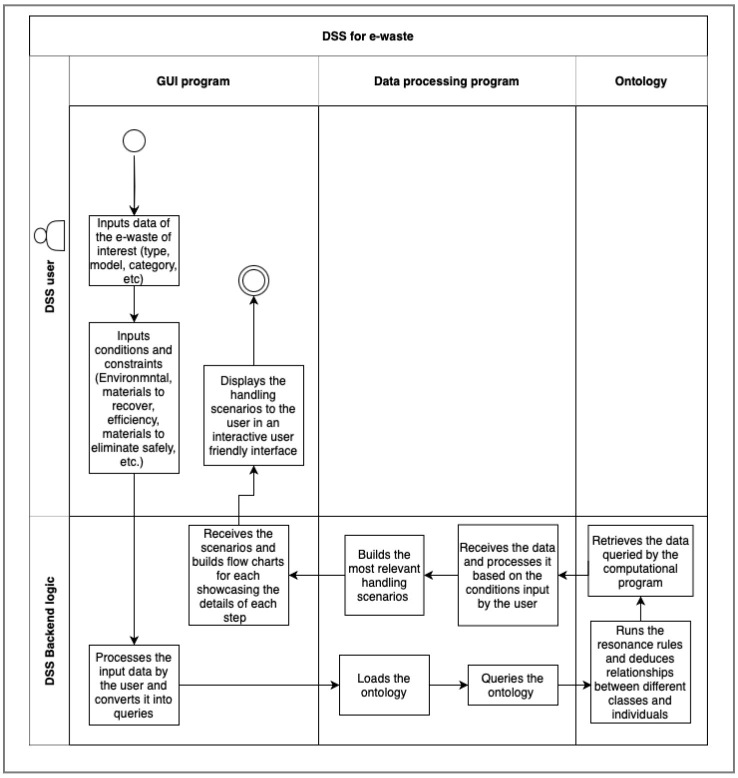
First name: Ahmed Tarek Ismail **LAST NAME**: MOHAMED

Topic: Computational model for the improved management of e-waste

Course year: 3rd **Tutor(s)**: Francesco LAVIANO, Debora FINO

Highlights of the research activity

The research focuses on developing a holistic framework for managing electronic waste (e-waste), with a particular emphasis on solar photovoltaics (solar PVs) and Printed Circuit Boards (PCBs). Central to this study is the design of an ontology-based Decision Support System (DSS) that integrates multidisciplinary knowledge related to e-waste, encompassing materials science, treatment methodologies, and environmental and health considerations. This DSS is intended to facilitate complex decision-making in e-waste handling for non-expert users by offering a simplified, knowledge-driven interface.In addition to the development of the DSS, the research involves extensive material characterization of various PCB types, including motherboards, RAM modules, and CPUs. Advanced analytical techniques such as ICP-OES, ICP-MS, and XRF are employed to quantify material composition. These analyses reveal significant variations in the material content of different PCB types and models, shedding light on trends in PCB composition over time.



Furthermore, the study explores the effect of solvent pre-treatment using dimethyl sulfoxide (DMSO) on PCBs of varying particle sizes, including fine powders, to enhance the efficiency of subsequent metal leaching processes. The impact of this pre-treatment on copper recovery is critically assessed, alongside an evaluation of the interplay between PCB composition and market value.
This interdisciplinary research integrates theoretical modeling through ontology development with experimental investigations into material analysis and treatment methodologies. By combining these approaches, the study aims to advance sustainable and efficient recycling practices for PCBs, contributing to the broader field of e-waste management with a focus on environmental responsibility and resource recovery.

External collaborations

- ENI S.p.A

Academic context

[1] E. A. Oke and H. Potgieter, "Recent chemical methods for metals recovery from printed circuit boards: A review," *J Mater Cycles Waste Manag*, vol. 26, no. 3, pp. 1349–1368, May 2024, doi: 10.1007/S10163-024-01944-4/METRICS.
[2] A. Priya and S. Hait, "Characterization of particle size-based deportment of metals in various waste printed circuit boards towards metal recovery," *Cleaner Materials*, vol. 1, p. 100013, Dec. 2021, doi: 10.1016/J.CLEMA.2021.100013.
[3] Udage Kankanamge, A. K. S., Erdiaw-Kwasie, M. O., & Abunyewah, M. (2024). Towards a Taxonomy of E-Waste Urban Mining Technology Design and Adoption: A Systematic Literature Review. *Sustainability*, *16*(15), 6389. https://doi.org/10.3390/su16156389

First name: Matteo **LAST NAME**: NICOLI

Topic: Investigation of innovative energy paradigms for the exploitation of nuclear fusion

Course year: 3rd **Tutor(s)**: Laura SAVOLDI, Anderson Rodrigo de Queiroz

Highlights of the research activity

Over the past year, my research activity in collaboration with the MAHTEP Group has focused on advancing energy system modeling, specifically through the development and application of the TEMOA-Italy open-source model to assess policy and technological impacts on energy transition. A significant aspect of my work has been exploring technology-specific hurdle rates, crucial for understanding investment behavior in clean energy. I developed a framework (see Figure 1) that integrates the weighted average cost of capital to evaluate how green finance measures, such as reduced hurdle rates for renewable technologies, affect the cost and competitiveness of energy systems. The analysis indicated that although lower hurdle rates can promote green investments, their effect alone is insufficient for a significant shift, implying the need for complementary policy measures.Another focus was on evaluating the marginal costs of GHG abatement in Italy under increasingly stringent decarbonization targets. By comparing marginal costs with emission reduction benefits, I identified that the power sector offers the lowest abatement costs, while industry faces the highest. This analysis highlighted the potential role of carbon pricing, suggesting that a tax of approximately 160 €/t could drive substantial emissions reductions. Additionally, I emphasized the importance of transparency in energy modeling through open-source approaches, ensuring that policymakers can better connect modeling insights to strategic goals like the Sustainable Development Goals (SDGs). I demonstrated how various decarbonization scenarios impact sustainability, revealing trade-offs between environmental, social, and geopolitical factors, especially when renewable energy reliance leads to increased import dependence.

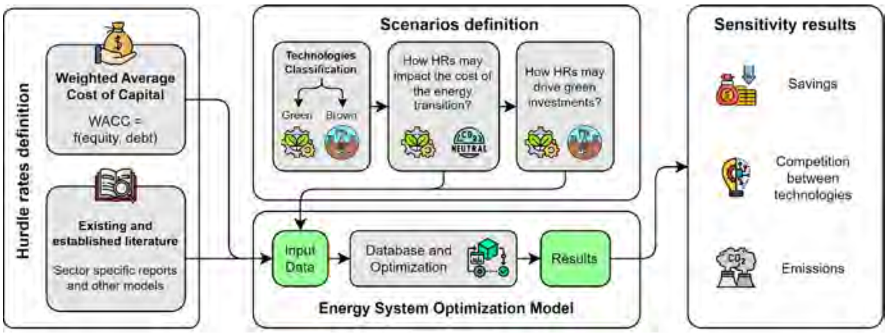


Figure 1. Methodological flowchart used to assess the impact of hurdle rates on the cost of the energy transition and on technological competition.

External collaborations

- Università di Torino
- North Carolina State University
- Eni S.p.A.

Academic context

[1] M. Nicoli et al., “Modeling energy storage in long-term capacity expansion energy planning: an analysis of the Italian system”, Journal of Energy Storage, 2024.
[2] M. Nicoli et al., “Evaluating the impact of hurdle rates on the Italian energy transition through TEMOA”, Applied Energy, 2025.
[3] M. Nicoli et al., “Enabling Coherence between Energy Policies and SDGs through Open Energy Models: the TEMOA-Italy Example,” in “Aligning the Energy Transition with the Sustainable Development Goals: Key Insights from Energy System Modeling”, Springer, 2024.

First name: Daniele **LAST NAME**: PLACIDO

Topic: Modeling innovative superconductive cables and magnets for future fusion machines

Course year: 3rd **Tutor(s)**: Laura SAVOLDI, Alessandro savino

Highlights of the research activity

The objective of the PhD is to develop OPENSC^2, a Python based, object oriented, open-source open-access software that enables the modelling of both thermal-hydraulic (TH) and electric transients in superconducting (SC) cables for nuclear fusion and power transport applications.

The initial two months of the 3rd year of the PhD were spent abroad at the MIT, where the candidate undertook the validation of the TH model of the OPENSC^2 against the experimental resulst from test on a VIPER-like cable at the SULTAN test facility. Furthermore, during this period, the candidate initiated additional validation of the TH model against esperimental measurements on a coil based on the PITVIPER cable. This ongoing validation process requires a thorough senvitivity analysis using Sobol indexes to identify of a representative value of the heat transfer coefficients between each object composing the cable cross section.

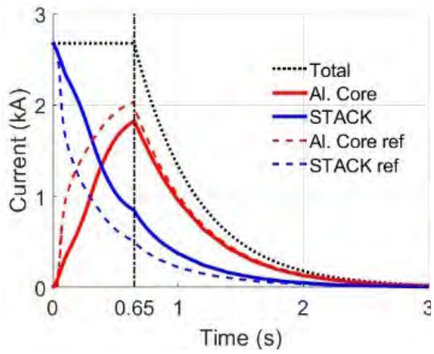


Figure 1: Comparison of OPENSC^2 current time evolution and redistribution against H4C code results (ref).

Additionally, the electric model was benchmarked against numerical results obtained with the H4C code, with the assistance of Master's student A. Mortara. The reference case study was a quench propagation analysis of the high temperature SC slotted core cable design proposed by ENEA. The aim was to reproduce the same output with OPENSC^2. Overall, the comparison demonstrates favorable qualitative outcomes for both the TH model (temperature evolution) and the electric model (current redistribution), the latter being illustrated in Figure 1. Quantitative discrepancies are mainly attributed to the different model implementations.

The implemementation of adaptive time step and adaptive mesh algorithms in OPENSC^2 is bases on ad-hoc strategies. In the former approach, the time variation of the solution is leveraged to calibrate the subsequent time step. In the latter strategy, the localization of quench fronts enables the identification of regions where the mesh requires local refinement. During the verification phases of the adaptive mesh algorithm, some spurious oscillations in the coolant temperature were identified. Following numerous attempts to detect and correct the source of the error, it became evident that this behaviour was inherent to the adopted upwind scheme, known as the balancing diffusion method. >Subsequently, it was demonstrated with a simplified case that the Petrov-Galerkin upwind scheme does not exhibit oscillations, and is currently being implemented in the software.

OPENSC^2 is currenlty being adopted as design tool of the feeders to be manufactured for the ENEA DTT test facility, in a collaboration with dr. De Marzi. Following the techno-economic analysis conducted in the second year of the PhD, an alternative cable design has been identified and is currently being investigated for feasibility. In addition to these duties, the candidate is assisting RSE with the design of an MgB_2 SuperConducting Energy Pipeline capable of transporting bot high current and hydrogen.

External collaborations

- MIT
- ENEA
- RSE

Academic context

[1] Wilson, Martin N. Superconducting Magnets. Clarendon Press: Oxford, 1983. Print. Monographs on Cryogenics 2.

[2] Van Sciver, Steven W. Helium Cryogenics. New York: Plenum, 1986. Print. The International Cryogenics Monograph Ser.

[3] L. Savoldi, F. Casella, B. Fiori, R. Zanino, Cryogenics, Volume 50, Issue 3, 2010, Pages 167-176, ISSN 0011-2275, https://doi.org/10.1016/j.cryogenics.2009.07.008

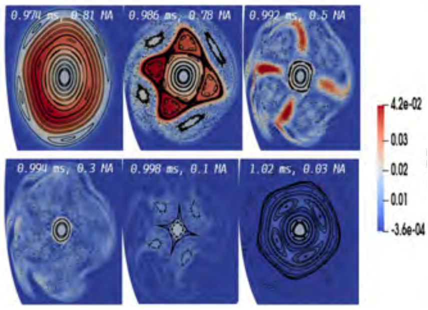
First name: Lovepreet **LAST NAME**: SINGH

Topic: Disruptions and runaway handling strategies in the next generation of tokamak reactors

Course year: 3rd **Tutor(s)**: 1st Tutor Fabio SUBBA, 2nd Daniela GRASSO

Highlights of the research activity

The main focus of the 2023-2024 activitiy was the modelling of the RE benign termination observed in JET pulse 95135, firstly carried out in [1], where the authors demonstrated the benign effect of the magnetic stochasticity on the RE loss. This numerical work used the nonlinear MHD code JOREK.



Evolution of magnetic stochasticity and RE current amplitude at different time points. The background color indicates the RE density.

The stochastization leads the magnetic field lines, which are normally well-organized in closed magnetic flux surfaces, to become disrupted and start to follow random, non-periodic paths. Previous simulations done by Bandaru et al (2021) had taken particular assumptions regarding the properties of the background plasma, e.g., regarding the resistivity, that might not be accurate due to the recombination following massive deuterium injection. Thus, the simulations were carried out with several sets of different assumptions regarding the accompanying plasma conditions. This part of the work was done in collaboration with researchers from CEA, Cadarache and IPP, Garching. It was observed that by reducing the plasma ion density, the amplitude of the RE current after the stochastic phase is higher, but the rate of RE loss is higher. This is caused by the rapid evolution of the plasma stochasticity with increasing plasma ion density. A higher degree of magnetic stochasticity means a broadening of the RE wetted are at the wall, highlighting the importance of plasma recombination (causing the reduction of ion species due to the formation of neutrals) for the benign termination of the RE current.
Through the scan in resistivity, it was possible to observe the benign effect of a higher plasma resistivity on the RE loss. A higher resistivity leads to a more stochastic plasma, similar to the ion density, which increases the RE loss to the wall. An example of such dynamics is shown in the figure, where the evolution of the stochasticity and its effect on the RE current amplitude is presented. As observed, the RE current amplitude reduces from 0.8 MA to 0.03 MA. Similar RE losses were seen at all resistivities. However, at high resistivity, a more intensive evolution of the stochasticity causes a broadening of the RE impact area, saving the wall from any possible damage due to the RE beam. This was confirmed by evaluating the heat loads using the JOREK particle tracing module. Indeed, with increasing resistivity, the heat loads were characterised by lower values.

External collaborations

- CEA, Cadarache, France
- IPP, Garching, Germany

Academic context (

[1] V. Bandaru et al., Plasma Physics and Controlled Fusion 63, 035024 (2021)
[2] E. Nardon et al., Physics of Plasmas, 30(9) (2023)
[3] H. Bergstrom et al, Plasma Physics and Controlled Fusion 66, 095001 (2024)

First name: Marco **LAST NAME**: CARAVELLO

Topic: Multi-physics modelling of Molten Salt Blanket
Course year: 2nd **Tutor(s)**: Antonio FROIO, Roberto ZANINO, Fabrizio PODENZANI (ENI)

Highlights of the research activity

My PhD research focuses on multi-physics modeling of molten salt blankets for nuclear fusion reactors, particularly the ARC reactor [1], a tokamak-based machine developed at MIT. The ARC reactor utilizes a fully liquid immersion blanket filled with FLiBe molten salt, which serves multiple crucial roles: coolant, heat carrier, neutron multiplier (due to Beryllium), tritium breeder (through Lithium), and neutron shield. These diverse functions make the molten salt essential for reactor safety and efficiency. One of the main challenges of this research is the interaction between the strong magnetic fields controlling the D-T plasma in tokamak reactors and the electrically conductive molten salt. This interaction generates Lorentz forces, leading to complex magnetohydrodynamic (MHD) effects. Accurately modeling these effects is vital for optimizing blanket performance and ensuring the reactor's long-term viability. My research focuses on coupling MHD with neutronics to address power management and production challenges in fusion reactors like ARC. In 2024, my research concentrated on advancing MHD modeling in turbulent flow regimes. These flows involve intricate interactions between the flow field, electromagnetic forces, and heat transfer mechanisms. I implemented several MHD turbulence models in OpenFOAM, including Kenjeres and Meng's k-epsilon models and Meng's Reynolds Stress Model (RSM). A significant breakthrough in 2024 was integrating Widlund's models, which use scalar transport equations for the turbulence anisotropy variable alpha. This approach improved simulations of turbulence suppression in strong magnetic fields, and model validation against experimental data showed promising results. Additionally, code verification followed Smolentsev's work [2], a key reference in MHD for fusion reactors. I also initiated heat transfer simulations within the MHD regime, yielding preliminary insights into how MHD effects influence heat transport in molten salt blankets. This is crucial for designing efficient cooling systems in fusion reactors. Part of my 2024 research took place at Centro Ricerche San Donato Milanese in collaboration with ENI, comparing OpenFOAM and Ansys Fluent for MHD simulations. The results highlighted the strengths of both platforms. In September 2024, I began a collaboration with MIT's Nuclear Science and Engineering Department, applying advanced turbulence models to industrial case studies. In 2024, I also published a paper on nemoFoam [3], a multiphysics code for coupling neutron and photon transport with thermal-hydraulics in nuclear reactor simulations. The paper benchmarked nemoFoam against Serpent for ARC reactor simulations, demonstrating its robustness and accuracy.

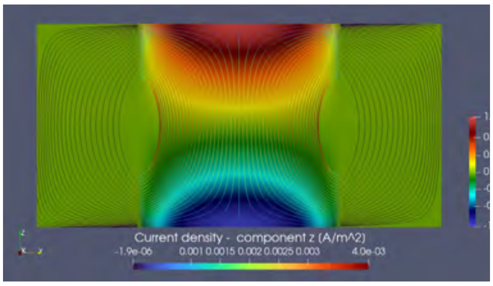


Fig. 1: Map of electric potential and streamlines of the induced current density, computed by the MHD code under development. The case study is defined by a square section pipe, with Hartmann walls in contact with the surrounding walls and side walls (top and bottom walls).

External collaborations

- ENI
- MIT – Nuclear Science and Engineering department

Academic context

[1] B.N. Sorbom, et al.; ARC: A compact, high-field, fusion nuclear science facility and demonstration power plant with demountable magnets. In Fusion Engineering and Design, Volume 100, 2015, Pages 378-405.
[2] S. Smolentsev et al.; An approach to verification and validation of MHD codes for fusion applications. In Fusion Engineering and Design, Volume 100, 2015, Pages 65-72.
[3] M. Caravello et al.; An OpenFOAM solver for multiphysics modeling of fusion reactor design: The nemoFoam code. In Nuclear Materials and Energy, Volume 40, 2024, 101693.

First name: Aldo **LAST NAME**: COLLAKU

Topic: Multi-physics and multi-phase modelling of Proton Exchange Membrane Fuel Cell technology

Course year: 2nd **Tutor(s)**: Laura SAVOLDI, Luca MAROCCO

Highlights of the research activity

The modeling of Proton Exchange Membrane Fuel Cells plays an important role in enhancing their performances, marking a fundamental step toward optimizing low-environmental-impact energy systems. The Computational approaches enable the analysis and improvement of key aspects such as channel design and flow distribution. However, a major challenge in this field is the lack of truly validated models capable of accurately representing the complex physical phenomena involved, including reactant and liquid mass transport, heat transfer, and electrochemical reactions. My doctoral research aims to address this gap by developing and validating a robust and reliable numerical model. The first step was to model an experimental PEMFC, characterized by parallel channel circuits and an active area of 10 cm², with three different CFD software: OpenFOAM, STAR-CCM+, and FLUENT. Each tool has its own electrochemical native module, which is (more or less) customizable. STAR-CCM+ allows some modifications to the existing equations by changing certain parameters through the assignment of UDFs. Fluent, on the other hand, enables modifications to the structure of some equations, such as the transfer current, via the source code pemfc_user.c. OpenFOAM, being an open-access code, allows the complete manipulation of the module. In terms of performances, the commercial software Fluent and STAR-CCM+ prove to be more stable and faster compared to OpenFOAM. Nevertheless, the assessment of numerical error is under investigation along with the validation against the experimental results. The main benchmark parameter is the polarization curve, in Figure 1 it is shown the comparison between the codes and the experimental data. Despite the three codes implements the same geometry, physics and operating conditions a non-negligible mismatch is found between the results. For this reason, further investigation of numerical errors and model implementation is under evaluation. On top of the polarization curve, the comparison accounts for local quantities such as liquid saturation in the porous regions (GDL, MPL and CL) and water content in the Nafion membrane.

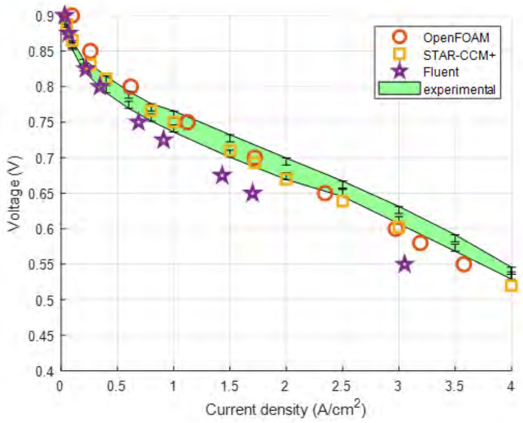


Figure 1: PEM Fuel Cell polarization curve computed with three different CFD codes against the experimental results.

External collaborations

- Politecnico di Milano, Energy Department

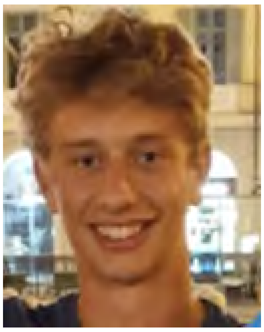
Academic context

[1] Bulgarini, M., Della Torre, A., Montenegro, G., Baricci, A. et al., "Application of a CFD Methodology for the Design of PEM Fuel Cell at the Channel Scale," SAE Technical Paper 2024-01-2186, 2024, https://doi.org/10.4271/2024-01-2186.

First name: Marino **LAST NAME**: CORRADO

Topic: Design and construction of a mock-up for the conditioning of spent ion exchange resins

Course year: 2nd **Tutor(s)**: SAVOLDI Laura, CAO Silvio



Highlights of the research activity

My PhD research, conducted in collaboration with Green-Land, focuses on developing an innovative geopolymer matrix (HYPEX®) designed to safely encapsulate spent radioactive ion exchange resins (IEXs), a particularly challenging type of Medium-Level Waste (MLW) generated by nuclear facilities. Additionally, the research emphasizes designing a mock-up system to validate the feasibility of the HYPEX® process on an industrial scale.

Figure 1 Experimental test on the "colloidal mill type E" of Probst&Class (DE) for resin grinding"

During the second year, experimental research on geopolymers has been carried out. Commercial metakaolin, such as BASF's Metamax®, was selected as the powdered precursor material. The study focused on the effect of temperature on the setting behavior of the geopolymer, particularly its final compressive strength and cation leachability.
Additionally, the potential of matrix depressurization during its formation was investigated as a strategy to minimize voids and enhance overall performance. The influence of ion exchange resin (IEX) particle size on water retention capacity (swelling pressure) was also examined through experimental studies conducted in collaboration with ETH Zürich.

The process of integrating ion exchange resins (IEXs) into the geopolymer matrix will be executed using a mobile plant consisting of two units. The first unit is designed to remotely extract the IEXs (waste) from their storage containers. In the second unit, the IEXs are combined with the geopolymer reagents to create the final matrix.Enhancements have been made to the mock-up design, focusing specifically on the development of the resin grinder (colloidal mill) and the evaporator. A market survey of potential colloidal mills within the European nuclear industry has been conducted, followed by preliminary industrial tests to validate the suitability of the selected equipment for this specific application (Fig. 1).

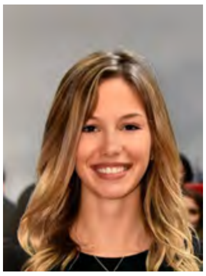
External collaborations

- SOGIN, italy
- ETH Zurich, Switzerland (Prof. Erich Pimentel)
- Probst & Class, Germany (Eng. Hector Sauri)

Academic context

[1] E. Phillip, T. F. Choo, N. W. A. Khairuddin, and R. O. Abdel Rahman, "On the Sustainable Utilization of Geopolymers for Safe Management of Radioactive Waste: A Review," Sustainability, vol. 15, no. 2, 2023, doi: 10.3390/su15021117.
[2] E. R. Vance and D. S. Perera, "8 - Development of geopolymers for nuclear waste immobilisation," in Handbook of Advanced Radioactive Waste Conditioning Technologies, M. I. Ojovan, Ed., Woodhead Publishing, 2011, pp. 207–229. doi: https://doi.org/10.1533/9780857090959.2.207.
[3] B. Kim, J. Lee, J. Kang, and W. Um, "Development of geopolymer waste form for immobilization of radioactive borate waste," J Hazard Mater, vol. 419, p. 126402, 2021, doi: https://doi.org/10.1016/j.jhazmat.2021.126402.

First name: Francesca **LAST NAME**: CRIVELLI



Topic: Treatment and disposal of radioactive ion exchange resins (IEXs)

Course year: 2nd **Tutor(s)**: Laura SAVOLDI, Giancarlo VENTURA

Highlights of the research activity

My PhD research focuses on developing a novel process for the treatment and conditioning of ion exchange resins (IEXs). This work is being carried out in collaboration with Green-Land S.r.l. IEXs represent the largest volume of Intermediate Level Waste (ILW) generated by nuclear power plants. These resins are primarily used to purify the primary circuit water in Light Water Reactors (LWRs) and to control water chemistry.

My PhD research aims to develop a novel process for conditioning ion exchange resins at ambient temperature.

To achieve this, a new geopolymer-based conditioning matrix has been developed, in which pre-hydrated and ground resin is incorporated. The studied geopolymer is a solid, inorganic product of the chemical reaction between metakaolin, a natural aluminosilicate resource, and a specific alkaline solution composed of sodium metasilicate, sodium hydroxide, and silica fume.

Over the past year, the formulation of the geopolymer has been optimized to maximize the amount of resin that can be incorporated. This optimization focused on studying the fundamental H_2O/Al ratio of the geopolymer and the degree of hydration of the resin. These parameters were adjusted to minimize the swelling pressure exerted by the resin when in contact with water. Additionally, the impact of mixing the geopolymer-resin mortar under reduced pressure was investigated in terms of compressive strength and immersion resistance. Vacuum conditions allow better penetration of the geopolymer mortar into the interstitial spaces of the resin, improving the homogeneity of the final product (Figure 1) and enhancing its mechanical properties.

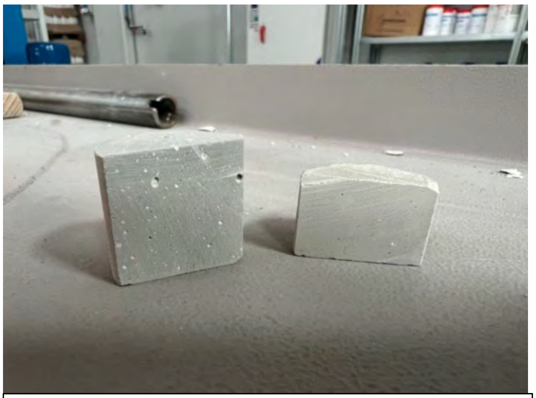


Figure 1. Sample of geopolymer embedding 30%wt of resin, mixed at ambient pressure (on the left) and in a depressurized environment (on the right)

This approach led to significant improvements in both compressive and immersion resistance.

Another critical parameter for qualifying a waste matrix for radioactive waste is its leaching resistance, particularly for Cesium, as per the Italian Waste Acceptance Criteria (WAC). To enhance the matrix's ability to retain radionuclides, the addition of silica fume and zeolites was studied. Zeolites are often used to improve the leaching resistance of conditioning matrices, but they are also highly hydrophilic and require a high water content in the mix. This disrupts the studied formulation, reducing the geopolymer's mechanical properties.

Silica fume, on the other hand, is a highly reactive form of SiO_2 that readily reacts with aluminum ions to form geopolymeric chains and with other ions, including cesium, to create silicates. These silicates are tightly bound within the matrix's chemical structure, preventing their migration. For this reason, silica fume was chosen as an additive in the final formulation to improve leaching resistance. These optimization studies have resulted in the ability to incorporate up to 30%wt of resin into the geopolymer while meeting the Italian Waste Acceptance Criteria (WAC). This significantly reduces disposal costs and waste volumes for the National Repository.

External collaborations

- SOGIN, italy

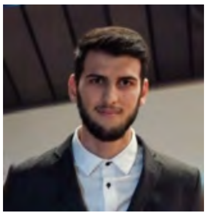
Academic context

[1] B. Kim, J. Lee, J. Kang, and W. Um, "Development of geopolymer waste form for immobilization of radioactive borate waste," J Hazard Mater, vol. 419, p. 126402, 2021, doi: https://doi.org/10.1016/j.jhazmat.2021.126402.

First name: Enrico **LAST NAME**: EMANUELLI

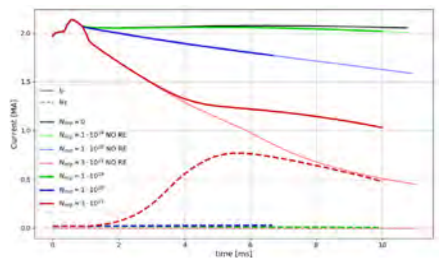
Topic: Simulation of runaway electron generation in DTT with the JOREK code

Course year: 2nd **Tutor(s)**: Fabio SUBBA, Giuseppe RAMOGIDA



Highlights of the research activity

The objective of this research activity is to study disruptions and Runaway Electrons (REs) formation and impact in the framework of the Divertor Tokamak Test (DTT) facility, an experimental nuclear fusion reactor that will be built in Frascati, Italy, as a part of the EUROfusion programme. During a disruption, the plasma quickly radiates the majority of its thermal energy (thermal quench, TQ), causing a sharp increase in plasma electrical resistivity which leads to a decay of the plasma current (current quench, CQ). The CQ induces a very strong electric field that is able to accelerate a portion of the electron population to relativistic speeds, leading to the formation of the so-called runaway electrons (REs). These REs can form beams of energies up to tens of MeV, posing a considerable threat to the plasma facing components of the future generations of fusion reactors, making it imperative to look for proper avoidance and mitigation strategies.



Plasma current (solid line) and runaway electron (RE) current (dashed line) for different values of impurity content, starting with an initial RE seed current of 20 kA.

In my PhD activity, I am exploiting the non-linear magnetohydrodynamic (MHD) code JOREK. It is a well-established tool for modeling phenomena in magnetically confined fusion devices and it can handle the complex dynamics associated with disruptions and REs formation. It implements a REs fluid model able to describe the non-linear coupled evolution of REs and the background plasma during disruptions self-consistently. In this kind of work we are carrying out an artificial thermal quench (ATQ), which mimics what occurs during a disruption by tuning some physical parameters (e.g., thermal diffusivities and electrical resistivity), serving as a simplified approach to reach a post-disruption phase, without running ad-hoc simulations that are much more complex and computationally expensive. The ATQ has already been used for simulations of disruptions in other tokamaks such as JET, ITER or EU-DEMO, since it provides a controlled environment to examine the evolution of the REs during the CQ phase. I have thoroughly simulated the Day-0 scenario of DTT, which will be the first operational phase of DTT, with a reduced plasma current of 2 MA, in contrast to the 5.5 MA of full power scenarios. The simulations took into account different levels of impurity content, injected to mitigate disruptions, and several orders of magnitude variation in the initial REs current seed. The picture on the right highlights that a non-negligible amount of REs is found only when combining the highest RE seed current (20kA) with the highest amount of impurities used in the simulations. Indeed, the red curve shows that the REs current modifies the CQ dynamics with respect to the case with the same level of impurities but without REs (light red solid line). This means that, if the disruption mitigation system is designed to avoid requiring such a high amount of impurities, the Day-0 scenario can be considered safe from REs threats. Future work will focus on the full power scenario, where significantly higher RE generation is anticipated.

External collaborations

- ENEA
- Max Planck Institute for Plasma Physics (IPP)
- Consorzio RFX

Academic context

[1] Hoelzl M., Huijsmans G.T.A. et al. Nuclear Fusion 61, 065001 (2021)

[2] Bandaru V., Hoelzl M., Reux C. et al. Plasma Physics and Controlled Fusion, 63, 035024 (2021)

[3] Schwarz N., Artola F.J., Vannini F. et al. Nuclear Fusion 63, 126016 (2023)

First name: Eleonora **LAST NAME**: GAJETTI

Topic: Multi-phase modelling of cooling systems equipped with structured porous media for the removal of high heat fluxes

Course year: 2nd **Tutor(s)**: Laura SAVOLDI, Gianluca BOCCARDO, Antonio BUFFO

Highlights of the research activity

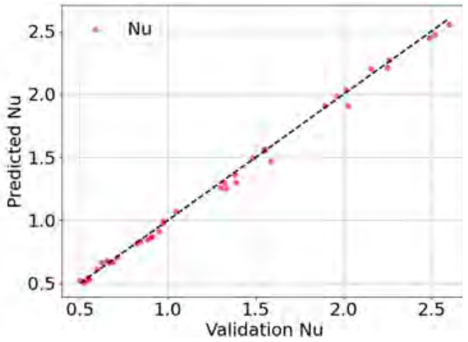


Figure 1: Comparison between the predictions and the validation points (computed with CFD)

The research activity focuses on the development of lumped models for Triply Periodic Minimal Surfaces (TPMS) structures. TPMS are mathematical surfaces that extend periodically in three dimensions and have zero mean curvature, minimizing surface area. They can be useful for heat management, as they have large surface area-to-volume ratios, making them highly efficient for heat dissipation. During this second year of the PhD, different TPMS topologies have been studied to assess a lumped hydraulic model based on the Darcy-Forchheimer's equation. CFD results have bene fitted to compute power-laws correlations for the permeability (for viscous regime) and inertial coefficient (for inertial regime), as function of the porosity as well as the tortuosity. This work is currently under review in the International Journal of Heat and Mass Transfer. Furthermore, in order to develop surrogate models, an automated workflow has been developed for the creation of a database to be used in the training of a neural network (NN). Using a training database of 200 points, giving as inputs the Re and the porosity, the neural network is able to predict the friction factor and the Nusselt number with a mean error of 5%. In Figure 1 the comparison between the predicted Nusselt numbers and the CFD results is plotted.
TPMS structures have also been employed in the design of cooling system for a real case application: a high-flux component in fusion reactors. Comparing the results of the new TPMS heat removal system to the previous design, TPMS are able to significantly reduce maximum temperatures and allow the fluid not to reach boiling point, an operating limit to avoid high rates of oxidation and erosion. This work has been presented at the 33rd Symposium on Fusion Technology (SOFT) in 2024.
An experimental campaign on hydraulic characteristic of TPMS has been conducted at Politecnico di Milano. The experimental results have been compared to CFD simulations using STAR-CCM+, Ansys Fluent and OpenFOAM, to assess the different codes performance. This work has been presented at the 9th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS) in 2024.

External collaborations

- Politecnico di Milano, Energy Department
- DTT S.C.a r.l., Via E. Fermi 45, Frascati, 00044, RM, Italy

Academic context

[1] M.G. Gado et al., "Triply Periodic Minimal Surface Structures: Design, Fabrication, 3D Printing Techniques, State-of-the-Art Studies, and Prospective Thermal Applications for Efficient Energy Utilization," *Energy Technology*, May 2024, doi: 10.1002/ENTE.202301287
[2] M.B. Hawken et al., "Characterization of pressure drop through Schwarz-Diamond triply periodic minimal surface porous media," *Chem Eng Sci*, doi: 10.1016/J.CES.2023.119039.
[3] N. Baobaid et al., "Fluid flow and heat transfer of porous TPMS architected heat sinks in free convection environment," *Case Studies in Thermal Engineering*, May 2022, doi: 10.1016/J.CSITE.2022.101944.

First name: Fabrizio **LAST NAME**: LISANTI

Topic: Macro-scale modeling of DTT cryogenic plant

Course year: 2nd **Tutor(s)**: Roberto BONIFETTO, Antonio FROIO

Highlights of the research activity

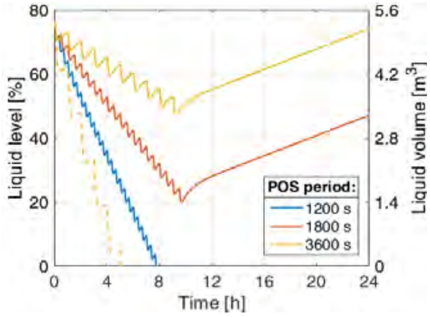


Fig 1. He level and volume in thermal buffer for different scenarios of the pulsed operation of DTT

The research activity carried out during my 2nd year of PhD focused on the development of system-level dynamic models for the cryogenic plant (cryoplant) of the Divertor Tokamak Test (DTT) superconducting tokamak [1].
To support the design of the DTT cryoplant, I developed dynamic, system-level models of the cooling circuits of the superconducting magnets [2] and of the refrigerator producing liquid He (LHe) at 4.2 K using the CryoModelica library of the 4C code, a state-of-the-art numerical tool developed at Politecnico di Torino. The CryoModelica library is based on the Modelica modelling language. During the last year, I developed the model for the cooling circuit of the poloidal-field (PF) coils and central solenoid (CS) coil and simulated them under the operating conditions foreseen for the plasma pulsed operation of the DTT machine. The development and simulations of the circuit models for the cooling of the TF coils (developed during my 1st PhD year) and of the PF and CS coils were presented in December 2023 at the Design Review Meeting of the DTT cryogenic system held at the ENEA Frascati research Centre. The main achievement was the development of the system-level model for a possible configuration of the DTT He refrigerator in Modelica, to support/qualify the executive project of the DTT He refrigerator. The model includes the main components of He refrigerators – e.g. LHe thermal buffer, heat exchangers, JT valves etc. – available within the CryoModelica library of the 4C code; the implementation of the model was presented in July 2024 at the CRYO-OPS conference in Grenoble, France, and the results of simulations performed assuming different scenarios for the pulsed operation of the DTT machine (i.e. shorted duty cycles for the plasma pulses, compared to the reference 3600 s-long pulses) were presented in September at the SOFT conference in Dublin, Ireland. They showed that for some proposed duty cycles, the daily operation could lead to empty the LHe thermal buffer, under the current design assumptions (see Fig 1).
In parallel, I also devoted some time to the system-level modelling of the lithium-lead (PbLi) circuit of the WCLL BB concept for the EU DEMO reactor. The model (implemented with the GETTHEM code, based on the same Modelica languaga of the DTT He refrigerator model) for the assessment of the generation and transport of Activated Corrosion Products (ACPs) developed during my 1st PhD year was extended in 2024 to account for the activation of corroded species carried within PbLi, when exposed to the neutron flux inside the BB, and for the radioactive decay of already activated species; this work was presented at the SOFT conference and will be submitted for publication in an international journal. Moreover, the GETTHEM model of the Permeator Against Vacuum (PAV, the reference technology for tritium extraction from PbLi in the EU DEMO) developed during my 1st PhD year was employed this year for a sizing analysis of the tritium extractor for the WCLL BB of DEMO, performing a parametric study to identify the optimal PAV design. A preliminary stage of this sizing analysis was presented at the WCLL BB and TER review meeting, held at Politecnico di Torino in July 2024.

External collaborations

- ENEA, Via E. Fermi 45 I, 00044 Frascati, Roma, Italy
- DTT S. c. a. r. l., c/o C.R. ENEA Via E. Fermi 45 I, 00044 Frascati, Roma, Italy
- Univ. Grenoble Alpes, CEA, IRIG, Département des Systèmes Basses Températures

Academic context

[1] F. Romanelli, "Divertor Tokamak Test facility Project: Status of Design and Implementation," Nuclear Fusion, 2024
[2] Lisanti, F., et al. "Design of the cryogenic loop for the superconducting toroidal-field magnets of the Divertor Tokamak Test." Cryogenics 136 (2023): 103757.

First name: Jihen **LAST NAME**: MAHDHI

Topic: Study and optimization of novel tubular absorbers for solar parabolic trough collectors

Course year: 2nd **Tutor(s)**: Laura SAVOLDI

Highlights of the research activity

This year, my research focused on the development and validation of numerical simulations for the performance of a non-evacuated Parabolic Trough Collector (PTC) with novel tubular absorbers. The primary step was to model and simulate the system's optical, hydraulic and thermal performances. In this regard, I developed a 3D CFD model using STAR CCM+ to simulate the heat transfer dynamics of the studied system. This included modeling the optical behavior of the system using SolTrace software, which simulates the path of sunlight reflecting from the parabolic trough and interacting with the absorber tube. The obtained solar flux distribution was then integrated into the CFD model as the thermal driver to predict the thermal behavior of the system under real solar conditions (Fig. 1a). The CFD model was designed to replicate the non-evacuated receiver environment, incorporating convection and radiation heat transfer, using Radiation models. After a grid independence study, the most appropriate mesh was selected for further simulations. Then, I proceed with validating the numerical models by comparing simulation results against the experimental data collected during the first year. This process focused on key parameters such as outlet temperature, temperature distribution on the absorber tube, and heat flux distribution. In analyzing the CFD results, it was seen that the absence of a vacuum led to increased thermal losses in the non-evacuated PTC, primarily from convection to ambient air and radiation from the glass tube. Air velocity streams observed on collector cross sections depicted two thermal loops form symmetrically around the absorber, illustrating the convection losses from the hot pipe to the cold glass (Fig. 1b). The work this year lays the foundation for future optimization of more complex absorber designs, such as sinusoidal and spiral absorbers (Fig. 1c), and provides valuable insights into the performance of small-scale PTC systems, and further refinements of the model are underway.

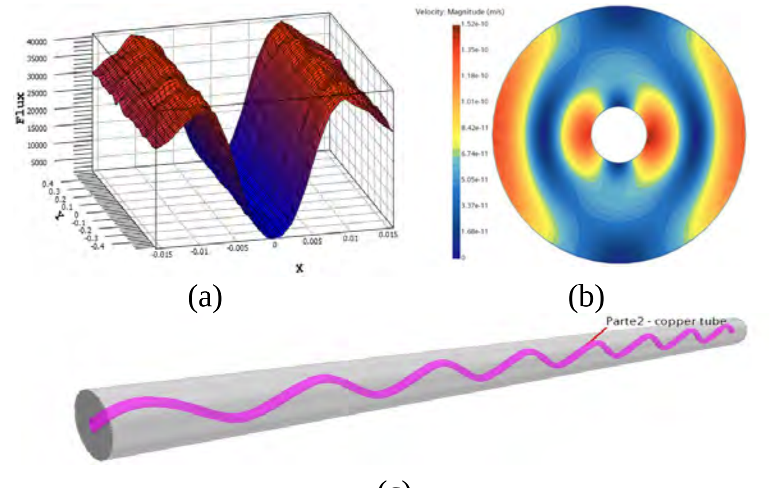


Figure 1: (a) 3D heat flux distribution on the absorber tube surface, (b) air velocity field in glass annulus cross section at the middle of the collector, and (c) physical model for the absorber with sinusoidal tube.

External collaborations

- M2EM Research Unit, university of Gabes, Tunisia.

Academic context

[1] Hossein Ebadi, Antonio Cammi, Laura Savoldi. *Energetic and Exergetic Analyses of a Double-Pass Tubular Absorber for Application in Solar Towers*. ASME. J. Sol. Energy Eng. 2024; 146(5): 051013. https://doi.org/10.1115/1.4066201

[2] Hossein Ebadi, Antonio Cammi, Eleonora Gajetti, Laura Savoldi. *Development, verification and experimental validation of a 3D numerical model for tubular solar receivers equipped with Raschig Ring porous inserts*. Solar Energy, 2024; 267, 112236. https://doi.org/10.1016/j.solener.2023.112236

First name: Arsham **LAST NAME**: MORTAZAVI

Topic: Performance optimization of concentrated solar thermal technologies equipped with structured porous media

Course year: 2nd **Tutor(s)**: Laura SAVOLDI, Luca MAROCCO

Highlights of the research activity

The research activity focuses on optimizing the performance of concentrated solar thermal technologies incorporating structured porous media. During this year, the research activity has been conducted both numerically and experimentally. In the first phase of the study, high temperature solar receivers equipped with different Triply Periodic Minimal Surface (TPMS) inserts were studied for Concentrating Solar Power applications. In the last phase of the PhD. studies, a Thermal Energy Storage (TES) unit equipped with a hollow cubic porous structure is under study.

Thanks to their smooth and interconnected flow channels, TPMS lattices significantly enhance heat transfer while maintaining a considerably lower pressure drop compared to unstructured porous structures. In a numerical study, four different TPMS inserts—Gyroid, Diamond, Lidinoid, and SplitP—were analysed with three square unit-cell sizes (10 mm, 15 mm, and 20 mm) inside a small section of a tubular receiver. The thermohydraulic behaviour of the lattices was compared, and performance optimization was carried out using the Entropy Generation Minimization (EGM) method. The Lidinoid and SplitP lattices demonstrated superior heat removal capabilities, albeit at the cost of higher pressure drop values. For all lattices, entropy generation was minimized at inlet temperatures ranging from 450 to 500 K.

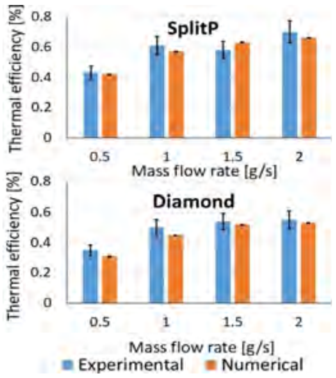


Figure1: Comparison of the numerical results with experimental data

In an experimental study conducted at the IMDEA Energy Institute in Madrid, Spain, two planar receivers equipped with Diamond and SplitP TPMS lattices were tested. The thermal performance of these mock-ups was evaluated under varying concentrated heat fluxes and mass flow rates (see Academic Context [1]). In all tests, the mock-up with the SplitP lattice consistently demonstrated superior thermal performance, a result also corroborated by the aforementioned numerical study.

In a subsequent study, the same mock-ups were investigated numerically, and the results were compared with experimental data, demonstrating good consistency. This study was presented as a poster at SolarPACES 2024. A comparison between the numerical and experimental results is shown in Figure 1.

In the final phase of the PhD studies, a Thermal Energy Storage (TES) device with phase change material (PCM) is being analysed. Due to the low thermal conductivity of the PCM, a hollow cubic lattice is employed to enhance the effective conductivity of the device. The objective is to optimize the shape and topology of the lattice to achieve higher heat absorption and improved effective thermal conductivity.

External collaborations

- IMDEA Energy Institute in Madrid, Spain

Academic context

[1] A. Mortazavi, et al., Experimental investigation of triply periodic minimal surfaces for high-temperature solar receivers, Case Stud. Therm. Eng. 60 (2024) 104771

[2] Mortazavi A., Ameri M., “Conventional and advanced exergy analysis of solar flat plate air collectors”, Energy, Vol. 142, pp. 277-288, 2018.

First name: Daniele **LAST NAME**: MOSSO

Topic: Modelling of the Climate-Land-Energy-Water Nexus

Course year: 2nd **Tutor(s)**: Laura SAVOLDI

Highlights of the research activity

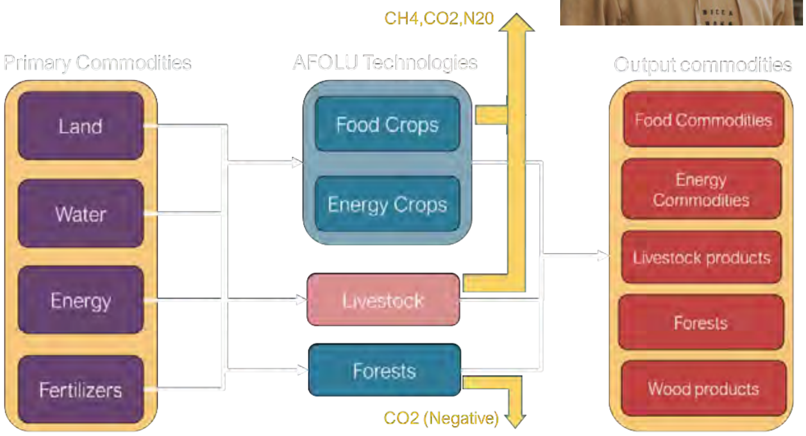


Figure 1 - AFOLU Reference Energy System

Over the past year, my research has focused on advancing integrated modeling of the Agriculture, Forestry, and Other Land Use (AFOLU) sector and its integration with energy system models to assess decarbonization policies and technologies. Collaborating with the Energy Modeling Lab in Copenhagen, my work has included literature review, model development, and application to case studies in Italy and Sweden.
Model Development and Validation
A robust AFOLU model was developed to represent interactions between primary resources (land, water, energy, fertilizers), technologies (e.g., food crops, energy crops, livestock, forests), and outputs (food, energy, wood products). The framework also includes emissions (CH_4, CO_2, N_2O) and forest-based negative emissions. Refinements ensured consistency in outputs.
Case Studies
Italy (TEMOA Framework): Explored AFOLU decarbonization pathways, revealing optimal resource allocation strategies and emission reduction potentials.
Sweden (TIMES Framework): Focused on forest management and bioenergy, highlighting synergies between sustainable forestry and energy transitions.
Key Findings
Integrating AFOLU with energy models is critical for capturing cross-sectoral dynamics. The Italian case emphasized emissions reduction through policies, while the Swedish study underscored opportunities in forest bioenergy. The model's adaptability across frameworks demonstrates its broad applicability to diverse contexts.

External collaborations

- Energy Modelling Lab
- E4SMA
- IFE

Academic context

[1] UN Sustainable Development Solutions Network and Fondazione Eni Enrico Mattei, "Roadmap to 2050 - The Land-Water-energy Nexus of Biofuels," 2021. Accessed: Mar. 06, 2023. [Online]. Available: https://roadmap2050.report/static/files/roadmap-to-2050-biofuels.pdf

[2] M. Howells *et al.*, "Integrated analysis of climate change, land-use, energy and water strategies," *Nat Clim Chang*, vol. 3, 2013, doi: 10.1038/NCLIMATE1789.

First name: Davide **LAST NAME**: PETTINARI

Topic: ARC safety and siting studies

Course year: 2^{nd} **Tutor(s)**: Raffaella TESTONI, Massimo ZUCCHETTI

Highlights of the research activity

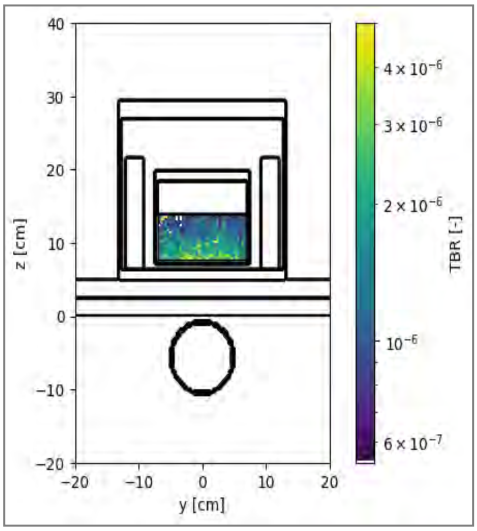


Figure 1. LIBRA experiment - 1L BABY model with TBR distribution map.

Over the past year, I have been actively engaged in the field of fusion energy technologies, with a focus on neutronics and reactor design. My work bridges theoretical research and practical applications, aiming to advance sustainable fusion energy solutions through innovative tools and methodologies. I developed advanced workflows for CAD importation and meshing, integrating tools like OpenMC, SolidWorks, Ansys and Coreform Cubit to conduct comprehensive neutron transport and activation studies. These workflows have improved the efficiency of complex simulation analyses. My research also includes decommissioning strategies, radioactive waste management, and siting criteria for fusion reactors. Notably, I analyzed the activation of compact tokamaks using Deuterium-Helium3 fuel.

During a two-month assignment at ENI in Porto Marghera, I designed a Neutron Attenuator for Gamma Detection and a Pellet Injection System. This project enhanced gamma detection sensitivity and involved selecting materials capable of withstanding extreme operational conditions. I also conducted detailed simulations to optimize neutron flux and spectrum behavior, contributing to improved system performance in demanding industrial environments.

Since September 2024, I have been conducting research at the Plasma Science and Fusion Center (PSFC) at MIT, focusing on validating OpenMC for fusion applications through the OKTAVIAN shielding benchmark. This involves comparing simulation results with experimental data and MCNP outputs using HDF5-based datasets from ACE files generated from ENDF/B-VIII.0, JEFF-3.3, and FENDL-3.2. I also contributed to the design of nuclear experiments and technologies, including the Liquid Immersion Blanket: Robust Accountancy (LIBRA) experiment at MIT. As part of this project, I worked on the design of Build A Better Yield (BABY 1L), shown in Fig.1, a key step in the progression to full-scale LIB technology. This involved collaborating with multidisciplinary teams to optimize reactor blanket designs by analyzing neutron backscattering effects and ensuring scalability toward full-scale implementations. I participated in key events such as the "15th ITER Neutronics Meeting and Fusion Neutronics Workshop" and the "Titans Project - Third Tritium School", where I shared my works and developed strategies for advancing fusion technologies. These experiences honed my ability to work in international teams and to communicate complex technical concepts effectively.

External collaborations

- Eni S.p.A.
- MIT Plasma Science and Fusion Center

Academic context

[1] Sorbom, B. N., et al. "ARC: A compact, high-field, fusion nuclear science facility and demonstration power plant with demountable magnets." Fusion Engineering and Design 100 (2015): 378-405.
[2] Kuang, A. Q., et al. "Conceptual design study for heat exhaust management in the ARC fusion pilot plant." Fusion Engineering and Design 137 (2018): 221-242.
[3] Romano, Paul K., et al. "OpenMC: A state-of-the-art Monte Carlo code for research and development." Annals of Nuclear Energy 82 (2015): 90-97.

First name: Alessandro **LAST NAME**: BALBO

Topic: Energy system model development and coupling with power dispatchment model

Course year: 1st **Tutor(s)**: Laura SAVOLDI, Matteo CHIESA

Highlights of the research activity

The PhD project, developed in collaboration with the MAHTEP Group, aims to propose novel and possibly more efficient methodologies to link energy system optimization models to power dispatchment models. These two classes of tools are nowadays acknowledged as reliable and useful means for short to long term decarbonization planning and system management. Yet, their functioning is mostly independent from each other, bringing to possible information gaps on the outcomes.
In particular, in the context of expected strong renewable energies development, the correct representation of the electricity grid can bring up their real possible exploitment according to peak demand and production, especially when combined to energy storage system as batteries or through chemical means.
So far, the most explored possibility to combine them is the so called "soft-linking" practice, which involves providing each model results (obtained separately) as input to the other one, with the purpose of reaching convergence iteratively.
The research activity wants to consider the implications and improvements (if any) that this coupling methodology present, and investigate the possibility of considering alternatives to be compared with it.
In order to dive into the activity, the Northern Norway region was taken as case study, thanks to the collaboration with the Arctic University of Norway, UiT, in Tromsø, and its preliminary energy system model has been developed during the first year of work. Moreover, during the first visiting period in the region, contacts where made with local DSO for data supply and collaboration, that are now undergoing the processing phase to be established, in order to build the power dispatchment model.
The expected outcome of the research is a thorough comparison between traditional linking methodology and a possible new ones, where pros and cons are balanced and evaluated.

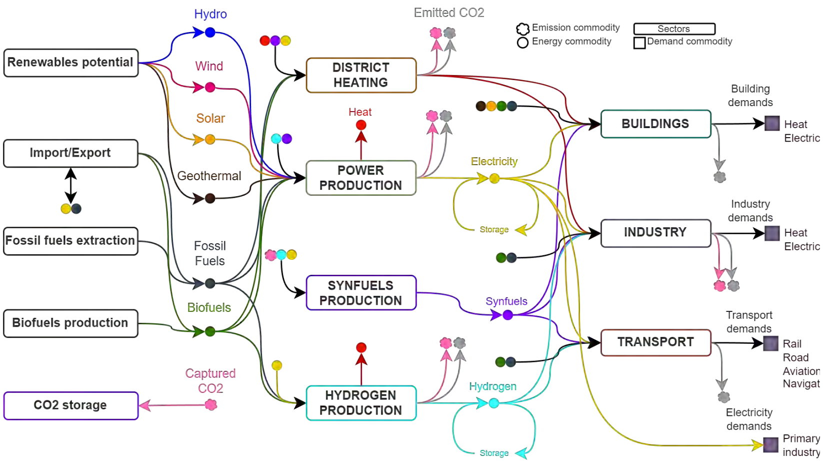


Figure 1: The Reference Energy System (RES) as represented in the Energy System Optimization Model (ESOM) TEMOA-Norway. As depicted, electricity is a fraction of the entire energy flow, yet, relevant for future development

External collaborations

- Arctic University of Norway, UiT

Academic context

[1] Chang, M. (2023). *Linking Energy System Models: Exploring analyses, methodologies, and theoretical dilemmas*. Aalborg Universitetsforlag. https://doi.org/10.54337/aau528189864
[2] Nicoli, M. *et al.* (2024). Enabling Coherence Between Energy Policies and SDGs Through Open Energy Models: The TEMOA-Italy Example. In: Labriet, M., Espegren, K., Giannakidis, G., Ó Gallachóir, B. (eds) Aligning the Energy Transition with the Sustainable Development Goals. Lecture Notes in Energy, vol 101. Springer, Cham. https://doi.org/10.1007/978-3-031-58897-6_5

First name: Elisabetta **LAST NAME**: BRAY

Topic: Development of self-consistent edge-core coupled transport models for impurities in Tokamaks

Course year: 1st **Tutor(s)**: 1st Fabio SUBBA, 2nd Giuseppe Francesco NALLO, 3rd Chiara MARCHETTO

Highlights of the research activity

The research activities for this first year of PhD started with a thorough review of the state of the art of impurity transport in the core plasma and integrated core-SOL (Scrape-Off-Layer) modeling. This study provided a solid foundation regarding the relevant physics, methodologies, and computational tools relevant for the PhD project.
Building on this knowledge, the technical work started with the interpretive analysis of an experimental campaign on the Asdex Upgrade (AUG) Tokamak, designed to study the behavior of Tin as a liquid metal divertor in a Tokamak.
Initial studies used the Aurora code to compute the radial impurity distribution in the core plasma, matching radiated power diagnosed by bolometers. These results were then used as inputs for the more comprehensive ASTRA simulation, which self-consistently models the transport of both main plasma species and impurities. ASTRA was coupled with subroutines such as TGLF and FACIT to calculate turbulent and neoclassical transport coefficients, respectively, for solving the diffusive transport equation. This approach led to a preliminary match with experimental results (Figure 1), and subsequent simulations were performed for two additional shots, one in H-mode (as in the case reported in Figure 1) and the other in L-mode, showing that the proposed modeling strategy is promising.
The study was then extended to include also simulations of the SOL region. To this aim, a new workflow was implemented in Python to facilitate case preparation, result visualization, and comparison in the overlapping core-SOL region. Specifically, the script extracts experimental data from the AUG database and iteratively calculates the impurity sources with the Aurora code. This result is implemented in the input file of the ASTRA code, integrating it into the other input files. Finally, post-processing tools for both core and SOL analysis are implemented, including specific routines for interpreting SOLPS-ITER (SOL transport code) results.
This represents an initial step toward integrating core and SOL transport modeling, with plans to develop a self-consistent strategy that iteratively updates core inputs based on SOL outputs and vice-versa.

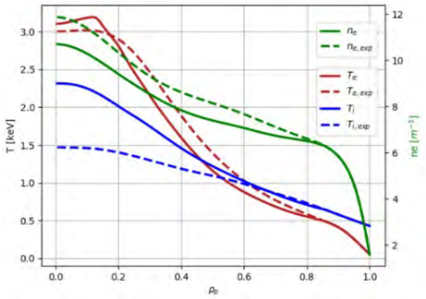


Figure 1: Core radial profiles of main plasma kinetic parameters. Dashed lines are experimental values and continuous ones are the results of the ASTRA simulation. The computed results are within the experimental uncertainty of the diagnostics.

During this first year, I also worked on two side projects, one related to the 0D modeling of the vapor shielding phenomenon associated to Liquid Metal Divertors, and the other aimed at the characterization of the ITER scenario in terms of target erosion using Aurora in support of the HeatLMD code, developed at IPP-CAS (Prague).

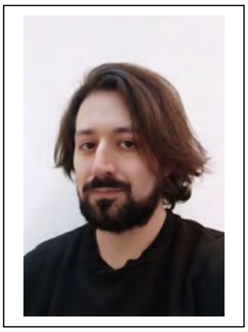
External collaborations

- Max Planck Institute for Plasma Physics (IPP)
- Institute of Plasma Physics of the Czech Academy of Sciences (IPP-CAS)

Academic context

[1] Nallo G.F. et al., *J. Fusion Energ* **42**, 41 (2023).
[2] Clemente A., *Plasma Phys. Control. Fusion* **63**, 073001 (2021)
[3] Scholte J.G.A. et al., *Nuclear Materials and Energy* **37**, 101522 (2023)

First name: Danilo **LAST NAME**: CATERINO



Topic: Experimental and numerical study of a bayonet tube heat exchanger for decay heat removal in LFR

Course year: 1st **Tutor(s)**: Roberto BONIFETTO, Giuseppe Francesco NALLO, Raffaella TESTONI

Highlights of the research activity

Generation IV lead-cooled fast reactors (LFRs) are among the most promising nuclear fission technologies in terms of inherent safety, reliability, and sustainability [1]. In this framework, *new*cleo plans to build a 30 MWe first-of-a-kind Lead-cooled Fast Reactor (LFR-AS-30) by 2031. To this aim, several experimental facilities dedicated to individual systems or components are envisaged by *new*cleo's roadmap. One of the targeted systems is the decay heat removal system.

Decay heat removal systems (DHRSs) are designed to remove the residual heat generated in the core by the radioactive decay of fission reaction products after a shutdown. One of the DHRS architectures to be employed in newcleo's LFR is based on the dip cooler concept: multiple bundles of parallel bayonet tubes are submerged into the reactor's primary coolant (lead) pool. Water enters by gravity through the feedwater pipeline, flows through each tube downcomer, then through each riser undergoing phase change. Steam is exhausted or condensed depending on the DHRS configuration: open-loop or closed-loop. Each bayonet tube features a double wall filled with pressurized helium to support prompt detection of leakages.

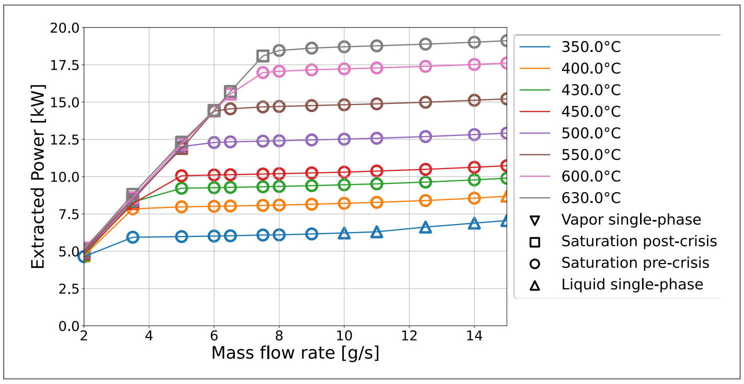


Figure 1: extracted power of a single bayonet tube for different wall temperatures at a system pressure of 10 bar. Markers indicate the outflow regime.

The experimental characterization of the DHRS will be supported by the Dip Cooler Instability (DCI) Test Facility. The facility is currently being assembled within the laboratory of the Energy Department at Politecnico di Torino, and it is planned to be operated from early 2025. To support the experimental investigation, several numerical models have been developed. The initial focus of the numerical analyses has been the thermal-hydraulic behavior of a single bayonet tube using the system code AC^2-ATHLET 3.4.1 [2]. A preliminary code verification has been performed through mesh convergence analyses and comparison against literature correlations. Then, a parametric study has been carried out to assess the influence of the operating conditions, identified for the Test Facility, on a single bayonet tube. Main results consist of operational maps concerning the extracted power (reported in Figure 1), pressure drop, and two-phase over single-phase pressure drop ratio.

The operational maps highlighted that the performance of a single bayonet tube drastically drops under operating conditions close to atmospheric due to the increasing intensity of two-phase phenomena. Future activities will concentrate on the thermal-hydraulic analysis of the entire DCI Test Facility. Additional efforts will be dedicated to Verification and Validation (V&V) thanks to the comparison against other computational tools and future experimental results.

External collaborations

- *new*cleo SrL

Academic context

[1] Alemberti A, Smirnov V, Smith CF, Takahashi M (2014) Overview of lead-cooled fast reactor activities. Progress in Nuclear Energy 77:300–307. doi: 10.1016/j.pnucene.2013.11.011
[2] P. Schoffel et al. (2023) ATHLET - Models and Methods. GRS

First name: Serena **LAST NAME**: CROBU

Topic: Tritium Technologies for the SORGENTINA-RF Facility

Course year: 1st **Tutor(s)**: Raffaella TESTONI, Massimo ZUCCHETTI

Highlights of the research activity

My PhD activity is focused on Tritium Technologies for the SORGENTINA-RF Facility. SORGENTINA-RF (SRF) is a project under development which should be carried out at the ENEA Brasimone Research Centre [1]. The scope is the production of ^{99}Mo (as precursor of ^{99m}Tc, used in nuclear medicine diagnostic procedures) with the development of a 14 MeV fusion neutron source using a rotating target and a deuterium-tritium ion accelerator.

The purpose of my PhD is to have a preliminary design for the Tritium Facility which has the following functions:

- receives the exhaust gas coming from the vacuum chamber
- removes the impurities
- re-introduces Q_2 (Q = D, T) isotopes in the fuel management system.

The core of the Tritium Facility is the Pd-Ag permeator unit which separates the impurities (He, Ar, Ti, O) from the exhaust gas stream in order to purify and recycle the deuterium and tritium as fuel. Basically, the exhaust gas enters the permeator, Q_2 starts permeating through the membrane, while the impurities remain inside. When impurities have reached a certain defined pressure, the permeator is emptied so that the process can restart from the beginning.

First, a literature review has been performed, in order to acquire an initial awareness of the research activity. The topics of the study concerned the physics of tritium permeation through Pd-Ag (palladium-silver) membranes [2] [3] and their application to SORGENTINA.

After that, the purpose was to develop a model (coded in Python) to predict the behaviour of the Pd-Ag permeator.

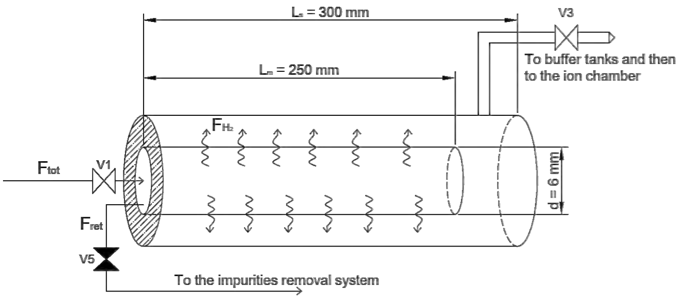


Figure 1 – Schematic representation of the permeator

In parallel to this activity, an initial study of the operation of the Simscape software has been carried out, in order to understand how the Tritium Facility can be modelled using this tool. The purpose of this activity is to implement the various sub-systems of the Tritium Facility, in order to have an engineering design.

External collaborations

- ENEA Brasimone Research Centre
- ENEA Frascati Research Centre

Academic context

[1] A. Pietropaolo et al., “SORGENTINA-RF project: fusion neutrons for 99 Mo medical radioisotope: SORGENTINA-RF,” Eur. Phys. J. Plus, vol. 136, no. 11, pp 136-1140, 2021.

[2] M. Vadrucci et al., “Hydrogen permeation through Pd-Ag membranes: Surface effects and Sieverts’ law”, Int. J. Hydrogen Energy 38, 4144-4152, 2013.

[3] R. Antunes et al., “Numerical study and experimental verification of protium permeation through Pd/Ag membranes for fusion applications”, Fusion Eng. Des. 146, 1286-1290, 2019.

First name: Marika **LAST NAME**: D'ADDAZIO

Topic: Design and multi-physics modeling of 20 T superconducting magnets for particle accelerators and for fusion machines

Course year: 1st **Tutor(s)**: Laura SAVOLDI, Paolo FERRACIN

Highlights of the research activity

The PhD research is conducted in collaboration with the Lawrence Berkeley National Laboratory and the main activities carried out during the first PhD year are briefly described.

The 2D magnetic and mechanical analysis of a 20 T hybrid cosθ dipole for future high-energy particle colliders is performed. The hybrid concept consists in the introduction of HTS conductors in the high field region and LTS conductors in the lower field region to reduce the overall cost of the magnet. The design of such high-field magnets presents numerous challenges, especially in managing the high Lorentz forces generated. Regarding the magnetic analysis, two dipole cross-sections are under development and the main difference lies in the conductor used for the magnet "insert" (Bi-2212 or REBCO STAR®/CORC® wires). Concerning the mechanical structure analysis, the cross-section under study is the one with Bi-2212 as "insert" and Nb_3Sn as "outsert". This work involved the analysis of the mechanics of the support structure, which plays a critical role in ensuring the structural integrity of the magnet under high-stress conditions. The described work was presented at the 8th Annual Collaboration Meeting of the US Magnet Development Program and at the Applied Superconductivity Conference 2024, where a research paper was submitted for publication.

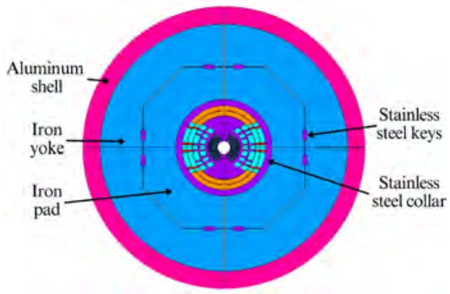


Fig. a) 2D structural cross-section of the 20 T hybrid cosθ dipole magnet.

To prove the feasibility of the hybrid concept, the first hybrid dipole with a nominal magnetic field of 9 T is currently under assembly and preparation for testing at LBNL. In this framework, the PhD research includes also the analysis of the 3D mechanical integration between the inner and the outer magnet. In this project is important to conduct a detailed stress analysis of the magnet to predict how it will behave under operational conditions. The final goal is to compare the predicted stresses with the results of the upcoming test to validate the simulation model.

Moreover, an experimental project is under development to understand the mechanical limits of the REBCO STAR® superconducting wire. This wire is being considered for use in high-field magnets but its mechanical behavior under electromagnetic forces is not yet fully understood. To perform this test, an impregnation mold is under development in order to simulate the real conditions experienced by the conductor in the magnet. The plan is to impregnate the wire with either pure or filled wax. Once impregnated, the wire will be compressed at room temperature inside the mold, mimicking the forces applied during the magnet operation, and then the critical current measurements will be performed at 77 K. By understanding the mechanical properties of the wires and cables used in these magnets, it is possible to design more reliable and robust systems capable of handling the conditions found in high-energy accelerators and other demanding applications.

External collaborations

- Lawrence Berkeley National Laboratory (CA, USA)

Academic context

[1] V. Marinozzi, *et al.*, "Conceptual design of a 20 T hybrid cos-theta dipole superconducting magnet for future high-energy particle accelerators", (2022).

[2] E. Galstyan, *et al.*, "High critical current STAR® wires with REBCO tapes by advanced MOCVD", in *Superconductor Science and Technology* (2023).

[3] L. G. Fajardo, *et al*., "Electromechanical Analysis for the Integration of a Nb_3Sn and a Bi-2212 CCT Dipole Magnet for a Hybrid Magnet Test," in *IEEE Transactions on Applied Superconductivity* (2023).

First name: Alessandro **LAST NAME**: MORANDI

Topic: Decommissioning of radioactive components from advanced fusion and fission nuclear reactors

Course year: 1nd **Tutor(s)**: Raffaella TESTONI, Massimo ZUCCHETTI

Highlights of the research activity

The primary objective of my PhD research is to explore the decommissioning of advanced fission and fusion reactors. While the decommissioning process for conventional fission reactors is well-established, future reactor designs and fusion systems may pose new challenges. This year, my research focused on two main areas: accident scenario analysis and neutronic analysis using OpenMC [1]. Both tools are integral to estimating radiological hazards and activation levels, which are critical for efficient and safe decommissioning planning.

I began with an extensive literature review to assess the current state of decommissioning, including the concept of clearance and advanced techniques to reduce activation in fusion devices [2]. I also explored existing regulatory frameworks for decommissioning, with a focus on assessing their applicability to fusion reactors and identifying any potential gaps or challenges unique to fusion technology.

Using OpenMC, a Monte Carlo-based neutron and photon transport simulation code, was used to analyze neutron-induced activation in fusion devices. My research this year concentrated on the impact of fuel choice on neutron flux and subsequent material activation. Specifically, I studied the neutron flux reduction achieved by using Deuterium-Helium-3 (D-He3) instead of deuterium-tritium (DT) fuel in a compact, high-field tokamak based on an ARC-class design. The reactor on which the analysis was performed is equipped with high-temperature superconducting (HTS) magnets and a molten salt (FLiBe) blanket. While the DHe3 reaction is aneutronic, neutrons are still generated in the Deuterium-Deuterium (DD) channel and secondary reactions involving Tritium produced by DD fusion also generate some high-energy neutrons. It was found that comparing the performance of the two fuels, at a fusion power output of 525 MW_{th}, the use of DHe3 can reduce the neutron flux by about an order of magnitude on critical components such as the first wall (Figure 1), blanket, and toroidal field coils. Furthermore, a preliminary analysis considering the substitution of the FLiBe blanket with Borated Water showed comparable neutron flux reduction, highlighting the potential to simplify the design by using a more technologically viable and more material compatible coolant.

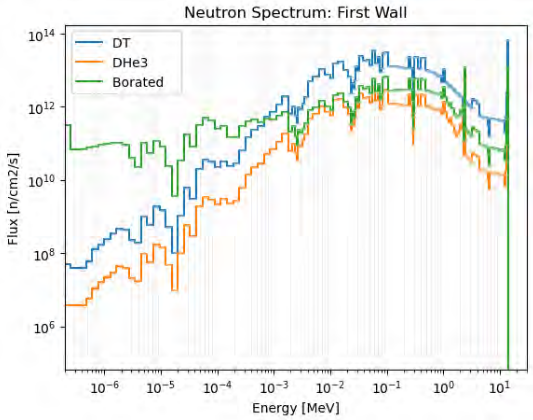


Fig.1 – Neutron spectra on the First Wall (FW) for the three reactions considered.

These findings were presented as a poster titled "Activation Analysis of a Compact Tokamak Using Deuterium-Helium-3 Fuel" at the 33rd Symposium on Fusion Technology (SOFT 2024) in Dublin.

External collaborations

- ENI

Academic context

[1] P. K. Romano et al. OpenMC: A state-of-the-art Monte Carlo code for research and development. Annals of Nuclear Energy, 82:90–97, 2015.

[2] IAEA. Global Status of Decommissioning of Nuclear Installations. IAEA NUCLEAR ENERGY SERIES NW-T-2.16. 2023.

[3] E. Pedretti and S. Rollet. Comparison of neutronic productions during operation of the Aries-III second stability D3He tokamak reactor without and with Tritium-assisted startup. In Emerging Nuclear Energy Systems: Icenes' 93 - Proceedings Of The Seventh International Conference, page 47. World Scientific, 1994.

First name: Elia **LAST NAME**: NOVARESE

Topic: Development of a digital twin for the operation of MW-class gyrotrons for plasma heating and current drive in fusion reactors

Course year: 1st **Tutor(s)**: Laura SAVOLDI, Antonio CAMMI

Highlights of the research activity

The Electron Cyclotron Resonance Heating (ECRH) and Current Drive (ECCD) systems are critical for preheating and stabilising the plasma during fusion reactor operation. Their power source, the Gyrotron, generates high-power, high-frequency electromagnetic waves through the electron cyclotron maser instability. The development of a complete model of this device is indispensable for its control; moreover, the concept of a digital twin is becoming more relevant in the research communtiy, providing a digital copy of the physical device to perform real-time, data-driven simulations. The Ph.D. research therefore focuses on the development of a complete physical-based model of the Gyrotron, and the first phase of the project required the identification of the main components to be modelled and integrated into the complete model. This task involved a deep and essential literature review to understand how the Gyrotron works, which components are relevant to the device, and what physics is important to capture the behaviour of each component and the device as a whole. Thanks to this research activity, six different components were selected:

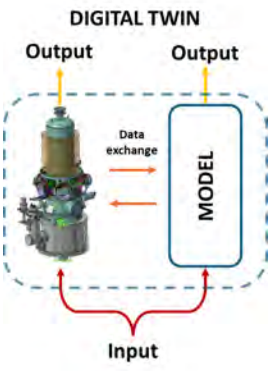


Figure 1 A visualization of the digital twin in which the data exchange between the physical device and the model allow to perform real time data-driven simulations essential for the

1. Magnetron Injection Gun, responsible for generating the electron beam;
2. Beam Tunnel, responsible for absorbing parasitic electromagnetic waves;
3. Resonant cavity, responsible for generating electromagnetic waves from resonance phenomenon between electron beam and magnetic field;
4. Quasi-Optical system, responsible for shaping the cavity electromagnetic mode wave into a Gaussian wave;
5. Window, responsible for transmitting the wave outside the Gyrotron;
6. Collector, responsible for absorbing spent electron beam from the cavity.

Regarding the physical models, the following have been selected:

1. Electromagnetism model;
2. Electrodynamic model;
3. Thermo-Hydraulic model;
4. Thermo-Mechanic model.

From the selection of physical models, the components were modelled and the complete model of the Gyrotorn was schematised, starting from the connection of the input/output parameters of the component model. This scheme was presented at the FuseNet conference and the Symposium of Fusion Technology (SOFT2024)) conference, and it's the argument of an article under development.

External collaborations

- Politecnico di Milano
- Fusion 4 Energy
- National Technical University of Athens

Academic context

[1] M. Thumm, Gyrotrons: High-Power Microwave and Millimeter Wave Technology
[2] M. K. Thumm, High-power gyrotrons for electron cyclotron heating and current drive
[3] A. Thelen, A comprehensive review of digital twin—part 1: modeling and twinning enabling technologies

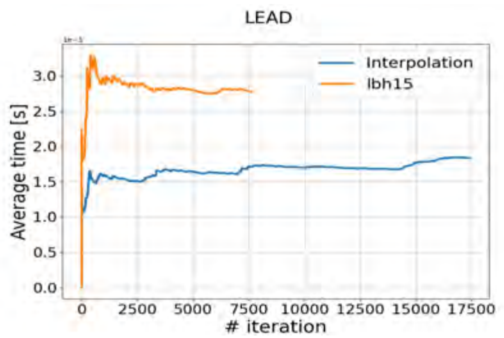
First name: Francesco **LAST NAME**: PEPE

Topic: Development of a subchannel code for full-core thermal-hydraulic analysis of lead-cooled fast reactors

Course year: 1st **Tutor(s)**: Roberto BONIFETTO
Giuseppe Francesco NALLO

Highlights of the research activity

The main objective of the research activity is to develop and improve subchannel codes for nuclear reactor core thermal-hydraulic analysis. In the first year, the research activity focused on the open-source sub-channel code DASSH (Ducted Assembly Steady-State Heat transfer software), originally developed at Argonne National Laboratory (IL, USA). This code is intended for both full-core and assembly level thermal-hydraulic analysis of liquid metal-cooled fission reactor cores. All subchannels are hydraulically isolated, while energy exchanges (due to turbulence, conduction and the presence of spacers) are modelled by means of a global energy mixing coefficient, computed through suitable correlations. While the domain is radially divided into subchannels, a 1D axial finite volume mesh is defined and the energy equation is solved at each volume with a forward-difference scheme.
During the first months, the main capabilities of DASSH have been studied, and necessary improvements were identified, particularly to remove restrictive assumptions and enhance accuracy and flexibility. DASSH was originally developed only for forced-convection problems, with the hypothesis of homogeneous, isotropic fluid properties in the axial direction, resulting in a simplified version of the energy equation, which is directly solved for temperature.
The solver of the code has therefore been updated removing the hypothesis of homogeneous properties. The energy equation is now solved for enthalpy and temperature is then evaluated from it. Additional correlations for the energy mixing coefficient were also added. Some modifications have also been made in the way DASSH computes the material properties. First of all, values in property tables, which are used for interpolation as the default option, that were inaccurate or not in accordance with the reference correlation, have been corrected. Moreover, some missing checks on the user-defined tables have been implemented (for example checking the strict monotonicity of temperature values before interpolation, and the presence of zero, negative or missing values for properties), to improve the code robustness. Additionally, a link of DASSH with the library of material properties for lead, bismuth and lead-bismuth eutectic *lbh15*, developed by *new*cleo, was implemented. The computational time of both options (interpolation and *lbh15* call) was studied and compared, resulting in slightly higher computational cost for *lbh15*, which remains very limited and may be justified by the increase in accuracy. Finally, the suite of tests for the material class has been updated, including tests on *lbh15*.



Computational time: comparison between properties from table interpolation and lbh15.

External collaborations

- *new*cleo

Academic context

[1] M. Atz, M. A. Smith and F. Heidet, "DASSH software for ducted assembly thermal hydraulics calculations – overview and benchmark," Transactions of the American Nuclear Society, vol. 123, pp. 1673-1676, 2020.
[2] G. Ottino, et al. "lbh15: a Python package for standard use and implementation of physical data of heavy liquid metals used in nuclear reactors." *Journal of Open Source Software* 9.96 (2024): 6383.
[3] L. Cinotti, et al. "Lead-Cooled Fast Reactor (LFR) Design: Safety, Neutronics, Thermal Hydraulics, Structural Mechanics, Fuel, Core, and Plant Design, pages 2749-2840. Springer US, Boston, MA, 2010.

First name: Cecilia **LAST NAME**: PIATTI

Topic: Cooling enhancement in high energy physics components applied in decarbonization: thermal hydraulics of next generation of porous structures

Course year: 1st **Tutor(s)**: Laura SAVOLDI, Luca MAROCCO, Nima FATHI

Highlights of the research activity

The research activity investigates the use of an innovative type of porous media, Triply Periodic Minimal Surfaces (TPMS), to improve cooling performance in high heat flux components. TPMS are defined by trigonometric functions in the 3D space and are characterized by their periodic, zero mean curvature surfaces that do not self-intersect. These geometries allow for the development of highly interconnected lattice structures, greatly improving heat transfer to the working fluid, due to the increase of the surface-to-volume ratio [1]. Additive Manufacturing (AM) technology makes the fabrication of such complex structures possible.
During the past year of PhD, experimental and computational activities have been carried out in parallel.
A first experimental campaign was performed in Madrid, at IMDEA Energy Institution. Two TPMS samples, namely Diamond and SplitP, were tested under high heat fluxes produced by a solar simulator, to assess the different thermal performance of the lattices.
Subsequently, hydraulic testing was carried out at different experimental facilities to explore the effects of the design parameters and the manufacturing procedures on the pressure drop of fluid flowing through TPMS structures. Water and air tests were performed respectively at Politecnico di Milano and Politecnico di Torino, on a set of samples, designed with different TPMS topologies (Diamond, Gyroid and SplitP), produced in stainless steel and in resin, and varying the design parameters. Both these experimental activities formed a large dataset that allowed the definition of correlations for the hydraulic dimensionless variables.
The results of this work were presented by some colleagues in June at the UIT Conference (Neaples, Italy) and at ECCOMAS Congress (Lisbon, Portugal) and are the object of a journal paper that will be published soon.

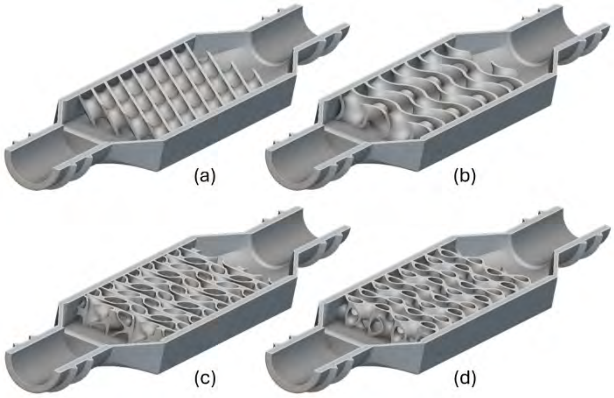


Figure 1: Longitudinal sections of the tested samples, Diamond (a), Gyroid (b), Lidinoid (c) and SplitP (d)

Further experiments were performed at the premises of Texas A&M University in Galveston (Texas, USA), during two visiting periods. In this case the main objective was the validation of two turbulence models used in the computational fluid dynamics (CFD) simulations. The results of this work were presented at the ASME VVUQ Symposium in May (College Station, Texas, USA) and at ECCOMAS Congress. For this second conference, the analysis was focused on the quantification of the discrepancies between test data and computational results through a Multivariate Metric.

External collaborations

- Texas A&M University, Galveston, Texas
- Politecnico di Milano

Academic context

[1] Gado, M.G., et al (2024), *Triply Periodic Minimal Surface Structures: Design, Fabrication, 3D Printing Techniques, State-of-the-Art Studies, and Prospective Thermal Applications for Efficient Energy Utilization*. Energy Technol., 12: 2301287. https://doi.org/10.1002/ente.202301287

First name: Alessio**LAST NAME**: QUAMORI TANZI

Topic: Design and optimization of Triply Periodic Minimal Surfaces as heat sinks for the cooling of high heat-flux components in fusion reactors

Course year: 1st **Tutor(s)**: Laura SAVOLDI, Antonio CAMMI

Highlights of the research activity

The work conducted during the first year of my PhD includes both theoretical aspects, suc and practical ones, such as design development and experimental campaigns. The design of a TPMS-based divertor tile for the W7-X fusion reactor has been successfully completed (Figure 1). The tile has demonstrated the ability to withstand a heat flux of 10 MW/m², distributed over a heated length of 10 cm, when a subcooled water mass flow rate of 1.25 kg/s is applied. This results in a pressure drop of less than 0.7 MPa and limits fluid boiling near the inlet and outlet manifolds. The initial phase of the project focused on selecting the most suitable TPMS candidate through a detailed thermal-hydraulic analysis conducted on a reduced computational model, maintaining the same layered structure as the tile. After selecting the optimal configuration, the analysis was expanded to the full tile to ensure compliance with operational constraints. This work has culminated in a paper publication in *Case Studies in Thermal Engineering* [1] and a poster presentation at the PhD event in Stuttgart, Germany, as well as the SOFT 2024 conference in Dublin, Ireland. A systematic review on the state of the art of TPMS is almost completed, with the goal of creating a comprehensive database of TPMS-related papers selected based on specific inclusion criteria. This database will serve as the basis for a comprehensive review paper that will be published next year. An extensive analysis of the thermofluidynamic properties of TPMS is also ongoing. Using CTfD simulations, the effects of topology, porosity, and displacement on heat transfer capabilities and pressure drops have been carefully examined. These simulation results are being validated through experimental campaigns. Two experimental campaigns have already been completed: one at the Energy Department of Politecnico di Torino and another at Politecnico di Milano. At Politecnico di Milano, water tests were conducted on a set of five samples, each designed with different TPMS topologies and orientations. These samples were manufactured using two techniques: stainless steel samples produced via LPBF (Laser Powder Bed Fusion) and resin samples made via SLA (Stereolithography). Additionally, nine samples were tested in an air circuit at the DENERG laboratories of Politecnico di Torino. The verification and validation of the numerical simulations have been thoroughly examined, supported by participation in the VVUQ PhD School held in Arona, Italy. Lastly, a new project is focusing on the development of a TPMS-based molten salt heat exchanger, encompassing activities from initial dimensioning and theoretical calculations to numerical simulations, conducted in parallel with an experimental campaign.

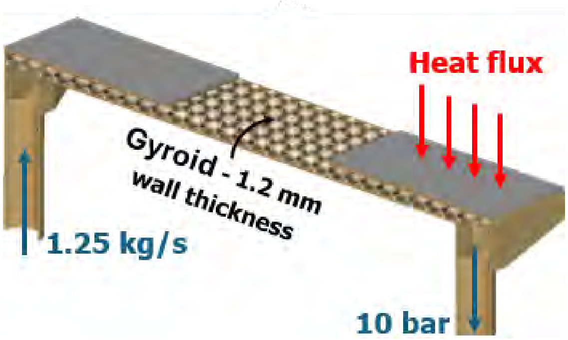


Figure 1: W7-X TPMS-based divertor tile design

External collaborations

- Energy Department of Politecnico di Milano
-

Academic context

[1] A. Quamori Tanzi, A. Cammi, L. Marocco, and L. Savoldi, 'Design of a 10 MW/m2-heat-flux removal system for a W7-X divertor tile using triply periodic minimal surfaces', *Case Stud. Therm. Eng.*, vol. 63, p. 105405, Nov. 2024, doi: 10.1016/j.csite.2024.105405.

First name: Mauro **LAST NAME**: SPRÒ

Topic: Modelling an in-cryostat Loss-Of-Coolant Accident in nuclear fusion reactors

Course year: 1st **Tutor(s)**: Antonio FROIO, Andrea ZAPPATORE, Roberto BONIFETTO

Highlights of the research activity

The research focuses on modeling a Loss-Of-Coolant-Accident (LOCA) in the cryostat of nuclear fusion reactors. The goal is to develop a detailed thermal-hydraulic model for analyzing accidental releases of pressurized supercritical fluids, as no numerical models currently exist for such events, despite similar accidents having occurred. One such incident happened at a test facility in San Diego, where a 15 kA discharge on an ITER Central Solenoid Module (CSM) caused an electrical arc that punctured two coaxial joints, leading to the leakage of supercritical helium (SHe).

The first step was to calculate the properties of SHe as a function of pressure and temperature, using the CoolProp software, over a temperature range of 3 K to 300 K and a pressure range of 0.01 bar to 20 bar. The results were then tabulated for integration into STAR-CCM+. The next phase involved a preliminary 2D CFD analysis aimed at determining the correct simulation setup, especially how to handle the complex thermophysical properties of SHe. To validate the multiphase model, a 2D simulation of a supercritical CO_2 release from high-pressure pipelines was conducted, comparing results with available experimental data.

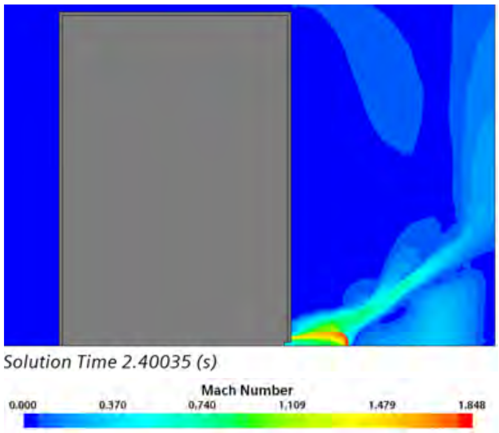


Fig. Mach number distribution of the SHe supersonic jet on a symmetry plane

Following this, a simplified 3D domain was developed by rotating the 2D domain to create a mesh refinement algorithm. This algorithm adapts the mesh based on Mach number gradients to refine or coarsen the mesh cells as required by the shock fronts formed during the release of the pressurized fluid into a vacuum environment. This step was essential because STAR-CCM+ supports AMR solvers only for 3D simulations and it also allows to check if the 2D setup needed some adjustments for the 3D analysis.

Finally, the actual 3D model of the accident, including CSM, insulation, and fluid volume, has been built in STAR-CCM+ and is currently being simulated, with completion expected in several weeks due to high computational demands. In parallel, a multiphysics model of the electric arc is being developed to assess the energy deposited on the electrodes and the time required for the arc to heat and melt them.

Academic context

[1] K. Khumthong *et al*., "ITER CS Module Test Facility Operational Lessons From CS Modules 1–4," in *IEEE Transactions on Applied Superconductivity*, vol. 34, no. 5, pp. 1-6, Aug. 2024

[2] N. Martovetsky *et al*., "Testing of the ITER Central Solenoid Modules," in *IEEE Transactions on Plasma Science*, vol. 50, no. 11, pp. 4292-4297, Nov. 2022

[3] M. Sprò *et al.,* "3D Transient CFD Simulation of an In-Vessel Loss-Of-Coolant Accident in the EU DEMO Breeding Blanket," in *Energies,* vol. 16, no. 9, Apr. 2023

First name: Christian **LAST NAME**: VITA

Topic: Advanced uncertainty quantification and propagation analysis to support lead fast reactor development

Course year: 1st **Tutor(s)**: Sandra DULLA, Nicolo' ABRATE

Highlights of the research activity

During my first PhD year, my research focused on the Lead-cooled Fast Reactor (LFR) designed by Westinghouse Electric Company. The goal, set with my academic and industrial tutors, was to conduct Uncertainty Quantification and Sensitivity Analysis (UQSA) on key transient parameters (e.g., power , cladding and fuel temperature, ..). UQSA requires extensive data and pre-calculations, but the high number of uncertain parameters often makes running all simulations infeasible due to the curse of dimensionality. Generating multi-group cross-sections (MGXS) using Monte Carlo (MC) simulations, while accurate, is computationally expensive and configuration-specific. To address this, a new approach was tested, leveraging three independent sub-system MC models for fuel assemblies, peripheral assemblies, and non-multiplying regions. As a first step, the full-core WEC LFR model in Serpent was defined and compared against reference results from the pyARC package. Subsequently, Python packages were developed to automate input generation, accounting for variations in material properties and system geometry. Once the full-core model in Serpent was successfully reconstructed, it became possible to compare the MGXS datasets generated by the full-core model and the mini-core models. Using mini-core models for MGXS generation, it was observed that deterministic solvers (in my study a home-made FreeFem-based neutron diffusion solver), achieved accuracy comparable to datasets generated with full-core simulations.

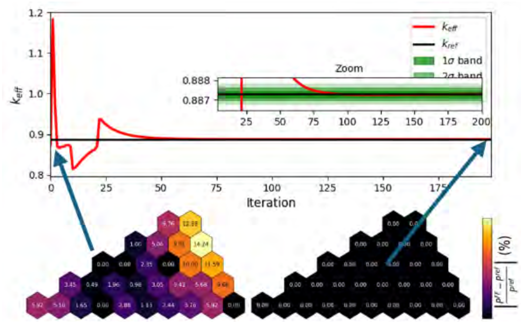


Figure 1: k_{eff} and $\Delta P/P_{ref}$ evolution

The potential application of the SPH method was also investigated to enhance the multi-MC model pipeline. SPH coefficients, derived by comparing neutron flux results from the deterministic code with Serpent MC reference data, were used to adjust datasets to reproduce reaction rates accurately. This method was applied to non-multiplying regions, yielding significant improvements in both the eigenvalue and power density distribution (P). Additionally, the feasibility of using a full-core MGXS dataset with SPH correction applied to each assembly was tested, with a remarkable reproduction of the k_{eff} and P (Figure 1).
Further studies included analysing the impact of SPH coefficients on the adjoint function and their effect on kinetic parameters (β_{eff}, Λ_{eff}), which appear insensitive to cross-section corrections. The role of photons was also examined, revealing non-negligible energy deposition due to photon kerma, particularly in reflecting regions. Finally, a preliminary uncertainty quantification and sensitivity studies based on Generalized Perturbation Theory (GPT) was conducted, highlighting the most impactful nuclide-reaction channels on the k_{eff} in steady-state condition.

External collaborations

- Argonne National Laboratory
- Westinghouse Electric Company

Academic context

[1] Bell, G.I. and S. Glasstone, *Nuclear Reactor Theory*, Van Nostrand Reinhold Company, 1970.
[2] Nikitin, E. Fridman, and K. Mikityuk. "On the use of the SPH method in nodal diffusion analyses of SFR core", *Annals of Nuclear Energy*, **85**, 544-551, 2015.
[3] A. Hebert. Développement de la méthode SPH: Homogénéisation de cellules dans un réseau non uniforme et calcul des parametres de réflector, *Ph.D thesis*, CEA-N-2209, 1981.

First name: Antonio **LAST NAME**: ZURZOLO

Topic: Modelling of laser-matter interaction for the sustainable energy production by nuclear fusion

Course year: 1st **Tutor(s)**: Roberto BONIFETTO, Raffaella TESTONI, Antonio FROIO

Highlights of the research activity

My PhD research focuses on modeling laser-matter interactions for sustainable energy production through nuclear fusion reactions. The aim is to analyze laser-plasma interactions using hydrodynamic and Particle-In-Cell (PIC) simulations to optimize target design for future inertial confinement fusion (ICF) devices, enhancing laser absorption and fusion reaction rates.

I started by studying laser-matter interactions to understand plasma formation and laser absorption mechanisms. I focused first on the hydrodynamic MULTI code, which relies on equations of state (EOS) to describe material properties. To overcome its limited material database, I developed a Python script to integrate EOS data from the SESAME library. I then worked with PIC codes, specifically SMILEI, reproducing published results to gain experience. Unlike hydrodynamic codes, PIC codes provide a kinetic model of plasma behavior by solving the Vlasov and Maxwell equations, though at a higher computational cost. My work aims to combine hydrodynamic and PIC simulations for more comprehensive analyses.

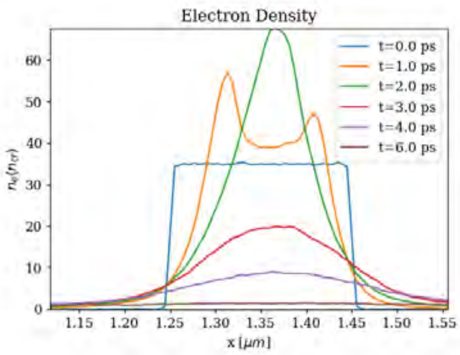


Fig.1 – Electron Density at different timesteps. Simulation with both Resonance and Collisional absorption.

Following the method in reference [1], I set up simulations to study laser interactions with solid-density foam, analyzing resonance and collisional absorption mechanisms. The results showed that both mechanisms play an important role: ablation of the solid filament creates a density gradient, enabling resonant interactions at the critical density, while electron-ion collisions also contribute significantly, leading to complete filament expansion within 6-7ps. These findings highlight the importance of both absorption mechanisms.

I studied parametric instabilities in laser-plasma interactions, such as Stimulated Raman Scattering (SRS), Stimulated Brillouin Scattering (SBS), and Two-Plasmon Decay (TPD), which can generate suprathermal particles and reduce laser absorption efficiency—key issues in inertial confinement fusion (ICF). Using the SMILEI code, I am simulating these instabilities. During a 2024 experimental campaign at the PALS laser facility in Prague, protons with unexpectedly high energies were observed. These protons resulted from a long pre-pulse (~1.5ns, 10^{14} W/cm^2) forming plasma, followed by a main pulse (~1 ns) that likely triggered instabilities. Based on hydrodynamic simulations from ENEA Frascati, I am setting up PIC simulations to investigate regions of the plasma where instabilities are expected, as simulating the entire laser profile is computationally prohibitive for ICF applications.

External collaborations

- ENEA (Italy)
- LULI (Laboratoire pour l'Utilisation des Lasers Intenses – Paris (France))

Academic context

[1] S. Shekhanov *et al.*, 'Kinetic modeling of laser absorption in foams', *Physics of Plasmas*, vol. 30, no. 1, p. 012708, Jan. 2023, doi: 10.1063/5.0131786.

Sustainable propulsion and energy systems

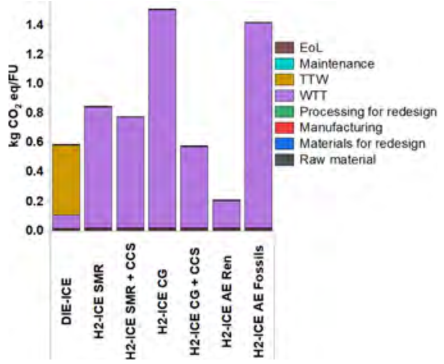
First name: Antonella **LAST NAME**: ACCARDO

Topic: Sustainability assessment of vehicles and automotive components through life cycle assessment

Course year: 3rd **Tutor(s)**: Ezio SPESSA, Giovanni DOTELLI

Highlights of the research activity

The relevance of the Life Cycle Assessment (LCA) is constantly growing as a result of the increasingly strict mandate to reduce the environmental effects of the transport sector. Nevertheless, even though several LCA studies of vehicles can be found in the literature, the comparability of the results among different studies is hampered by their disparity in the underlying assumptions. This limited comparability is due to the absence of methodology guidelines. The aim of this research activity is to contribute to the development of the methodology to apply LCA on vehicles. To do so, the third year of the PhD course was focused on strengthening the methodologies applied to batteries and electric drivetrains so far. Furthermore, attention was given to hydrogen engines and hydrogen production paths. In fact, hydrogen can be essential in achieving environmental objectives. However, the outcome depends on the underlying energy source and the specific conversion method employed for hydrogen production. This section has investigated the comprehensive environmental impacts of hydrogen production, comparing the environmental impacts of six different production paths (i.e., steam methane reforming (SMR), steam methane reforming with carbon capture and storage (SMR+CCS), coal gasification (CG), coal gasification with carbon capture and storage (CG+CCS), fossil-based alkaline electrolysis (AE Fossils), and renewables based-alkaline electrolysis (AE Ren)). Then, results have been exploited to estimate the life cycle environmental impacts of a hydrogen engine (H2-ICE) against its diesel counterpart (DIE-ICE), both assumed to be mounted on pickup trucks. An insight into the life cycle GHG emissions of all the investigated scenarios is given in the chart below.



Life cycle GHG emissions of H2-ICE against DIE-ICE.

External collaborations

- Dumarey
- IVECO Group
- Stellantis

Academic context

[1] A. Accardo, A. Garofalo, G. Dotelli and E. Spessa, "Prospective LCA of Next-Generation Cells for Electric Vehicle Applications," in IEEE Access, vol. 12, pp. 19584-19597, 2024, doi: 10.1109/ACCESS.2024.3361312
[2] Accardo, A.; Costantino, T.; Spessa, E. LCA of Recycled (NdDy)FeB Permanent Magnets through Hydrogen Decrepitation. Energies 2024, 17, 908. https://doi.org/10.3390/en17040908
[3] A Accardo, T Costantino, G Malagrinò, M Pensato, E Spessa. Greenhouse Gas Emissions of a Hydrogen Engine for Automotive Application through Life-Cycle Assessment. Energies, 2024, 17(11), 2571; https://doi.org/10.3390/en17112571

First name: Matteo **LAST NAME**: ACQUARONE

Topic: Advancing vehicle electrification: control strategies for hybrid electric vehicles and battery management algorithms for state estimation

Course year: 3rd **Tutor(s)**: Daniela Anna Misul

Highlights of the research activity

During my PhD, I mainly focused on energy management strategies (EMSs) for hybrid electric vehicles (HEVs) and battery state estimation.

Hybrid electric vehicles

During the first two years of my PhD, I focused on developing innovative control strategies for HEVs to optimize the power split between ICE and battery. Exergy-based control strategies were formulated to improve vehicle efficiency and minimize thermal detection risk in military applications. Moreover, while investigating the potential of machine learning techniques for HEV control, a reinforcement learning-based control strategy was enhanced with an innovative exploration strategy to speed up the training process and boost controller performance, reducing fuel consumption.

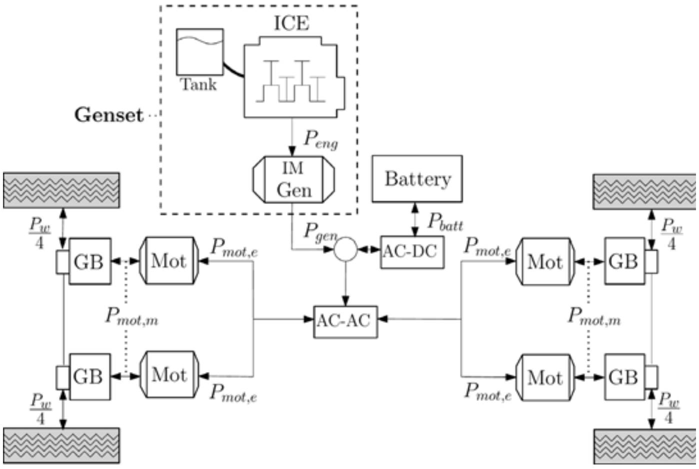


Figura 1 Schematic of an hybrid electric vehicle powertrain

Battery management system

During the third year of my PhD, I developed BMS algorithms for the estimation of critical battery states, i.e., state of charge (SOC) and state of health (SOH). First, we formulated and validated a novel data-driven approach for SOH estimation during fast-charging events using experimental data from multiple fast-charging protocols. Afterward, a hybrid SOC and SOH estimation algorithm was developed to combine the advantages of model-based and data-driven techniques. In particular, the main drawbacks of the state-of-the-art dual extended Kalman filter were addressed by leveraging available capacity information coming from the data-driven algorithm.

Most of the methodologies developed during these three years were compared against state-of-the-art techniques, demonstrating their potential to improve both HEV control and battery state estimation. My PhD work could contribute to the advancement of electrified vehicle technology, supporting the transition toward more sustainable transportation solutions.)

External collaborations

- McMaster University, Stanford University

Academic context

[1] Biswas, A., Acquarone, M., Wang, H., Miretti, F., Misul, D. A., & Emadi, A. (2024). Safe Reinforcement Learning for Energy Management of Electrified Vehicle with Novel Physics-Informed Exploration Strategy. IEEE Transactions on Transportation Electrification.

[2] Acquarone, M., Pozzato, G., James, C., & Onori, S. (2024). Exergy Management Strategies for Hybrid Electric Ground Vehicles: A Dynamic Programming Solution. Journal of Dynamic Systems, Measurement, and Control, 146(3), 031004.

[3] Acquarone, M., Miretti, F., Misul, D., & Onori, S. (2024). Sleek dual Extended Kalman Filter for Battery State of Charge and State of Health Estimation in Electric Vehicle Applications (No. 2024-24-0023). SAE Technical Paper.

First name: Angelo **LAST NAME**: BORNEO

Topic: Innovative Solutions for Sustainable Mobility

Course year: 3rd **Tutor(s)**: Daniela Anna MISUL

Highlights of the research activity

The research activity carried out during the 3rd year involves further development of ADASs. The focus was on improving the fuel efficiency of Adaptive Cruise Control (ACC) systems, especially for internal combustion engine (ICE) vehicles. ACC improves driving safety and comfort by automatically adjusting vehicle speed, but it also has potential for fuel savings through smoother driving dynamics.

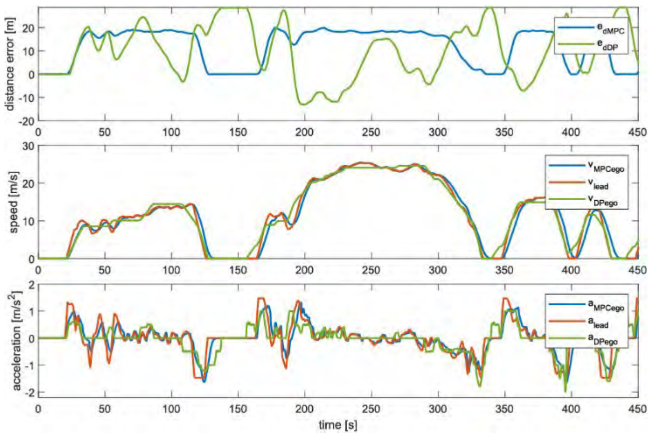


Figure 1. Comparison of velocity and acceleration profiles of ego equipped with fuel consumption

Two Model Predictive Control (MPC)-based approaches were explored. The first used a quadratic cost function to indirectly minimize fuel consumption by balancing state tracking and control effort. The second approach directly integrated a fuel consumption map into the MPC cost function to explicitly minimize fuel use. Both methods were benchmarked against an optimal dynamic programming solution.

Results showed that the simpler quadratic approach, with proper tuning, could achieve fuel savings comparable to the method that explicitly targets fuel. This makes the quadratic approach more practical for real-time implementation due to its lower computational demands. This study highlights the potential of MPC-based ACC to deliver fuel efficiency improvements while maintaining similar performance to more complex methods and is under review for publication.

External collaborations

- MCA Engineering

Academic context

[1] Borneo, Angelo; Miretti, Federico; Misul, DANIELA ANNA (2024)
Fuel Efficiency Optimization in Adaptive Cruise Control: A Comparative Study of Model Predictive Control-Based Approaches. In: APPLIED SCIENCES. ISSN 2076-3417

[2] Borneo, Angelo; Miretti, Federico; Acquarone, Matteo; Misul, Daniela (2023); “Battery Electric Vehicle Control Strategy for String Stability based on Deep Reinforcement Learning in V2V Driving.” In: 16th International Conference on Engines & Vehicles, Capri, Italy, 2023.

[3] Borneo, Angelo; Zerbato, Luca; Miretti, Federico; Tota, Antonio; Galvagno, Enrico; ... (2023); “Platooning Cooperative Adaptive Cruise Control for Dynamic Performance and Energy Saving: A Comparative Study of Linear Quadratic and Reinforcement Learning-Based Controllers.” In: APPLIED SCIENCES, vol. 13. ISSN 2076-3417

First name: Giuseppe **LAST NAME**: CASTELLANO

Topic: Phoenice (PHev towards zerO EmissioNs & ultimate ICE efficiency)

Course year: 3rd **Tutor(s)**: Federico MILLO; Luciano ROLANDO

Highlights of the research activity

To mitigate carbon footprint and pollutant emissions in the transportation sector, many governments aim for a fully electrified fleet of light-duty vehicles by 2035. However, research suggests that relying solely on electrification may not ensure carbon neutrality by 2050. A diversified approach, including innovative hybrid-oriented internal combustion engines, could more effectively achieve sustainability goals. Within this context, the EU-funded PHOENICE project is developing a plug-in hybrid (P0/P4) C-SUV demonstrator focusing on an advanced spark ignition engine concept coupled with a Euro 7 compliant aftertreatment system, seeking to improve fuel efficiency and minimize pollutant emissions beyond current standards.

The PHOENICE engine incorporates cutting-edge features: a high compression ratio of 13.6, variable valve actuation for Miller cycle operation, a 48V electric turbocharger, long-route cooled EGR, and swirl-enhanced intake ports enabling ultra-lean combustion. The exhaust system includes an electrically heated TWC, a coated GPF, and an underfloor SCR for NOx reduction under lean exhaust conditions.

My research contributed to PHOENICE by optimizing engine calibration under steady-state and transient operation using both 1D-CFD simulations and experimental testing. Initially, a 1D-CFD combustion model was developed for virtual calibration. Findings revealed a 47% peak gross indicated efficiency and a brake thermal efficiencies above 40% at part load using lean combustion, EGR, high CR, and EIVC.

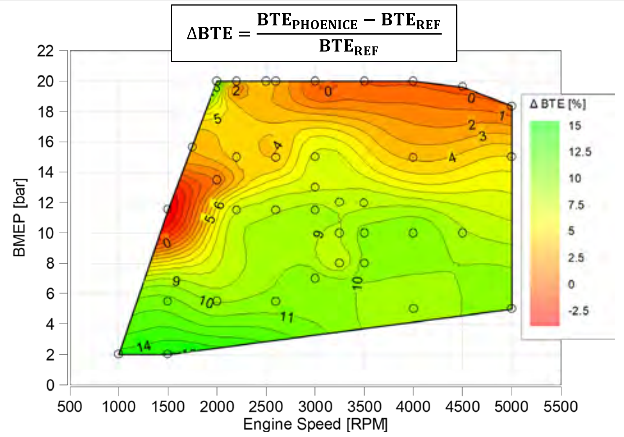


Figure 1 - Relative improvement in BTE in comparison with the baseline engine.

Experimental testing on the PoliTO dynamic bench refined transient calibration and developed control strategies for combustion mode transitions, including $\lambda = 1$ operation, EGR activation, and lean combustion. Various driving cycles were evaluated under diverse conditions (hot/cold starts, with/without EGR and electrical turbo assistance), refining actuator controls and stabilizing engine behavior against knock and lambda fluctuations. The tests demonstrated effective engine control functionality for all target cycles.

The final project phase focuses on testing the demonstrator vehicle with PEMS to evaluate dual dilution combustion efficiency and emissions reduction potential under real driving conditions.

External collaborations

- FEV Italia
- Stellantis
- IFP Energies Nouvelles

Academic context

[1] Martinez, S., Irimescu, A., Merola, S.S., Lacava, P. et al., “Flame Front Propagation in an Optical GDI Engine under Stoichiometric and Lean Burn Conditions,” Energies, 2017, 10(9):1337, https://doi.org/10.3390/en10091337.

[2] Tornatore, C., Bozza, F., Bellis, V., de, Teodosio, L. et al., “Experimental and Numerical Study on the Influence of Cooled EGR on Knock Tendency, Performance and Emissions of a Downsized Spark-Ignition Engine,” Energy 172:968–976, 2019, https://doi.org/10.1016/j.energy.2019.02.031.

[3] Cordier, M., Laget, O., Duffour, F., Gautrot, X. et al., "Increasing Modern Spark Ignition Engine Efficiency: A Comprehension Study of High CR and Atkinson Cycle," SAE Technical Paper 2016-01-2172, 2016, https://doi.org/10.4271/2016-01-2172.

First name: Giovanni **LAST NAME**: CECERE

Topic: Hydrogen efficient use in small size spark ignition engine

Course year: 3rd **Tutor(s)**: Federico MILLO, Luciano ROLANDO

Highlights of the research activity

Within the above topic framework, the research activity mainly focused on the characterization of the hydrogen combustion through the use of optical investigation techniques. A single cylinder engine was used for this purpose and experimental test campaigns with CH_4 – H_2 blends (H_2 volumetric concentration 20 - 50%, λ 1.0 – 1.3) and solely H_2 (λ 1.9 – 3.0) were planned. The data obtained from natural flame emissions were exploited for the analysis of main morphological aspects as well as a the study of the radical species emissions by performing a spectroscopic analysis. The first objective of the activity was to examine the main phenomena governing the development of the flame front from the start and how they relate to cycle-to-cycle performance, the spectroscopic for the detection of flame and radical emissions directly relating it to the air-fuel ratio (AFR). As far as the blended conditions, once fixed the spark timing the results showed the beneficial influence of hydrogen additon to methane, with the COV - IMEP that dropped to less than half respect to the solely methane case, i.e. 1.6 to 0.6%, while keeping the IMEP on comparable values to the baseline (CH_4), i.e. from 6.9 to 6.6 bar. Diffferently, the ignition trigger played an opposite role as it quickly led to an increase of the maximum pressure rise rate (MPRR). The optical analysis revealed that since its inception, the cases with the highest content of hydrogen resulted in a narrower area of spark arc dislocation. The reduced arc dispersion and the repeatability of the flame front propagation revealed the stabilising role of hydrogen during the entire combustion process. The luminous analysis carried out on the natural flame emissions showed how the increased velocity of the flame front makes the latter poorly influenced by transition phenomena due to turbulent motions, suggesting a partial detachment of hydrogen from the need for sophisticated turbulent – based strategies (a large number of investigations are planned to verify above statement). As far the spectroscopic investigation, the use of H_2-air mixtures leads to the analysis of the OH, NH and atomic H_2 emissions, which can be well resolved after 400 μs after the ignition trigger. The outcomes draw from this study revealed the suitability of using OH and NH intensities to correlate with the equivalent ratio, more importantly the diatomic molecule of Hydrogen resulted a viable option. The latter consists of a valuable option to detach this kind of analysis form the need of more sophisticated devices as its emissions fall within the visible spectra.

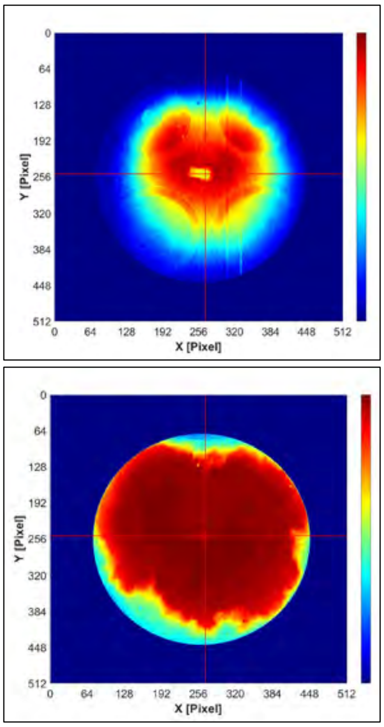


Figure 1. Colored flame front intensity: Methane (top) and H_2 – CH_4 (bottom), 16.8 CAD aST, λ 1.0.

External collaborations

- CNR - Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili (STEMS), Napoli (IT).

Academic context

[1] Merola, S.S., Irimescu, A., Cecere, G. (2025). 0D/1D Modeling of Lean-Burn Conditions in a Hydrogen SI Engine for Closer Correlation of In-Cylinder Chemical Species with Optical Data. In: Chiru, A., Covaciu, D. (eds) CONAT 2024 International Congress of Automotive and Transport Engineering. CONAT 2024. Proceedings in Automotive Engineering. Springer, Cham. https://doi.org/10.1007/978-3-031-77627-4_1

First name: Panagiotis **LAST NAME**: GALLIS

Topic: Unsteady numerical simulations of the interactions between the pressure-gain combustors & high-pressure turbines

Course year: 3rd **Tutor(s)**: Daniela Anna MISUL, Simone SALVADORI

Highlights of the research activity

Under the prism of introducing more efficient propulsion systems, Pressure Gain Combustion (PGC) cycles came under the spotlight of the research community. PGC cycles exploit either detonative or isochoric deflagrative combustion mode to augment the total pressure and temperature along the combustion process. In contrast to the conventional quasi iso-baric burners, PGC increase the stagnation quantities of the medium leading to higher theoretical thermal efficiency. Nonetheless, the alternative combustion mode results in unsteady outflow. Thus, it is necessary to investigate how this unsteadiness affects the subsequent turbine performance when integrating PGC into gas turbines.

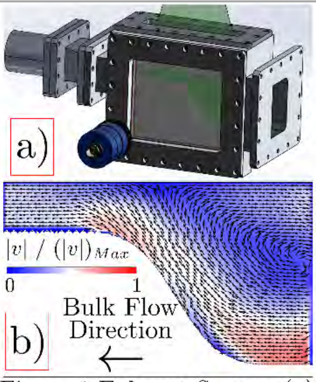


Figure 1 Exhaust System (a) & PIV Flow Field (b)

During the last year of the research activity, the doctoral student focused on the Constant-Volume Combustor (CVC). A 1D numerical analysis of the test rig, 3D CFD simulation of the existing exhaust system and the new exhaust system had been conducted during the 1st and 2nd year. In fact, the new conceptual exhaust system of CVC consists of a rectangular plenum, a transition duct to damp the total pressure fluctuations and a High-Pressure Turbine (HPT) vane. The transition duct was manufactured and tested under inactive and reactive conditions of the CVC. The HPT vane was replaced by a circular converging-diverging nozzle for reasons of simplicity. The experimental apparatus included fast response pressure measurements sensor upstream and downstream of the transition duct. In addition, two windows were placed in the lateral and upper side of the duct allowing for the laser penetration and the visual inspection of this component. Thus, Particle Velocimetry Image (PIV) analysis of high frequency (1 kHz) was conducted for the unsteady flow field of the transition duct.

In Fig.1 a), the configuration of the PIV system is portrayed, while in Fig.1 b) a Phased-Locked Averaging PIV velocity flow field is shown. When, the exhaust valves were open a strong vortex was generated. At the outlet, it is evident that the vortex was effectively suppressed from the transition duct. In particular, the transition piece was able to subtract the spatio-temporal variation of the velocity unsteadiness produced by the CVC for every moment of the cycle. A parametric analysis of the cycle frequency (15-40 Hz) offered valuable remarks for the periodic operation of this unconventional combustor with the new exhaust system. In conclusion, it was portrayed and investigated in details for the first time the pulsating exhaust flow field of the CVC paving the way for the future integration of such machine with a HPT stage.

External collaborations

- PPrime Institute, ENSMA, Poitiers, France
- University of Purdue, West Lafayette, U.S.A.
- Technical University of Berlin, Berlin, Germany

Academic context

[1] Gallis, P., Misul, D. A., Boust, B., Bellenoue, M., & Salvadori, S. (2024). Development of 1D Model of Constant-Volume Combustor and Numerical Analysis of the Exhaust Nozzle. *Energies*, *17*(5), 1191.

[2] Gallis, P., Misul, D. A., Boust, B., Bellenoue, M., & Salvadori, S. (2025). Numerical Analysis and Design of New Exhaust Section Downstream of Constant Volume Combustor. *Journal of Engineering for Gas Turbines and Power*, *147*(2).

[3] Gallis, P., Salvadori, S., & Misul, D. A. (2024, June). Numerical Analysis of a Flow Control System for High-Pressure Turbine Vanes Subject to Highly Oscillating Inflow Conditions. In *Turbo Expo: Power for Land, Sea, and Air* (Vol. 87974, p. V005T06A021). American Society of Mechanical Engineers.

First name: Simona **LAST NAME**: GURRI’

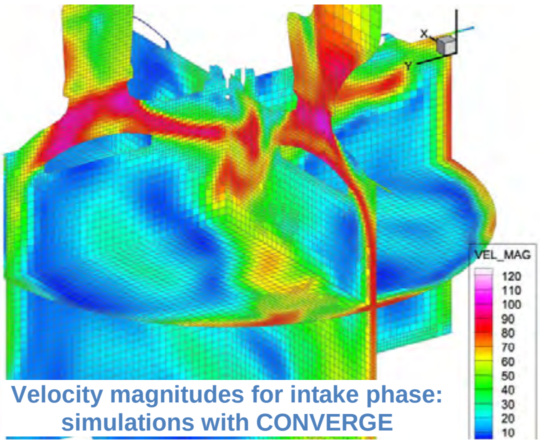
Topic: Synergies of Bimodal Freight Electric Train (F-EMU) and Advanced ICE Technologies for Sustainable Intermodal Freight Transport

Course year: 3rd **Tutor(s)**: Alessandro FERRARI, Bruno DALLA CHIARA

Highlights of the research activity

The imperative for sustainability in freight transportation continues to grow, driven by policy frameworks like the European Green Deal and Fit for 55, notwithstanding the need to reconcile these objectives with other *declinations of sustainability*, the economic and social as well as the technical and market demand response, and to complete the reasoning on the *overall energy chain* and *life cycle in transport systems*.

My research in 2024 has been focused on advancing sustainable freight solutions by bridging academic inquiry with industry practices, pursuing EU objectives. Key achievements include:



Velocity magnitudes for intake phase: simulations with CONVERGE

- **Systematic Literature Review on Mass Quantity Injection Systems**: this review provided critical insights into the adaptation of ICEs for alternative fuels, guiding future simulation and modelling efforts.
- **A DES model** using ARENA software evaluated the F-EMU's performance in **intermodal transport** versus all-road solutions, showing its superior efficiency and environmental benefits in terms of flow time, WTW energy consumption, and GHG emissions.
- **3D CFD Analysis of Alternative-Fuel ICEs**: advanced 3D CFD simulations were employed to model the combustion in heavy-duty spark ignition engines. These used RANS k-ε turbulence models for optimising air-fuel mixing and combustion efficiency. Data derived from 3D simulations are supporting the refinement of a 1D turbulence model for more computationally efficient predictive models, to be used for the FEMU powertrain.
- **RAMS for FEMU Monitoring System**: In collaboration with Alstom Ferroviaria, I finalized the design of an Integrated Monitoring System for FEMU. This system, validated in Simulink, enhances RAMS (Reliability, Availability, Maintainability, Safety) for the train by integrating diagnostics and control features.
- **An LCA of propulsion technologies for trains,** in collaboration with Alstom Ecodesign, found that alternative-fuel ICEs offer the best balance of environmental and economic performance, while H_2 fuel cells have higher lifecycle impacts due to resource use in production, supporting the adoption of alternative-fuels ICEs for FEMUs in non-electrified scenarios**.**

These achievements, supported by industrial collaborations and disseminated through publications, including conferences, have contributed to the development of sustainable, efficient freight transportation systems. My research advances the integration of alternative propulsion technologies, optimised transport operations, and environmental assessments, aligning with the broader goal of decarbonising inland freight transport.

External collaborations

- Alstom Ferroviaria S.p.A.; FPT Industrial; Blue Engineering

Academic context

[1] Gandini, L.M., Ricci, S., Verrascina, F. (2023). *Hydrogen-powered trains operation. Normative constraints and assessment on a case study.* Ingegneria Ferroviaria. doi: 10.57597/IF.10.2023.ART.1
[2] Gurri’, S., Bocchieri, M., Galasso, D., Operti V., Dalla Chiara B. (2023). *Assessing the speed of an electric multiple-unit freight train on high-speed lines.* INGEGNERIA FERROVIARIA. doi: 10.57597/IF.05.2023.ART.1
[3] Dulbecco, A., Richard, S., Laget, O., and Aubret, P. (2016). *Development of a Quasi-Dimensional K-k Turbulence Model for Direct Injection Spark Ignition (DISI) Engines Based on the Formal Reduction of a 3D CFD Approach.* SAE Technical Paper 2016-01-2229, doi: 10.4271/2016-01-2229

First name: Lorenzo **LAST NAME**: LAVENEZIANA

Topic: Clean energy transition of airport energy systems

Course year: 3rd **Tutor(s)**: David CHIARAMONTI, Matteo PRUSSI

Highlights of the research activity

The objective of my research is to analyse and model the energy system of Torino Airport, developing a long-term decarbonisation strategy aligned with ambitious environmental goals. In the third year of my PhD, I conducted a techno-economic assessment of three alternative pathways: one based solely on renewable generation and electrification; another integrating multiple energy vectors, such as biomethane and locally produced hydrogen for tri-generation; and a third combining on-site production with green hydrogen supply from a nearby hydrogen valley. These pathways were compared using a set of technical and economic indicators, some of which are shown in the figure below.

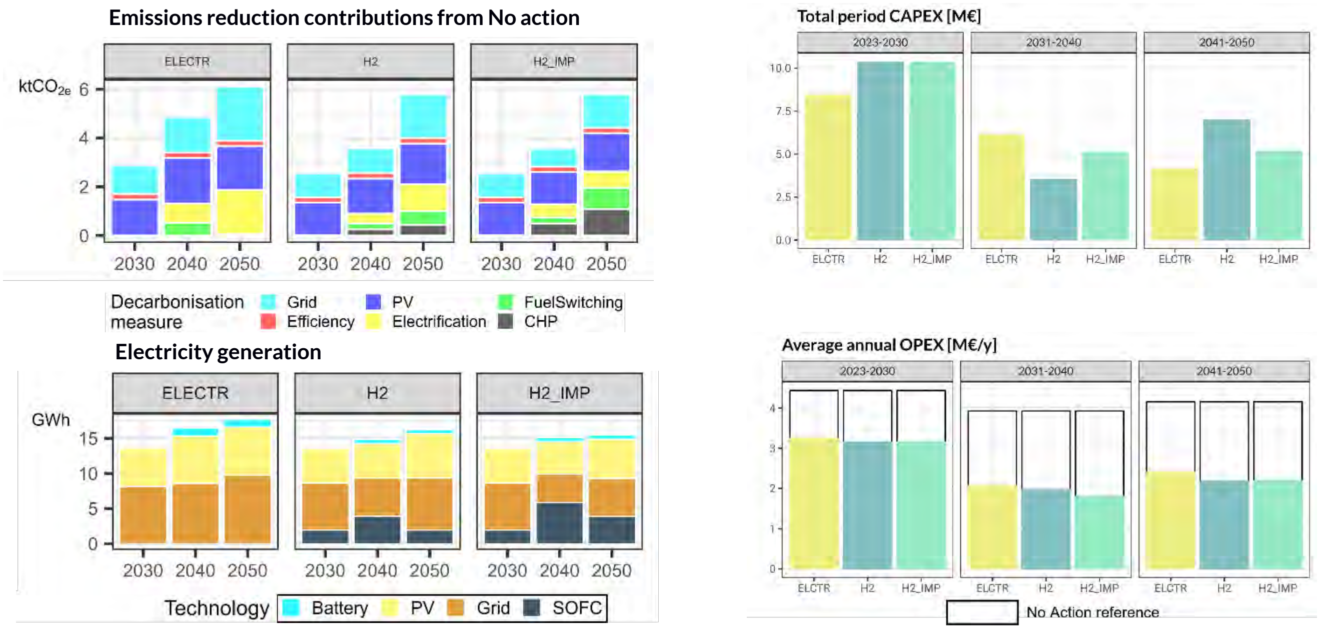


Figure 1 – Techno-economic performance indicators of the three development pathways examined. ELECTR: sole electrification; H2: multiple energy vectors; H2_IMP: hydrogen supply.

The comparison of the scenarios highlighted both similarities and differences between the technological strategies. All pathways rely on significant on-site renewable capacity and storage (via batteries or electrolysis), reducing OPEX compared to a no-action scenario where all energy is externally sourced. However, once the on-site renewable potential is saturated, access to external green energy vectors—grid electricity, biomethane, or green hydrogen—becomes crucial for the energy transition.

External collaborations

- Sustainable, Smart and Safe Mobility Unit, Joint Research Centre, JRC, Ispra

Academic context

[1] S. Ortega Alba and M. Manana, *“Characterization and analysis of energy demand patterns in airports,”* Energies, vol. 10, no. 1, Jan. 2017.

[2] M. Welsch, et al., *“Modelling elements of Smart Grids - Enhancing the OSeMOSYS (Open Source Energy Modelling System) code,”* Energy, vol. 46, no. 1, pp. 337–350, 2012.

First name: Chiara **LAST NAME**: MONZANI

Topic: Decarbonization of district heating systems

Course year: 3rd **Tutor(s)**: Alberto POGGIO

Highlights of the research activity

As part of PhD research, a novel simulation tool has been developed to model district heating systems (DHSs). The tool enables simultaneous simulation of heat generation and user demand, facilitating the analysis of decarbonization scenarios by integrating diverse user-profiles and generation operating conditions. User thermal demand is defined using different methodologies tailored to the specific case study and available data types. For existing DHSs, historical operating data can be utilized as a subset of connected users. By leveraging the XGBoost machine learning algorithm, the tool can estimate hourly thermal demand crucial to evaluate: (i) actual thermal demand (ii) network extension and (iii) variations in demand due to energy efficiency interventions in buildings. A comprehensive case study on the Turin DHS, which includes hourly data from approximately 200 heat exchange substations over nine heating seasons, evaluates the comparative effectiveness of various forecasting approaches regarding prediction accuracy and computational efficiency. The findings provide valuable insights to guide DHS operators and planners in selecting the most appropriate forecasting approach based on input data availability, accuracy requirements, and computational constraints, thereby supporting efficient DHS strategic planning and development. The model estimates hourly thermal demand using climatic conditions (hourly outdoor temperature), calendar factors (day type), building construction characteristics (heated volume, construction period, loss coefficient), and substation thermal capacity data. Data can be entered at the individual building level or the average of the served building stock. The estimation can, therefore, be carried out at the level of the individual building (approach S) by aggregating the load curves of the individual buildings (approach A) or by directly obtaining the aggregated curve known from the average data of the served building stock (approach W). The model demonstrates robust performance for approaches A and W, with Approach W emerging as the most advantageous due to its lower data requirements and reduced execution time. Under Approach W, relative percentage errors of less than 20% are achieved in 70% of simulated hours, and the model demonstrates an R^2 value of 0.95 when comparing estimated versus actual daily thermal consumption.

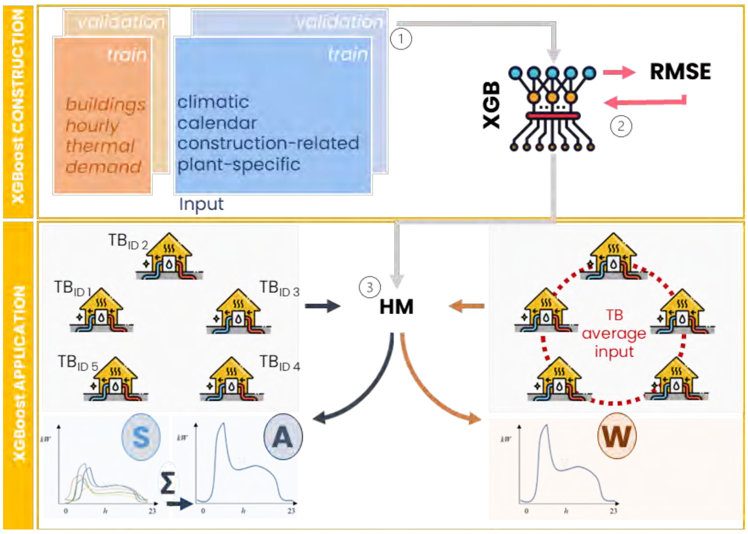


Fig. 1

External collaborations

- IREN Spa

Academic context

[1] C. Monzani, G. Cerino Abdin, A. Poggio and G. Montanari, Modelling Hourly Thermal Energy Demand: A Machine Learning Approach of Residential District Heating Substations in Turin, Renewable Energies and Power Quality (ICREPQ'24), vol. 22, 2024
[2] XGBoost Python Package https://xgboost.readthedocs.io/en/stable/python/
[3] K. B. Debnath, M. Mourshed, Forecasting methods in energy planning models, Renewable and Sustainable Energy Reviews (2018), Vol. 88, pp. 297-325

First name: Rosario **LAST NAME**: NASTASI

Topic: Green - Tecnologie innovative per la gestione termica e soluzioni per una aviazione pulita

Course year: 3rd **Tutor(s)**: Daniela Anna MISUL, Simone SALVADORI

Highlights of the research activity

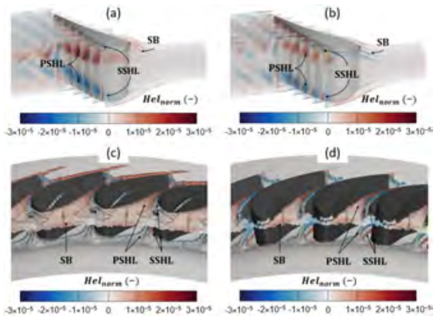


Figure 1. secondary flows: (a) baseline, (b) optimized, (c) baseline design flow structures, and (d) optimized design flow structures

One of the main topics of the research activity is to find a robust and reliable numerical approach for studying complex physical phenomena occurring in cooling applications for High-Pressure Turbines (HPT). In this context, film cooling is characterized by a complex mechanism of mixing, which is difficult to simulate accurately using conventional RANS-based methods. To overcome this problem, high-fidelity numerical approaches such as Stress-Blended Eddy simulations (SBES), and Scale-Adaptive Simulations (SAS) are considered during the analysis of a discrete film cooling hole which operates at realistic conditions. The results demonstrated that these approaches effectively capture turbulent phenomena at various length scales, including coolant mixing with hot gases and flow separation. As a result, the cooling coverage was characterized more accurately than by conventional RANS methods. Another important research topic is the development of optimization strategies that utilize machine learning techniques for the shape optimization of HPT components. The test case considered is a diffusive high-pressure turbine vane designed to ingest a high-subsonic flow from a Rotating Detonation Combustor. The airfoil and the diffusive endwalls were parameterized using splines and control points, and then deformed to explore new geometrical configurations. Shape optimization was performed using stator aerodynamic efficiency, inlet Mach number, and exit flow angle as objective functions. The geometrical parameters were varied within a predefined design space using Latin Hypercube sampling to create a Design of Experiment (DOE), which was then used to train machine learning models. Among various models, Artificial Neural Networks (ANN) and Random Forest (RF) were selected for their efficiency in regression tasks. The dataset was first simulated using RANS CFD and then splitted into training, validation, and test sets for performance evaluation. Hyperparameters were optimized using a random search approach to maximize the R^2 coefficient on the test set, with cross-validation assessing train-test split impacts. Results showed the ANN model outperformed RF, achieving $R^2 \approx 0.98$-0.99 compared to 0.89 for RF. The models were then coupled with a genetic algorithm to identify the optimal solution, which reduced secondary flow intensity and improved the stator efficiency. The current objective of the research activity is to combine the advantage of machine learning models and gradient-based approaches (Adjoint method) to find new design practices for internal blade cooling channels. Convection cooling in HPT blades still represent the most used cooling technology and thus require further studies aimed at optimizing heat exchange to reduce the metal temperature and enhance the cooling efficiency of the component.

External collaborations

- Avio Aero

Academic context

[1] Nastasi, R.; Rosafio, N.; Salvadori, S.; Misul, D.A. Evaluation of Film Cooling Adiabatic Effectiveness and Net Heat Flux Reduction on a Flat Plate Using Scale-Adaptive Simulation and Stress-Blended Eddy Simulation Approaches. https://doi.org/10.3390/en17112782

[2] Nastasi, R.; Labrini, G.; Salvadori, S.; Misul, D.A. Shape Optimization of a Diffusive High-Pressure Turbine Vane Using Machine Learning Tools. https://doi.org/10.3390/en17225642

[3] He, Ping & Mader, Charles & Martins, Joaquim & Maki, Kevin. (2018). Aerothermal Optimization of Internal Cooling Passages Using a Discrete Adjoint Method. 10.2514/6.2018-4080.

First name: Francesco **LAST NAME**: PUCILLO

Topic: H2-HD: Hydrogen as a fuel for internal combustion engines for heavy-duty applications

Course year: 3rd **Tutor(s)**: Federico MILLO, Andrea PIANO,

Highlights of the research activity

The need to move towards a decarbonized transport sector has led to the search for different technological solutions: hydrogen, used as fuel in internal combustion engines (ICEs), is gaining momentum due to its combustion properties, which are characterized by near-zero harmful emissions and high flame speed. However, particularly for direct injection applications, additional calibration efforts are required to optimize the mixture preparation and combustion processes. In this context, the research activity, sponsored by FPT Industrial, focuses on evaluating, through numerical simulation, the potential of hydrogen as a fuel for internal combustion engines in heavy-duty applications. A comprehensive optimization of critical components and operating parameters is carried out to achieve torque, power, efficiency, and emissions targets.

Thanks to the analysis of a wide experimental dataset, a detailed characterization of hydrogen combustion peculiarities has highlighted the decisive influence of mixture formation on performance, combustion stability, and NO_X emissions.

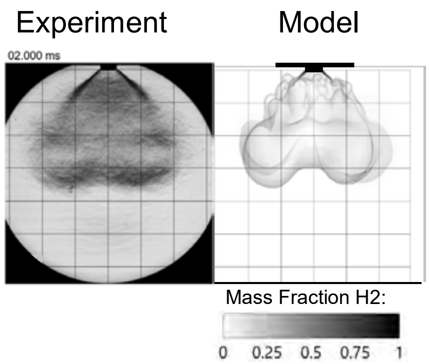


Figure 1: *Hydrogen jet validation. Comparison between experiment and simulation.*

This year, mixture formation was investigated through 3D-CFD numerical simulation. First, the hydrogen jet was validated in a constant volume vessel (CVV) against experimental measurements obtained through the Schlieren technique. A simplified methodology, which exploits synergies with 1D-CFD simulations, has been validated to limit the computational effort required for the simulation of hydrogen injection. Subsequently, the analysis focused on the mixing process in the engine setup, to evaluate mixture stratification under different operating conditions. The outcomes have been employed for the development of a 1D-CFD predictive combustion model (SITurb). Furthermore, the analysis of the abnormal combustion phenomena (knock, pre-ignition, misfire) and cyclic combustion variability will enhance the predictiveness of the 1D model, providing further insight into the main limitations of hydrogen combustion in internal combustion engines.

External collaborations

- FPT Industrial S.p.A.
- Garrett Motion Inc.
- Robert Bosch GmbH

Academic context

[1] Millo, F., Piano, A., Rolando, L., Accurso, F. et al., "Synergetic Application of Zero-, One-, and Three-Dimensional Computational Fluid Dynamics Approaches for Hydrogen-Fuelled Spark Ignition Engine Simulation," SAE Int. J. Engines 15(4):561-580, 2022, https://doi.org/10.4271/03-15-04-0030.
[2] Golisano, R., Scalabrini, S., Arpaia, A., Pesce, F., et al. “PUNCH Hydrogen Internal Combustion Engine & KERS: An Appealing Value-Proposition for Green Power Pack,” presented at Vienna Motor Symposium 2021, April 29-30, 2021.
[3] Rezaei, R., Kovacs, D., Hayduk, C., Mennig, M. et al., “Euro VII and Beyond with Hydrogen Combustion for Commercial Vehicle Applications: From Concept to Series Development,” SAE Int. J. Advances & Curr. Prac. in Mobility 4(2):559-569, 2022, doi:10.4271/2021-01-1196

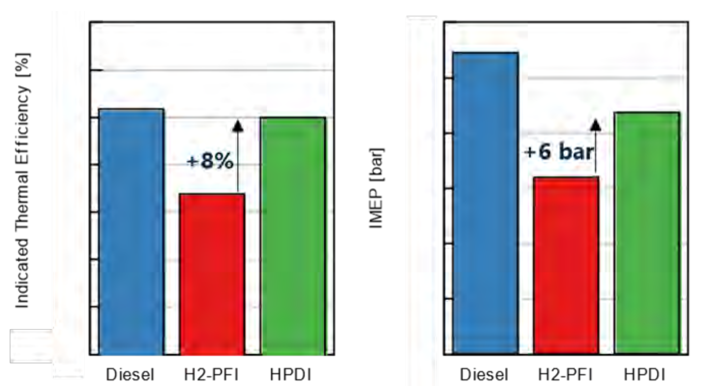
First name: Gianpaolo LAST NAME: QUATTRONE

Topic: Optimization of H2 fuelled ICE from Fuel Injection to Exhaust Aftertreatment

Course year: 3rd Tutor(s): Federico MILLO, Andrea PIANO

Highlights of the research activity

The main scope of the research activity, carried out in collaboration with DUMAREY Torino, Westport Fuel Systems and Cornaglia Group, is to investigate the potential benefits of the usage of hydrogen in Internal Combustion Engines, considering Port Fuel Injection (PFI) [1] and High-Pressure Direct Injection (HPDI) [2] technologies. The H2-HPDI, patented by Westport Fuel Systems, is an innovative combustion system characterized by the hydrogen direct injection into the combustion chamber near to the top dead center of firing. A Diesel pilot is injected just before the gas injection and acts as ignition source. This combustion systems eliminates the risk of knock and pre-ignition, allowing high compression ratios and thermal efficiencies. Its potentialities have been demonstrated in heavy-duty (HD) applications [3]. However, its effectiveness in light-duty (LD) engines remains unexplored in the existing literature. For these reasons, this research aims to assess the H2-HPDI technology for LD applications, and to directly compare the H2-PFI and H2-HPDI technologies. To this end, a 3D-CFD predictive combustion model was developed and validated against the experimental data coming from a HD HPDI application. The simulations, encompassing both hydrogen and compressed natural gas scenarios, showcased strong predictive accuracy across varying engine speeds and loads. This approach facilitated a detailed analysis of H2-HPDI combustion phenomena, enabling the identification of the key combustion phases. Subsequently, the 3D-CFD combustion model was adapted to explore the potential of HPDI technology for LD engines. Results indicate that the light-duty HPDI engine concept exhibits significant promise, achieving indicated efficiency comparable to the baseline heavy-duty configuration and demonstrating, at peak torque, an 8% improvement in indicated efficiency over the H2-PFI application on a similar 0.5L engine.



Diesel, H2-PFI and H2-HPDI technologies: Indicated Efficiency and IMEP comparison.

External collaborations

- DUMAREY Torino
- Westport Fuel Systems
- Cornaglia Group

Academic context

[1] Millo F., Piano A., et al., “Synergetic Application of Zero-, One-, and Three-Dimensional Computational Fluid Dynamics Approaches for Hydrogen-Fuelled Spark Ignition Engine Simulation”, SAE International Journal of Engines, DOI:10.4271/03-15-04-0030

[2] Munshi S., Huang J. et al., “The Potential for a High Efficiency Hydrogen Engine Using Westport Fuel Systems Commercially Available HPDI Fuel System”, Vienna Motor Simposium, 2021

[3] D. Mumford, S. Baker, et al., “Application of Westport’s H2 HPDITM Fuel System to a Demonstration Truck”, Vienna Motor Simposium, 2023

First name: Andrea **LAST NAME**: SCALAMBRO

Topic: H2GT - Hydrogen as a ICE fuel for Ground Transportation

Course year: 3rd **Tutor(s)**: Federico MILLO, Andrea PIANO

Highlights of the research activity

Among the different hydrogen premixed combustion system concepts, direct injection (DI) seems to be one of the most promising since it minimizes the volumetric efficiency reduction induced by the gaseous injection and decreases the risks of abnormal combustions (i.e., backfire). Nonetheless, to fully exploit the benefits of this technical solution, the optimization of the mixture preparation process is of paramount importance. Indeed, a highly homogeneous mixture allows the reduction of NOx emissions and decreases the risk of knocking combustion phenomena at the same time.

Within this framework, my research activity was focused on the study and optimization of the mixture formation process in a DI H2-ICE, retrofitted from a diesel ICE, through 3D-CFD simulations. In the numerical environment, a sweep of injection timing was initially performed to find the optimal timing, i.e. the one that allows to achieve the highest mixture uniformity, with a negligible reduction of the volumetric efficiency. Then, several injector spray caps (i.e. small chambers positioned downstream of the injector valve) were designed and tested. They proved to be able of providing to the injected gas the desired direction and enhance hydrogen distribution. Successively, swirl intensity was varied, by acting on the intake valve seat eccentricity. Five levels of swirl ratios were tested. Among them, the configuration that led to an almost nil swirl motion proved to be the one capable of maximizing mixture homogeneity. Afterward, an engine prototype was built according to the main outcomes of the numerical analysis and tested at the dynamic test bench. The engine successfully met the performance targets, i.e., the same full load curve of the original diesel engine (max. load 16 bar BMEP), with a maximum indicated thermal efficiency (ITE) comparable to the diesel one (ITE~40.5%). Lastly, also a 3D-CFD flamelet-based combustion model, i.e., relying on tabulated flame speed maps, was developed and validated against experimental data gathered from the engine prototype. First, standard laminar flame speed maps were adopted. Nevertheless, the recalibration of the combustion model parameters was required when changing the operating air-to-fuel ratio. Hence, a second set of flame speed maps was developed, considering thermo-diffusive instabilities that characterize hydrogen flames in lean environments. This approach allowed to improve the correlation between experimental data and numerical simulations keeping fixed combustion model parameters.

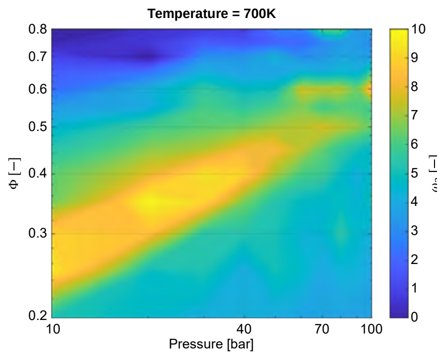


Figure 1. Instability parameter ω_2 at 700K as a function of pressure and equivalence ratio (Φ)

External collaborations

- FEV Italy/Europe
- CNR STEMS
- GammaTech Engineering

Academic context

[1] White, C. M., Steeper, R. R., and Lutz, A. E., "The hydrogen-fueled internal combustion engine: a technical review," International Journal of Hydrogen Energy 31.10 (2006): 1292-1305.

[2] Addepalli, S. K., Pei, Y., Zhang, Y., and Scarcelli, R., "Multi-dimensional modeling of mixture preparation in a direct injection engine fueled with gaseous hydrogen," International Journal of Hydrogen Energy 47.67 (2022): 29085-29101

[3] Howarth, T., Hunt, E., Aspden, A., "Thermodiffusively-unstable lean premixed hydrogen flames: Phenomenology, empirical modelling, and thermal leading points," Combustion and Flame 253 (2023): 112811

First name: Afanasie **LAST NAME**: VINOGRADOV

Topic: A Comprehensive Methodology for the Development of Electrified Powertrain Solutions for off-road Applications

Course year: 3rd **Tutors**: Federico MILLO, Luciano ROLANDO

Highlights of the research activity

In the last decades, the automotive industry proved the benefits of powertrain electrification and fostered its adoption in other fields such as Non-Road Mobile Machinery (NRMM). Nevertheless, in this sector, the impact of the hybridization may be significantly different according to the wide range of specific application.

The first activities of the the first PhD year focused on investigating the performance of a hybrid powertrainfeaturing a 56 kW engine coupled with a 16 kW electric motor and aiming to minimize fuel consumption and emissions. During the second year, exploration of different architectures was performed for a Skid Steer Loader (SSL) application. Using several Dynamic Programming (DP) optimizations, the study pointed out the maximum fuel economy potential of different powertrain layout, providing, at the same time, relevant information to design implementable and suboptimal control strategies. The third year focused on the integration of a specific parallel hybrid powertrain to the skid steer loader. The industrial partner installed the hybrid unit on an SSL prototype, and it performed an extensive experimental campaign to collected duty cycles under specific working conditions. These acquisitions played a key role for evaluating the hybrid potential using the DP framework and for testing real time capable Energy Management Strategies (EMS). Among real time approaches two EMSs were analyzed: a rule based (RB) which nowadays represent the standard for this kind of application and a more advanced Reinforcement Learning approach. The Rule Based was developed by exploiting insights from the powertrain characteristic with guidance from DP analysis. Meanwhile RL was chosen for its ability to learn by directly interacting with the environment, presenting itself as possible flexible solution to adapt to different duty cycles and applications. In the initial phase of the activity, a Deep Q-Learning (DQL) agent was chosen for its simplicity and for its extensive use in the literature, allowing for straightforward workflow development and environment testing. Given the continuous nature of the action space, a Soft-Actor-Critic (SAC), a state-of-the-art agent, was also tested. SAC and RB strategies, demonstrated near optimality capability, compared to DP, suggesting that once given a priority to the ICE, the powertrain may present a low sensitivity to the EMS for the given case study. SAC and RB provided similar results in terms of fuel consumption; however, the RL-SAC was able to adapt better to the periodicity of the duty cycle, typical of the skid steer, ensuring more consistent battery usage.

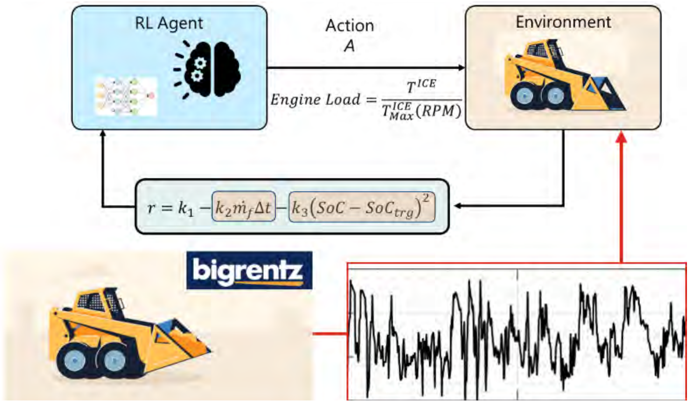


Figure 1 Reinforcement Learning based energy management for a hybrid Non-Road Mobile Machinery

External collaborations

- Lombardini - Kohler Engines

Academic context

[1] *Un-Noor, F.; Wu, G.; Perugu, H.; Collier, S.; Yoon, S.; Barth, M.; Boriboonsomsin, K.* Off-Road Construction and Agricultural Equipment Electrification: Review, Challenges, and Opportunities. *Vehicles 2022, 4, 780-807. https://doi.org/10.3390/vehicles4030044*

[2] *A. Bertini, M. Ceraolo, G. Lutzemberger*, Systematic approach in the hybridization of a hydraulic skid loader, *Automation in Construction*, *2015, https://doi.org/10.1016/j.autcon.2015.07.013*

[3] *Luigi Tresca, Luca Pulvirenti, Luciano Rolando, Federico Millo,* Development of a deep Q-learning energy management system for a hybrid electric vehicle, *Transportation Engineering, 2024, https://doi.org/10.1016/j.treng.2024.100241*

First name: Filippo**LAST NAME**: AGLIETTI

Topic: Physics informed neural networks

Course year: 2nd **Tutor(s)**: 1st Federico MILLO, 2nd Andrea PIANO, 3rd Francesco DELLA SANTA

Highlights of the research activity

During the second year of my PhD, I focused on integrating prior physics knowhow into Machine Learning models to improve the accuracy and generalization of emission predictions in Diesel engines. Traditional data-driven models often struggle with limited data, especially in complex nonlinear problems. By incorporating physics-informed constraints, it is possible to develop robust models requiring less training data, streamlining virtual engine calibration processes and reducing costs.

A new deep learning model, GradINN (Gradient Informed Neural Network), was developed to introduce a general prior belief on the gradients of the target function during training. Since many physical problems exhibit inherently smooth behaviors and continuity, the focus was placed on encoding smooth prior beliefs into the auxiliary network. This approach demonstrated improved accuracy and stability in both synthetic functions and real-world datasets from diverse engineering domains (from the UCI repository) particularly in scenarios with limited training data.

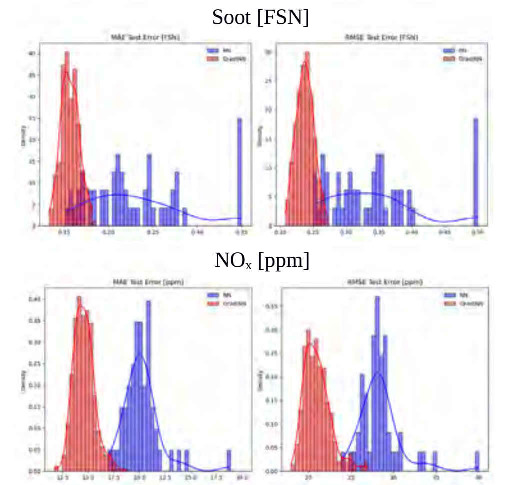


Fig.1 Errors Distribution of GradINN and NN for each tested hyperparamiter ccombination

GradINN was then applied to diesel emission prediction using a dataset derived from 12 Design of Experiments (DoEs), originally developed in past experimental campaigns. Each DoE corresponded to a fixed combination of engine speed (RPM) and load (BMEP), resulting in 12 unique RPM × BMEP pairs. For each combination, approximately 100 measurements were collected, representing distinct sets of engine control variables such as Boost, Rail Pressure, and the Start of Injection (SOI) for the main injection. It is important to note that the experimental campaign was not specifically designed to optimize the distribution of points or operational conditions for modeling purposes, as the data was collected in the context of previous activities. The dataset was split into two subsets: 50% allocated for training and validation, and the remaining 50% reserved for testing. This division ensured an unbiased evaluation of model performance on unseen data. The performance of the models was assessed using two metrics: Root Mean Square Error (RMSE) and Mean Absolute Error (MAE). A DoE was conducted to evaluate the performance of GradINN and standard NN (s-NN) across a wide range of hyperparameter configurations, including variations in the number of neurons, number of hidden layers, activation functions, and batch sizes. Figure 1 illustrates the distribution of RMSE and MAE values for both the NOx and Soot models across all tested hyperparameter combinations. The results show that GradINN generally achieved lower errors compared to s-NN, indicating superior performance of GradINN across a wide range of configurations. For NOx emissions, GradINN achieved a 26% lower RMSE in the best configuration (17.8 ppm vs. 24.1 ppm for standard NN). Similarly, for Soot emissions, GradINN reduced RMSE by 20% (0.20 vs. 0.25). Additionally, GradINN demonstrated greater robustness, as indicated by narrower error distributions and reduced sensitivity to hyperparameter variations, making it a reliable choice for this application.

External collaborations

- Dumarey Automotive Italia S.p.A.

Academic context

[1] Czarnecki, W. M., Osindero, S., Jaderberg, M., Swirszcz, G., and Pascanu, R. Sobolev training for neural networks. CoRR, abs/1706.04859, 2017. URL http://arxiv. org/abs/1706.04859.

First name: Salvatore **LAST NAME**: CARUSOTTO

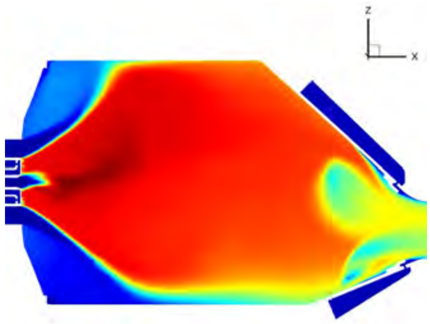
Topic: Fuel-flexible gas turbines for decarbonization

Course year: 2nd **Tutors**: Daniela Anna MISUL, Simone SALVADORI

Highlights of the research activity

Developing fuel-flexible combustion systems for gas turbines, especially those adopting hydrogen as a fuel in a premixed configuration, requires extensive studies regarding temperature distributions, emissions and stability. By continuing the activity started in the first year, 3D-CFD combustion models are now applied to a lean premixed case. To reduce the overall computational costs, a fluid-dynamic characterization of the pressure-swirl atomizer injector mounted on this machine has been investigated by using 1D/3D CFD simulations. The results of this analysis have been presented at ASME TurboExpo2024 in London.

The acquired information regarding the burner air split and the velocity, species concentrations and temperature profiles extracted from the injector simulation are used to couple the injector with the annular chamber under investigation. Furthermore, the complex simulation domain has been simplified to guarantee a reasonable computational cost. Just to cite some of the actions the application of a perforated wall model to simulate the presence of the effusion cooling for the liner has been applied, while the heat transfer coefficients for the dome cooling and for the ribbed liner walls were estimated from literature data.



Resulting temperature distribution for the annular combustion chamber under investigations – Base Load conditions, natural gas

A dedicated routine has been developed in MATLAB© to duplicate and translate the resulting profiles from the injector.

The obtained setup has been compared to some available performance tests for the base load conditions. The results are aligned in terms of temperature distributions, mass flow rates and emissions with the available data. For these reasons, it is hence possible to move on with the simulation of hydrogen blends for the studied configurations.

External collaborations

- Ethos Energy Italia S.p.A.
- Technische Universität Berlin - Institut für Strömungsmechanik und technische Akustik

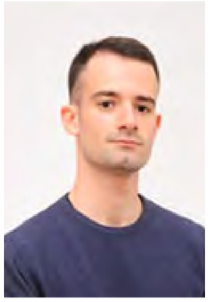
Academic context

[1] Carusotto, S, Salvadori, S, Cavalli, A, Casto, E, Cardile, F, & Misul, DA. "Characterization of a Premixed Gas Turbine Injector for Light-Duty and Low Emissions Applications." *Proceedings of the ASME Turbo Expo 2024: Turbomachinery Technical Conference and Exposition*. *Volume 3B: Combustion, Fuels, and Emissions*. London, United Kingdom. June 24–28, 2024. V03BT04A069. ASME.

[2] Carusotto, S., Labrini, G., Salvadori, S., Baratta, M., Cardile, F., Toppino, M., Valsania, M., and Misul, D. (October 26, 2023). "Evaluation of No_x Emissions Associated to Non-Premixed Combustion of H_2/Natural Gas Blends in a 40 MW Heavy-Duty Gas Turbine." ASME. *J. Eng. Gas Turbines Power*. December 2023; 145(12): 121020

[3] zur Nedden, PM, Eck, MEG, Lückoff, F, Panek, L, Orchini, A, & Paschereit, CO. "Flame Transfer Function and Emissions of a Piloted Single Jet Burner: Influence of Hydrogen Content." *Proceedings of the ASME Turbo Expo 2023: Turbomachinery Technical Conference and Exposition*. *Volume 3B: Combustion, Fuels, and Emissions*. Boston, Massachusetts, USA. June 26–30, 2023. V03BT04A017. ASME

First name: Trentalessandro **LAST NAME**: COSTANTINO

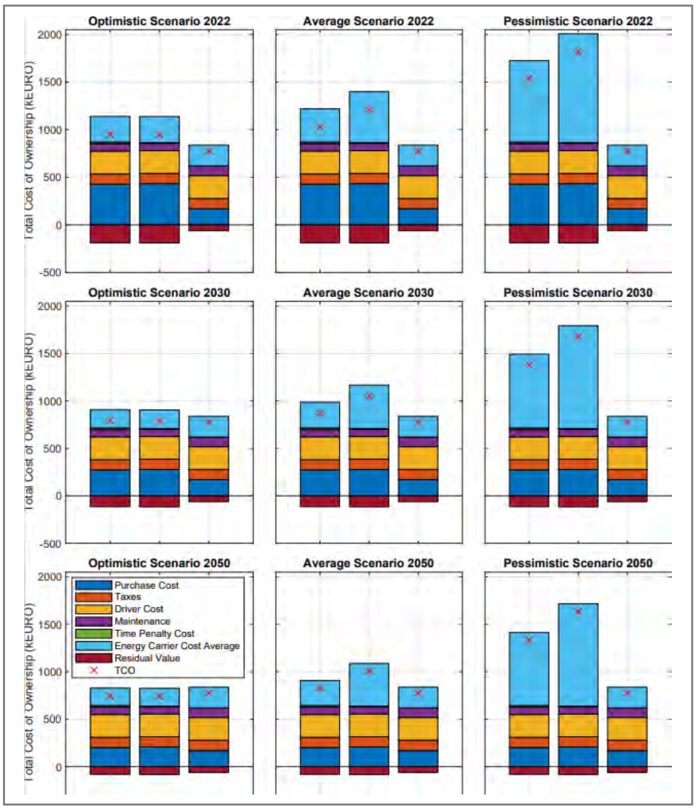


Topic: Sustainability assessment of advanced propulsion systems and fuel pathways for Commercial Vehicles

Course year: 2nd **Tutor(s)**: Ezio SPESSA, CHIARAMONTI, DOTELLI

Highlights of the research activity

In the second year of my research, I published a study on the environmental impact of recycling NdDyFeB permanent magnets using a hydrogen-decrepitation-based technique, demonstrating significant carbon footprint reductions (DOI: 10.3390/en17040908). I also presented my work on converting diesel engines to hydrogen-powered internal combustion engines at the SAE World Congress, emphasizing the potential for reducing greenhouse gas emissions. This research led to a journal publication showing that hydrogen engines, especially with green hydrogen, could reduce emissions by over 90% (DOI: 10.3390/en17112571).



Additionally, I conducted a techno-economic analysis of Dynamic Wireless Power Transfer (DWPT) systems in long-haul freight transport, comparing them with BEVs and diesel trucks. The results, published in *Applied Energy*, provide insights into the cost-effectiveness of DWPT from a fleet operator's perspective (DOI: 10.1016/j.apenergy.2024.124839).

Beyond research, I contributed to the Energy Management in Hybrid Electric Vehicles course, further developing my skills in powertrain simulation and controls. I also began working at IVECO, the company that co-funded my fellowship, customizing the techno-economic model to align with their specific needs. Currently, I am collaborating with IFP Energies Nouvelles to advance sustainability assessments and finalize research papers in partnership with industry stakeholders.

Through these activities, I have enhanced my technical expertise and contributed to innovative solutions for decarbonizing transport.

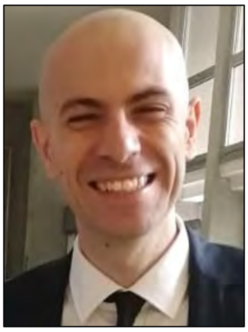
External collaborations

- IFP Energies Nouvelles

Academic context

[1] Burke et al, Projections of the costs of medium- and heavy-duty battery-electric and fuel cell vehicles (2020-2040) and related economic issues, https://doi.org/10.1016/j.esd.2023.101343.
[2] European Commission, Directorate-General for Climate Action, Hill, N., Amaral, S., Morgan-Price, S. et al., Determining the environmental impacts of conventional and alternatively fuelled vehicles through LCA – Final report, Publications Office of the European Union, 2020, https://data.europa.eu/doi/10.2834/91418
[3] Prussi, M., Yugo, M., De Prada, L., Padella, M. and Edwards, R., JEC Well-To-Wheels report v5, EUR 30284 EN, Publications Office of the European Union, Luxembourg, 2020, ISBN 978-92-76-20109-0, doi:10.2760/100379, JRC121213.

First name: Giuseppe **LAST NAME**: DI LUCA



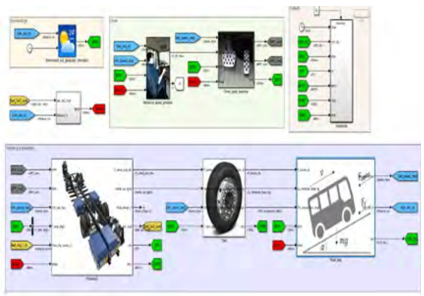
Topic: Advanced Battery Management System Solutions for a Smart and Connected Electrified Mobility

Course year: 2nd **Tutor(s)**: Daniela Anna MISUL, Ezio SPESSA

Highlights of the research activity

The research conducted during the reference period has been focused on Battery Electric Buses (BEBs). An extensive literature review was carried out highlighting their benefits and challenges. A critical point is assessing the battery State of Health and Remaining Useful life to improve BEB operational efficiency. In this context, a detailed electric bus model was developed in the Matlab/Simulink environment. A forward modeling approach was chosen for a more realistic simulation, including driver behavior to generate acceleration and braking commands. In this approach, the vehicle behavior is determined by a set of inputs, such as speed profiles, road gradients, and passenger load. The purpose of the model is to assess energy consumption across different bus routes under various load conditions (e.g., number of passengers). The required input data, including current, voltage, battery capacity, and vehicle characteristics, were sourced from published data repositories. Furthermore, a custom script was implemented to simulate passenger boarding and alighting at each bus stop, allowing for dynamic load conditions. The energy consumption estimation serves as a foundation for understanding how different load conditions affect battery aging and performance. Key parameters such as high discharge rates, deep cycles, and extreme temperatures are known to accelerate degradation. Moreover, the power demand of HVAC and auxiliary systems represents a non-negligible factor to consider. High power demands, particularly during rapid acceleration or while climbing steep gradients, significantly increase the depth of discharge, leading to capacity fade and resistance growth in the battery. Consequently, battery capacity and efficiency degrade over time, negatively impacting both the range and performance of the vehicle. In this context, the implementation of a battery aging model is currently under investigation as part of ongoing research.

BEB model block diagram



External collaborations

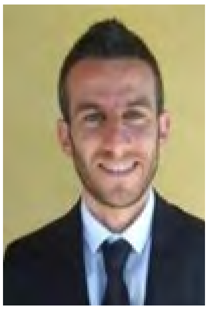
- CNR-STEMS
- Center for Automotive Research (CAR)-Ohio State University
- Teoresi SPA

Academic context

[1] Di Luca, G.; Di Blasio, G.; Gimelli, A.; Misul, D.A. Review on Battery State Estimation and Management Solutions for Next-Generation Connected Vehicles. *Energies* 2024, *17*, 202. https://doi.org/10.3390/en17010202

[2] Basma, H.; Mansour, C.; Haddad, M.; Nemer, M.; Stabat, P. Comprehensive energy modeling methodology for battery electric buses, Energy, Volume 207, 2020, 118241, ISSN 0360-5442, https://doi.org/10.1016/j.energy.2020.118241.

[3] Göhlich, D.; Fay, T.A.; Jefferies, D.; Lauth, E.; Kunith, A.; Zhang, X. Design of urban electric bus systems. *Design Science*, *4*, e15,2018. doi:10.1017/dsj.2018.10



First name: Salvatore **LAST NAME**: MAFRICI

Topic: Electric Motor Design for Circular Economy

Course year: 2nd **Tutor(s)**: Alberto TENCONI, Giovanni Andrea BLENGINI, Luca SETTINERI

Highlights of the research activity

The research I'm carrying on within the Industrial PhD on going at Politecnico di Torino and at PUNCH Torino, where I'm currently working, is focused on the Design for Circular Economy of Electric Motors. The paradigm for which a technology is considered clean on the base of the emission produced during its usage phase should change taking into consideration the complete product life cycle; my research, indeed is coupling technological aspects with methodological ones aiming to re-think an industrial product featuring circular design aspects. In this process product environmental impacts are taken into consideration since the first development phase with the implementation of various design options characterized by new features that will be enabler of circular loops (Durability, Maintenance, Reuse, Refurbishment/Remanufacturing, Recycle, …) of the product in its lifecycle. Environmental impacts are evaluated through Life Cycle Assessment (LCA) and together with other conventional key performance indicators, like performance and economic impact, will be part of a balanced review. The first portion of research activity was dedicated to the definition of Circular Strategies suitable for an electric motor, and to the identification and implementation of design features that allow a complete motor disassembly. Also a LCA model for the assessment of electric motor has been built with the scope to evaluate the various circular strategies implemented. The model at the moment has been used to provide Permanent Magnet Synchronous Machine (PMSM) assessment with evaluation of most influencing cycle phase and sub-components. Furthermore I provided results investigating two alternative scenarios, including the most impacting factors like the production and usage country (considering also material extraction) and the vehicle application and showing relevance of electricity mix production. In addition the model has been used to provide comparison between a conventional PMSM and a magnet free switched reluctance machine that is the product analyzed in my research activity. In this perspective it has been also investigated an Eco-Design strategy like the replacement of conventional copper windings with aluminum ones. A purposely re-designed machine with a virtually rewound stator was consiered. In Figure 1 is summarized this comparison between mainstream motor topology (PMSM), a magnet free motor topology (SRM) featuring both copper and aluminum winding. In third year, research will be focused on the assessment of circular strategies.

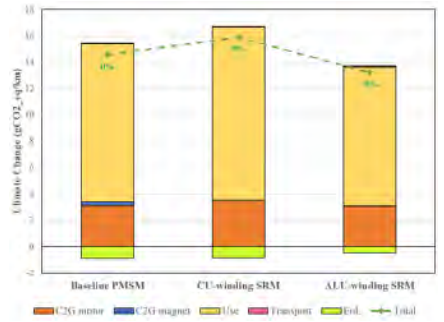


Figure 1. LCA comparison of a PMSM with a SRM featuring copper and Aluminum winding

External collaborations

- Dumarey Automotive Italia

Academic context

[1] Mafrici, S., Madonna, V., Meano, C., Hansen, K, Tenconi, A., "Switched Reluctance Machine for Transportation and Eco-Design: A Life Cycle Assessment" IEEE ACCESS 2024, https://dx.doi.org/10.1109/access.2024.3400324

[2] Mafrici, S., Accardo, A., Spessa, E., Tenconi, A., "A Novel Scenario Analysis Framework for the Life Cycle Assessment of Permanent Magnet Synchronous Motors for Electric Vehicles", IEEE ACCESS 2024 https://dx.doi.org/10.1109/access.2024.3486380

[3] Madonna, V., Meano, C., Mafrici, S., Hansen, K, "Copper vs. Aluminium Winding SRMs: a Multidisciplinary Performance Assessment", PEMD 2023, https://doi.org/10.1049/icp.2023.1978

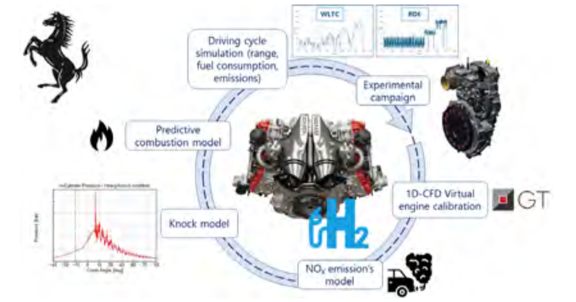
First name: Giancarlo **LAST NAME**: MONTANARO

Topic: Hydrogen-Fueled High-Performance Powertrains

Course year: 2nd **Tutor(s)**: ROLANDO, MILLO

Highlights of the research activity

The urgent need to address climate change has accelerated the global transition to sustainable energy sources. In this scenario, the European Green Deal aims to make Europe the first climate-neutral continent by 2050. Central to this vision is the promotion of alternative fuels such as hydrogen, a versatile and sustainable energy carrier. It offers unique advantages for high-performance internal combustion engines (ICEs), including rapid mixing and fast flame speed, high efficiency, and potentially zero carbon emissions during its lifecycle. Moreover, it can maintain the engine sounds ensuring the *fun-to-drive* of a sport car. These peculiarities make it an ideal candidate for sustainable and high-performance mobility solutions. In the first year, extensive experiments on a spark ignition Single-Cylinder Engine (SCE) were conducted to understand hydrogen combustion peculiarities. Concurrently, a detailed digital twin of the real engine was developed with a focus on the combustion process. In the second year of this research, substantial efforts have been devoted to improving the virtual model of the single-cylinder engine, focusing on accurate modeling of heat transfer processes. This refinement allows better predictions of energy flows, distinguishing between useful power and energy lost to cooling or exhaust. To accurately calibrate the predictive combustion model, a one-dimensional turbulence model has been calibrated against 3D-CFD data across a wide range of operating conditions, including variations in speed, load, and fuel injection parameters. Hydrogen-specific challenges, such as thermo-diffusive instabilities in ultra-lean mixtures and the impact of charge stratification on NOx emissions, have been rigorously investigated. A novel Laminar Flame Speed model has been developed to consider the increase of flame speed observed experimentally in combustion with lean mixtures due to the thermo-diffusive instability. Contemporarily, a Zeldovich-based NOx emissions model has been calibrated using experimental data, demonstrating satisfactory predictive capabilities, though the influence of stratification remains complex. Current efforts aim to refine the model further to account for multidimensional effects. Lastly, during this second year, experimental work has evaluated techniques like water injection (WI) and exhaust gas recirculation (EGR) to mitigate NOx emissions and prevent abnormal combustion. These strategies aim to balance engine efficiency and performance. The ultimate goal is to develop a virtual test bench capable of simulating various driving scenarios, enabling the assessment of hydrogen-fueled engines' performance and emission reduction strategies, paving the way for cleaner and more efficient mobility.



Path for the development of a reliable simulation platform for a hydrogen-fueled high-performance internal combustion engine

External collaborations

- Ferrari Powertrain Simulation & Know-How, www.ferrari.com

Academic context

[1] V. De Bellis, et al., "Development and validation of a phenomenological model for hydrogen fueled PFI internal combustion engines considering Thermo-Diffusive effects on flame speed propagation"
[2] S. Verhelst, et al., "Laminar and unstable burning velocities and Markstein lengths of hydrogen–air mixtures at engine-like conditions"
[3] Grabner, P., et al., "Formation Mechanisms and Characterization of abnormal Combustion Phenomena of Hydrogen Engines," SAE Technical Paper 2023-32-0168, 2023

First name: Teodosio **LAST NAME**: NACCI

Topic: Robust Design of High Temperature Components for Innovative Gas Turbine Cycles

Course year: 2nd **Tutor(s)**: Daniela Anna MISUL, Simone SALVADORI

Highlights of the research activity

The research activity carried out during my second year of Ph.D. studies focused on analyzing high-pressure turbine stages and related thermo-fluid-dynamic phenomena. The specific topics are the analysis of the impact of cavity flows on the first stage of an HP turbine and the flow distribution and vorticity structures in the cavities between the stator and rotor in an HP turbine's first stage. The activity concerns the simulation of a turbine stage with an attached internal cavity, located between the stator blade and the rotor blade, dedicated to controlling part of the cooling flow that enters the main flow, referred to as Purge flow, and analysis of the relative fluid-dynamic impact. Unsteady 3D-CFD simulations were carried out using Ansys CFX software and were validated by experimental data obtained at the Von Karman Institute (VKI) of Brussels. The idea was to use the CFD data to explore the thermo-fluid-dynamic performance of the turbine in greater detail and to figure out how the variation of the rotor angular speed and the purge flow rate affected the results. Three conditions were tested: one without injection into the cavity and two with positive Purge flow entering the mainstream. The geometry used to perform the Unsteady simulations, obtained using the Domain Scaling technique, is characterized by 2 stators and 3 rotors and a cavity with two inlets, one radial and the other axial. In addition to analyzing the results for comparison with experimental data, secondary flows on the rotor blade were identified, and the influence of the Purge flow on these structures was defined. In addition, the spanwise movement of the hub Passage Vortex, influenced by the contribution of the purge flow, was quantified as the rotor blade passed in front of the stator blade.

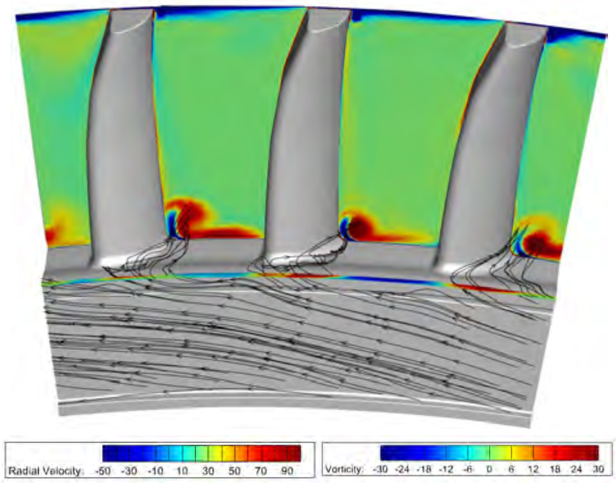


Fig. Cavity and main flows Interaction

The axial velocity gradient due to the rotation of the rotor part concerning the fixed stator part, the variation of the pressure profile at the cavity outlet, and the lid-driven effect led to a certain internal flow distribution and the genesis of vortical structures inside the cavity. To isolate these unstable vortex phenomena, detailed simulations of the cavity itself were carried out. Circumferential static pressure profiles, extracted from the previous simulations, were used as boundary conditions at the cavity outlet, while the flow rate and total temperature were set at the inlet. A SPOD (Spectral Proper Orthogonality Decomposition) analysis was performed on characteristic planes of the cavity to isolate the main energy modes, separating the various phenomena on different time scales.

External collaborations

- Technische Universität Berlin
- Technische Universität Graz
- Purdue University

Academic context

[1] Graikos, D., Carnevale, M., Sangan, C. M., Lock, G. D., and Scobie, J. A. (September 27, 2021). "Influence of Flow Coefficient on Ingress Through Turbine Rim Seals." ASME. *J. Eng. Gas Turbines Power*. November 2021; 143(11): 111010
[2] Jagerhofer, P. R., Patinios, M., Erlacher, G., Glasenapp, T., Göttlich, E., and Farisco, F. (April 21, 2021). "A Sector-Cascade Test Rig for Measurements of Heat Transfer in Turbine Center Frames." ASME. *J. Turbomach*. July 2021; 143(7): 071015

First name: Gerardo **LAST NAME**: STANZIONE

Topic: H_2 ICE – H_2 as an ICE fuel for marine & industrial

Course year: 2nd **Tutor(s)**: Federico MILLO, Andrea PIANO

Highlights of the research activity

The objective of this research activity, sponsored by YANMAR, is to explore the feasibility of converting a medium-speed diesel engine into an H_2-Diesel dual-fuel engine. In this concept, the hydrogen is injected into the intake port while the diesel fuel is directly injected into the cylinder at the end of the compression stroke to trigger the premixed combustion process.

In the first year of the PhD, the activity was divided into two distinct phases. In the first phase, the analysis of the experimental data was focused on gathering details not only on normal flame propagation but also on pre-ignition, ringing, and knocking phenomena. Subsequently, a previously developed 0/1D-CFD predictive combustion model was exploited. It accounts for two combustion modes, diesel spray combustion and turbulence flame propagation of the hydrogen. To do so, the 1D-CFD turbulence model was adopted and calibrated having as a target the outcomes of the 3D-CFD simulations in terms of turbulence kinetic energy (TKE) and the length scale. Then, the combustion model has been modified to take into account the influence of hydrogen on diesel ignition. More in detail, a dedicated ignition delay correlation was developed based on the outcomes of 0D-CFD detailed chemistry calculation. The correlation was defined through a meta-model that relies on an artificial neural network trained with 0D-CFD results. The modified version of the dual-fuel combustion model was calibrated over a wide range of operating conditions, proving its robustness and reliability.

Lastly, the emissions model based on the well-known Extended Zeldovich Mechanism (EZM) has been implemented. This model includes a stratified approach to compute lambda and temperature stratification, which highly affect NO_x formation. As highlighted in Figure 2, the model allowed an accurate prediction of the NO_x emissions.

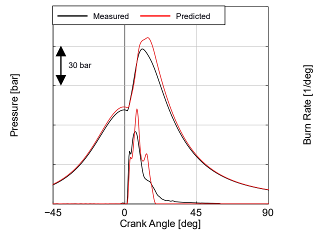


Figure 1 – Measured and Predicted pressure and Burn Rate with 94% H_2

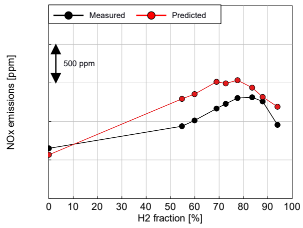


Figure 2 - NOx emissions as a function of H_2 fraction

External collaborations

- YANMAR
- Gamma Technologies LLC

Academic context

[1] Rouleau, L., Duffour, F., Walter, B., Kumar, R. et al., "Experimental and Numerical Investigation on Hydrogen Internal Combustion Engine," SAE Technical Paper 2021-24-0060, 2021, doi:10.4271/2021-24-0060

[2] Millo, F., Accurso, F., Piano, A., Fogla, N. et al., "Development and Validation of a Multi-zone Predictive Combustion Model for Large-Bore Dual-Fuel Engines," *SAE Int. J. Engines* 15(5):703-718, 2022, https://doi.org/10.4271/03-15-05-0038.

[3] Mancaruso, E., De Robbio, R., and Vaglieco, B.M., "Hydrogen/Diesel Combustion Analysis in a Single Cylinder Research Engine," SAE Technical Paper 2022-24-0012, 2022, doi:10.4271/2022-24-0012.

First name: Luigi **LAST NAME**: TRESCA

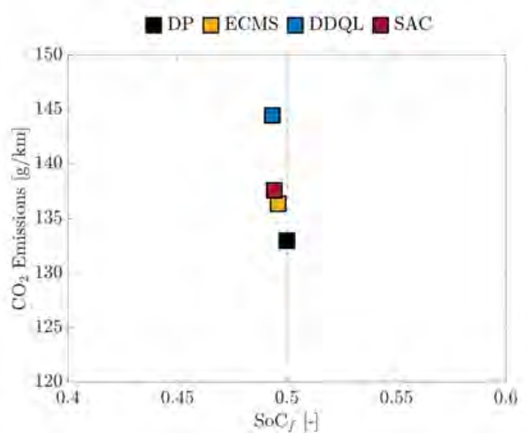
Topic: Machine Learning techniques application for the improvement of the Energy Management System of Hybrid Electric Vehicles with the goal of minimizing the CO2 emissions

Course year: 2nd **Tutor(s)**: Luciano ROLANO, Andrea PIANO

Highlights of the research activity

The transportation sector, responsible for 35% of global energy consumption, plays a critical role in achieving carbon neutrality by 2050 under the EU Green Deal. Hybrid powertrains, supported by advanced Energy Management Systems (EMS), represent a practical short-term solution to reduce greenhouse gas (GHG) emissions while mitigating the limitations of Battery Electric Vehicles (BEVs).

During the first year of research, an EMS using Recurrent Neural Networks (RNN) trained via Dynamic Programming (DP) was developed for a hybrid electric vehicle. This system optimized fuel consumption supporting Charge Sustaining (CS) and Charge Depleting (CD) modes. Additionally, an optimal eco-driving strategy was proposed using DP for multi-objective optimization. The natural evolution of this work regards the exploration of Reinforcement Learning (RL) in EMS design revealed its potential for self-learning optimization. Thus, RL-based EMS development was prioritized, focusing on Deep Q-Learning (DQL) and Soft Actor-Critic (SAC) agents. SAC, utilizing entropy-based exploration, demonstrated superior training efficiency and generalization capabilities, achieving near-optimal fuel efficiency (-0.47% from DP) and charge sustainability (-1.6% from initial SoC). A research activity carried out in collaboration with the mechanical department allows integrating traffic data, such as speed forecasts and congestion levels, into the RL framework, enhancing its performance in dynamic scenarios through the use of the software CarMaker. During an internship as visiting scholar at Stanford University I expanded this work to fleet-level optimization for Autonomous Mobility on Demand (AMoD) systems. Using SUMO, a micro-traffic simulator was developed to test RL-based fleet control in Luxembourg City. A graph-based SAC agent outperformed heuristic approaches and achieved performance comparable to Model Predictive Control (MPC), with significantly reduced computational demands.



Future research will further explore RL applications at vehicle and fleet levels, aiming to synergize these technologies for global emission reductions.

External collaborations

- Stanford University

Academic context

[1] L. Tresca, L. Pulvirenti, L. Rolando, F. Millo, Development of a deep q-learning energy management system for a hybrid electric vehicle, Transportation Engineering 16 (2024) 100241. doi: https://doi.org/10.1016/j.treng.2024.100241

[2] L. Rolando, N. Campanelli, L. Tresca, L. Pulvirenti, F. Millo, Development of a soft-actor critic reinforcement learning algorithm for the energy management of a hybrid electric vehicle, Tech. rep., SAE Technical Paper (2024). doi: https://doi.org/10.4271/2024-37-0011

[3] Tresca, L., Gammelli, D., Harrison, J., Pavone, M.: Benchmarking Reinforcement Learning for Network-level Coordination of Autonomous Mobility-on-Demand Systems Across Scales. In: Workshop on Autonomous Vehicles Across Scales at Robotic Science and Systems (2024)

First name: Massimiliano **LAST NAME**: ZANATTA

Topic: Combustion system development for alternative low and net zero carbon fuels

Course year: 2nd **Tutor(s)**: Federico MILLO, Luciano ROLANDO, Andrea PIANO

Highlights of the research activity

In 2024, the research activity, sponsored and supported by Dumarey Automotive Italia S.p.A., continued to build on the work initiated in 2023, expanding the investigation of innovative combustion systems with a particular focus on active prechambers (aPC). The CFD model previously developed for passive prechamber (pPC) systems was adapted to simulate the behavior and specific features of active prechambers. This adaptation enabled an extensive 3D-CFD numerical simulation campaign, providing a detailed analysis of the potential and limitations of both systems (pPC and aPC) and facilitating a direct comparison between them. The simplicity of passive prechamber systems (as they do not require a dedicated fuel line) is contrasted by the higher ignition energy associated to the stoichiometric aPC system. This results in narrower air-fuel ratio ignitability limits for passive prechambers and, consequently, lower efficiencies. The analysis revealed that exceeding lambda values of >2 requires the use of active prechambers, where it is possible to achieve competitive peak Indicated Thermal Efficiencies (ITE). From an emissions standpoint, NOx levels for the two systems were found to be approximately comparable, as the higher combustion temperatures of active systems are offset by their ability to operate at higher air-fuel ratios. In both systems, hydrocarbon (HC) emissions remain significant, indicating that further effort should be dedicated to addressing this issue.
Starting from September 2024, the research has turned to integrating these combustion systems with carbon-free fuels, particularly ammonia. Although ammonia offers high energy density and ease of transport, its low laminar flame speed and high minimum ignition energy pose significant challenges. The research aims to adapt these systems to optimize ammonia combustion, exploring innovative strategies such as prechamber applications and multi-fuel approaches. The work focuses on balancing efficiency and emissions, paving the way for sustainable propulsion solutions in large-bore engines. By the end of this research, the focus will shift to dual and tri-fuel systems (+diesel and H2), exploring compression ignition concepts and dual-fuel (+H2) spark-ignition systems with prechamber technology.

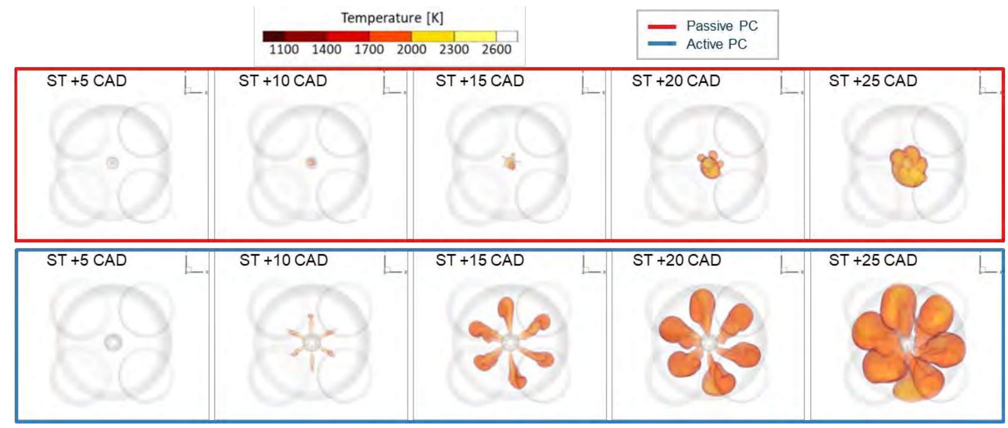


Figure 1 – Comparison of the combustion process between passive (top-red) and active (bottom-blue) prechamber systems.

External collaborations

- Dumarey Automotive Italia S.p.A.

Academic context

[1] Eicheldinger, S., Nguyen, H., et al, 2018, "Mitteldruck 30 bar bei Gasmotoren", Hrsg.: Forschungsvereinigung Verbrennungskraftmaschinen e.V.. Nummer 1201
[2] Wermuth, N., et al, 2023, "The Ammonia Combustion Engine for Future Power Generation Applications. Energy Technology", https://doi.org/10.1002/ente.202301008
[3] Matsunaga, D., et al, 2023, "A Study on Combustion and Emission Characteristics of Ammonia, Hydrogen, and Diesel Tri-Fuel Engines", SAE Technical Paper 2023-32-0103

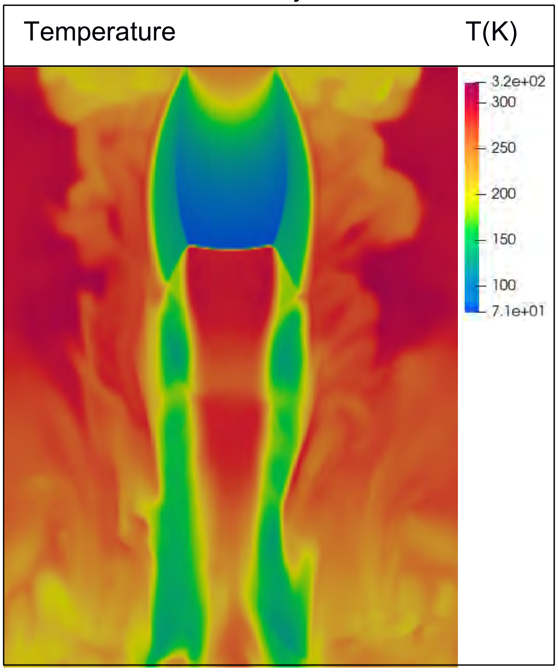
First name: Carmelo **LAST NAME**: BARONETTO

Topic: Numerical investigation of H_2-Air mixture formation in innovative green hydrogen direct-injection engines

Course year: 1st **Tutor(s)**: Alessandro FERRARI, Oscar VENTO, Alberto VASSALLO

Highlights of the research activity

The PhD scholarship regards the numerical simulation of highly under-expanded hydrogen jets. The complex structures which arise in supersonic compressible flows include gas dynamics shocks and Mach disk, and they strongly affect the jet in terms of tip penetration, jet opening and mass flow rate. The objective of this research is to carry out numerical simulations of hydrogen injections in order to characterize how these phenomena affect the mixture formation in hydrogen fueled direct injection (DI) engines. The findings of this study will be exploited for the optimization of the nozzle design for hydrogen DI injectors. Simulations are performed in OpenFOAM, an opensource software developed in C++. The literature review pointed out that *rhoCentralFoam* is one of the most employed solver for supersonic compressible flow, among those available in the OpenFOAM library. The activity started by performing two dimensional, single component (air-in-air) simulations which showed satisfactory shock capturing capabilities of *rhoCentralFoam*. The standard version of the solver has been then modified by adding a species-transport equation, and by replacing the Euler temporal discretization with a 4th order Runge-Kutta scheme. These modifications allow to solve multi-component flows and improve numerical stability, by increasing the temporal order of accuracy. The new solver has been successfully tested in two- and three-dimensional simulations of hydrogen-in-air injections. The picture shows the results at 50 μs of a 3D hydrogen jet, injected into the air (ratio of total upstream pressure to downstream pressure equal to 10). The preliminary numerical results, obtained using a LES turbulence model, are in good agreement with the experimental Schlieren images and the numerical data available in the literature. In parallel, an in-depth study of fluid dynamics and state of the art of numerical methods for multi-dimensional compressible flows has been done. Based on this activity, new numerical schemes for the discretization of inviscid fluxes have been implemented in OpenFOAM.



External collaborations

- Dumarey

Academic context

[1] Toro, Eleuterio F. *Riemann solvers and numerical methods for fluid dynamics: a practical introduction*. Springer Science & Business Media, 2013.
[2] Hamzehloo, A., and P. G. Aleiferis. "Large eddy simulation of near-nozzle shock structure and mixing characteristics of hydrogen jets for direct-injection spark-ignition engines." International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics, 2014.
[3] Yip, Ho Lung, et al. "Visualization of hydrogen jet evolution and combustion under simulated direct-injection compression-ignition engine conditions." *International Journal of Hydrogen Energy* 45.56 (2020): 32562-32578.

First name: Payam **LAST NAME**: DANESH

Topic: Modelling waste to biomaterial, energy, and critical material recovery

Course year: 1st **Tutor(s)**: 1st Matteo PRUSSI, 2nd David CHIARAMONTI

Highlights of the research activity

My Ph.D. work aims to model a slow pyrolysis process, for biochar production. The work of this year focuses on developing correlations based on physical models and experimental data, to predict biochar yield under varying process conditions. This involved analyzing the effects of key different parameters such as pyrolysis temperature, mean residence time, heating rate, and biomass characteristics, including type (sewage sludge, etc.) and moisture content. The modeling phase is functional to support the design and optimization of a rotary kiln slow pyrolysis reactor, emphasizing the geometrical aspects of the reactor (i.e. its length and diameter) to ensure heat transfer and energy recovery. Through sensitivity analyses, I am aiming to optimize system operation while minimizing investment costs. This integrated approach aims to contribute to developing a robust design tool, offering valuable insights for scaling biochar production sustainably and economically. In conclusion, the main goal of my research is to improve biochar's application as a catalyst in methane decomposition and its potential for recovering valuable materials like phosphorus and nitrogen. Comparison of different chemical and physical upgrading techniques for biochar (e.g., acid, alkali, metal impregnation, and heat treatments) and evaluate their effects on biochar's surface characteristics, adsorption capacity, and catalytic performance (Fig.1).

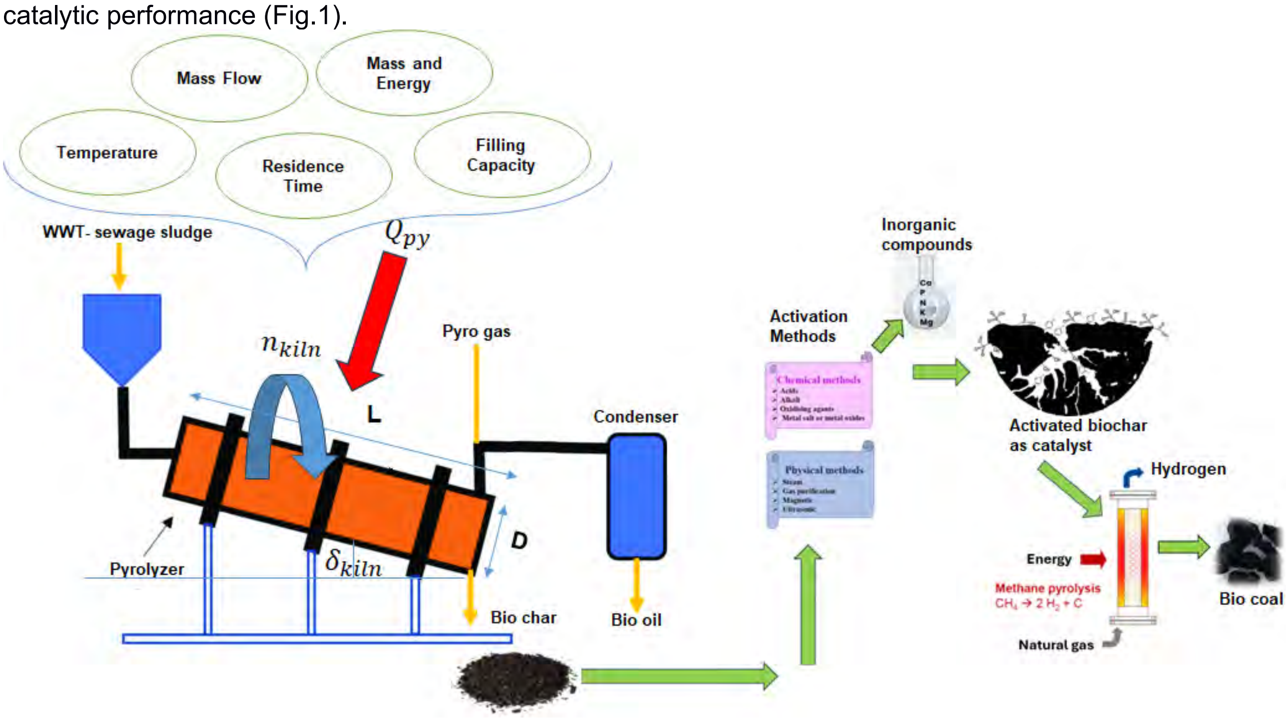


Figure 1. Conceptual modeling waste to biomaterial, energy, and critical material recovery

External collaborations

- Renewable Energy Consortium for Research and Demonstration (RE-CORD)

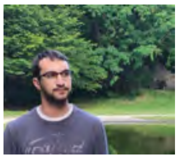
Academic context

[1] Fambri G, et al. "Energy Assessment of a Slow Pyrolysis Plant for Biochar and Heat Cogeneration." *Chemical Engineering Transactions* 109 (2024): 571-576.
[2] Salimbeni A, et al. "Techno-Economic feasibility of integrating biomass slow pyrolysis in an EAF steelmaking site: a case study." *Applied Energy* 339 (2023): 120991.

First name: Andrea **LAST NAME**: FRANZOSO

Topic: Optimal orchestration of energy flows with an energy and environmental perspective

Course year: 1st **Tutor(s)**: Marco BADAMI, Gabriele FAMBRI



Highlights of the research activity

The work developed this year was aimed at exploring the use of Deep Reinforcement Learning (DRL) algorithms to optimize different kinds of energy systems under high Renewable Energy Sources (RES) penetration scenarios. In literature, the utilization of DRL methods for the optimization and control of complex and interconnected energy systems is a topic of growing interest as they have proven to enable real-time decision-making and have been shown to outperform traditional optimization and control methods in terms of both speed and accuracy while handling high-dimensional state and action spaces efficiently. Different case studies have been developed to identify the strengths and weaknesses.

Initially, DRL was applied to simpler energy systems to test its capabilities and performance. These included the management of PV connected with Battery Energy Storage Systems (BESS), where the agent optimized auto-consumption and reduced costs tracking grid prices correctly, and a heat pump for house heating modeled in Simscape, where the agent leveraged thermal inertia to minimize costs while maintaining comfort, showing advantages over traditional PID control.

Building on the insights gained from these simpler systems, DRL was then applied to more complex energy systems. A significant focus was on optimizing a Multi-Energy System (MES) that integrates CHP, heat pumps (HP), BESS, and Power-to-Gas (P2G) technologies.

This study had two purposes: first, to investigate how DRL algorithms can effectively explore the behavior of complex MES systems and identify optimal strategies, and second, to evaluate the performance of the individual components in the MES by varying their sizes through sensitivity analysis to capture various operational contexts.

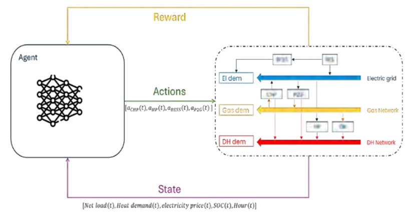


Fig: MES optimization with DRL.

The DRL agents identified HP technology as the most cost-effective and frequently used in synergy with RES and CHP production, followed by P2G and BESS, which are only used if surplus is available.

Concerning the evaluation of the performance of individual components, it was observed that as RES penetration increases, the use of centralized CHP production becomes less advantageous (acting as a peaking unit), while the direct use of renewable electricity (when available) and HP becomes more favorable for heat production. The DRL agent made limited use of P2G technology, primarily because its conversion efficiency was inferior to the other options. The results of this work have been described in a paper ("Deep Reinforcement Learning for optimizing the control of energy storage and conversion technologies in Multi-Energy Systems") under review in Applied Enegy.

External collaborations

- Trigenia S.r.l.

Academic context

[1] G. Ghione et al., Comparison of Genetic and Reinforcement Learning Algorithms for Energy Cogeneration Optimization, doi: 10.23919/SpliTech58164.2023.10193518.
[2] Dafeng Zhu et al., Energy management based on multi-agent deep reinforcement learning for a multi-energy industrial park, doi: 10.1016/j.apenergy.2022.118636.
[3] Imen Jendoubi et al., Multi-agent hierarchical reinforcement learning for energy management, doi: 10.1016/j.apenergy.2022.120500.

First name: Gaia | **LAST NAME**: GENTILUCCI

Topic: Environmental and cost assessment of climate-neutral solutions for bus and truck applications

Course year: 1st **Tutor(s)**: Ezio SPESSA, Daniela MISUL

Highlights of the research activity

The Life Cycle Assessment (LCA) is a critical methodology for evaluating the environmental impacts of a product throughout its entire life cycle, from raw material extraction to end of- life. This approach has become especially relevant in the automotive industry, where it serves as a key tool to assess and compare the environmental impacts of conventional vehicles with emerging zero-emission alternatives. In the first year of the PhD, the focus of research has been primarily on the application of LCA methodology to heavy duty vehicles and their components. The initial work involved a comprehensive literature review to identify existing methods, data challenges, and gaps in current LCA studies on heavy duty trucks. The aim was to evaluate the state of the art in this field and provide a foundation for further research. At the vehicle level, the research has concentrated on developing an LCA model to assess the environmental impact of two diesel heavy-duty trucks of VECTO group 9, as well as conducting a preliminary evaluation of two prototypes of zero-emission trucks: a Battery Electric Vehicle (BEV), designed for regional distribution mission profiles with a maximum uncharged driving range of 400 km and a Fuel Cell Electric Vehicle (FCEV) suitable for long-haul operation conditions with a maximum unrefueled range of 750 km. These efforts are part of the European project namely EMPOWER (i.e., Eco-operated, Modular, highly efficient, and flexible multi-POWERtrain for long-haul heavy-duty vehicles). At the component level, research efforts have focused on fuel cells (FC), specifically a 200kW Proton Exchange Membrane (PEM) FC system used in long-haul heavy-duty trucks. An LCA evaluation was conducted analyzing various scenarios to understand how changes in parameters such as material composition, electricity mix, performance characteristics (i.e., fuel consumption, the system size and durability) and hydrogen production routes affect overall environmental impacts.

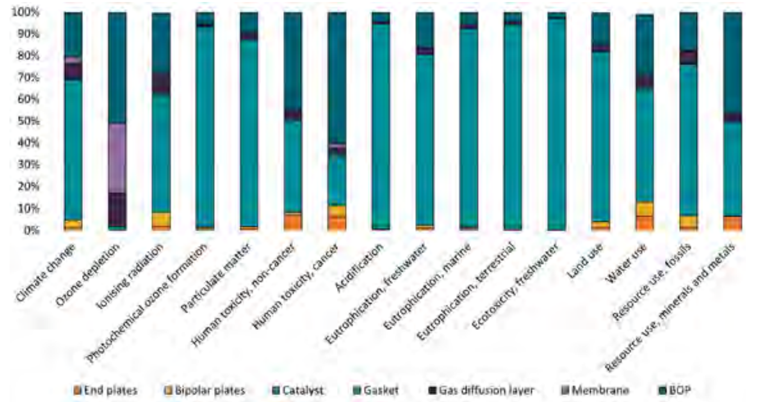


Fig: LCA comprehensive results from cradle-to-gate boundary of PEM fuel cell system

External collaborations

- IVECO Group

Academic context

[1] Gentilucci, G.; Accardo, A.; Spessa, E.. Life Cycle Analysis of a PEM Fuel Cell System for Long-Haul Heavy-Duty Trucks. SAE Technical Paper, 2024. https://doi.org/10.4271/2024-24-0020

[2] Hill, N.; Amaral, S.; Morgan-Price, S.; Nokes, T.; Bates, J.; Helms, H.; Fehrenbach, H.; Biemann, K.; Abdalla, N.; Jöhrens, J.; Cotton, E.; German, L.; Harris, A.; Haye, S.; Sim, C.; Bauen, A.; Ziem-Milojevic, S.. Determining the environmental impacts of conventional and alternatively fuelled vehicles through LCA. Final Report for the European Commission, 2020. https://doi.org/10.2834/91418

[3] Miotti, M.; Hofer, J.; Baueruse, C. Integrated environmental and economic assessment of current and future fuel cell vehicles. Int J Life Cycle Assess (2017) 22:94–110. https://doi.org/10.1007/s11367-015-0986-4

First name: Giovanni **LAST NAME**: LABRINI

Topic: Innovative cooling solutions for novel energy and propulsion systems

Course year: 1st **Tutor(s)**: Daniela Anna MISUL, Simone SALVADORI

Highlights of the research activity

The research activity is focused on the optimization of high-pressure Turbine Vane, in the context of the aeroengine field. More specifically, external aerodynamic and thermal performance are key parameters to improve components behavior, with the target to reduce fuel consumption and engine emissions.
Machine Learning tools are able to explore in a more efficient way the design space respect to traditional Computational Fluid Dynamics (CFD) analysis, which requires a higher computational cost.
In the current activity, the selected test case is represented by a high-pressure turbine vane with diffusive endwalls, in order to ingest a high-subsonic flow (Ma=0.6) delivered by a Rotating Detonation Engine (RDE). Optimization consists in finding the best configuration of the endwalls and blade profiles that increase the stator efficiency of the vane. These profiles are reconstructed with splines, whose form is controlled by control points that are used as input parameters to build the Desing of Experiments (DOE). The DOE employs CFD RANS simulations to build a database where design points are linked with correspondent value of stator efficiency, inlet Mach number, mass flow rate of the main flow.
In previous activities, this DOE is used to train machine learning models such as Deep Neural Networks and Random Forest, which are able to find correlations between the design point used to build the profiles and the stator efficiency. This method coupled with a Genetic Algorithm allowed to explore the design space in a limited amount of time and produces a new blade configuration with a higher aerodynamic efficiency respect to the nominal test case.
One of the limitations of the traditional machine learning model is that the input parameters are weakly linked with the real geometry of the blade and the physics of the problem. An interesting improvement can be made by exploiting a different type of ML model which is the Convolutional Neural Network. This methodology operates with images as input which are transformed into tensors using different combination of hyperparameters, with the objective to obtain a scalar value or a set of values.
In the actual case study, the input image is represented of a black and white image of the endwalls on the left side and blade profile on the right, while the output of this model is the stator efficiency. The CNN model is used as fitness function of a Particle Swarm Optimization (PSO) algorithm which produces a blade configuration with an improvement of stator efficiency of +3.5% respect to nominal case.
The results of this methodology can be applied also to different case studies. For the future, the idea is to apply CNN to a system of internal cooling channels in order to investigate the best geometrical configuration of these structures in order to improve the metal blade temperature without exceeding the coolant mass flow rate.

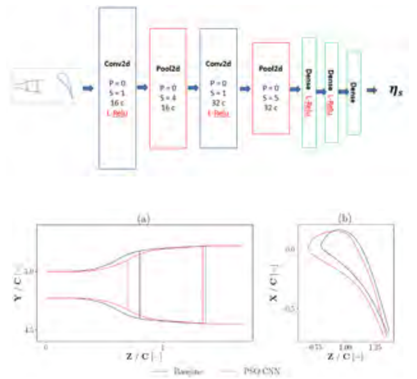


Fig. CNN structure and results of the optimization respect to baseline.

Academic context

[1] Nastasi, R. et al. "Shape Optimization of a Diffusive High-Pressure Turbine Vane Using Machine Learning Tools." (2024)
[2] Wang, Y. et al. “Dual-convolutional neural network based aerodynamic prediction and multi-objective optimization of a compact turbine rotor.” (2021)
[3] Dong, Z. et al. “Optimization of film cooling arrays on a gas turbine vane by using an integrated approach of numerical simulation and parameterized design.” (2022)

First name: MRZIEH **LAST NAME**: GOLABCHI

Topic: Prospective LCA of next-generation battery systems for automotive applications

Course year: 1st **Tutor(s)**: Ezio SPESSA, Daniela MISUL

Highlights of the research activity

During the 2023-2024 academic year, I concentrated my research efforts on two pivotal areas: collaborating with Stellantis on battery life cycle assessment (LCA), with a specific focus on end-of-life (EOL) strategies and participating in interdisciplinary research on artificial intelligence (AI) applications in engineering contexts at DIMEAS. These projects significantly enhanced my understanding of sustainable technologies, regulatory frameworks, and their practical application in industrial and academic settings.

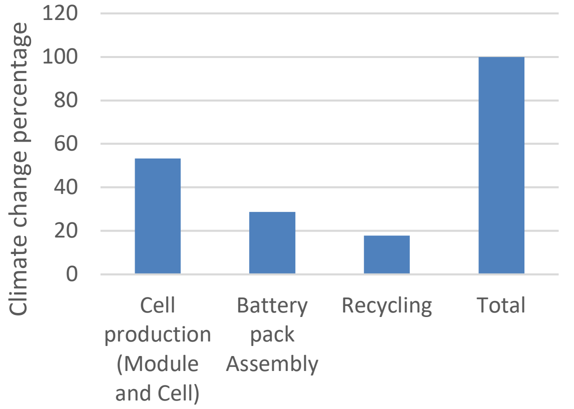


Fig: Climate change impact of LCA

In my collaboration with Stellantis, I conducted research with the objective of understanding and optimizing the environmental impacts of lithium-ion batteries throughout their life cycle, with a particular emphasis on end-of-life management. An extensive literature review was conducted to analyze various recycling techniques, including hydrometallurgy and pyrometallurgy, as well as second-life applications, where used batteries are repurposed for stationary energy storage. This work underscored the importance of a circular economy approach to maximize resource efficiency and minimize waste, emphasizing the critical challenges of recovering valuable materials like lithium, cobalt, and nickel from spent batteries.

In addition, I investigated the European Union's Circular Footprint Formula (CFF), a pivotal regulatory framework devised to standardize environmental impact assessments across industrial sectors. By examining the implications for battery manufacturers, including the challenges posed by data collection and reporting requirements, I provided insights and recommendations to Stellantis on aligning its LCA practices with these evolving regulations. Furthermore, I applied this regulatory knowledge by constructing LCA models based on primary industry data, though confidentiality agreements limited the disclosure of specific details. This hands-on work bridged the gap between theoretical frameworks and their real-world implementation.

External collaborations

- Stellantis

Academic context

[1] Šimaitis, J., Allen, S., & Vagg, C. (2023). Are future recycling benefits misleading? Prospective life cycle assessment of lithium-ion batteries. *Journal of Industrial Ecology*, 27, 1291–1303. DOI: 10.1111/jiec.13413 (jiec.13413).

[2] Accardo, A., Garofalo, A., Dotelli, G., & Spessa, E. (2024). Prospective LCA of Next-Generation Cells for Electric Vehicle Applications. *IEEE Access*. DOI: 10.1109/ACCESS.2024.3361312 (3. Prospective_LCA_of_N…).

[3] Haupt, J., Kononova, N., Cerdas, F., Zellmer, S., & Herrmann, C. (2023). Challenges of prospective life cycle assessment of emerging recycling processes: Case study of battery materials recovery. *Procedia CIRP*, 116, 23–28. DOI: 10.1016/j.procir.2023.02.005(1-s2.0-S221282712300009…).

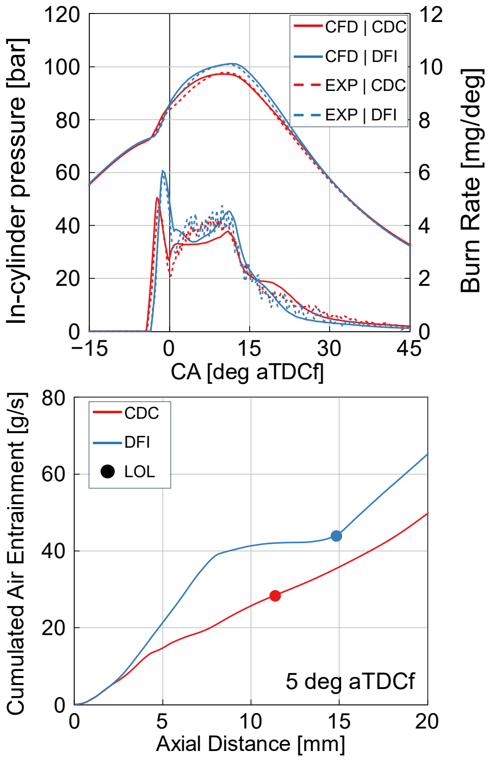
First name: Marco **LAST NAME**: ORLANDO

Topic: Development of suitable modeling methodologies to support the exploitation of hydrogen and e-fuels in internal combustion engines.

Course year: 1st **Tutor(s)**: Andrea PIANO, Federico MILLO

Highlights of the research activity

Electrification is considered the main driver for transport decarbonization, but still compression-ignition engines remain essential for heavy-duty applications despite they are respondible of high soot and NO_x emissions. In this context, Ducted Fuel Injection (DFI) is a promising solution for drastically reducing soot without increasing NOx emissions, through enhanced fuel mixing and air entrainment. Further investigations, supported by 3D-CFD simulations, are crucial for its integration into production engines.
The core of this year research activity, in collaboration with Sandia National Laboratories, is the development of a 3D-CFD model for the Sandia Compression Ignition Optical Research Engine (SCORE), for both conventional diesel combustion (CDC) and DFI configuration, on the base of experimental data from Sandia National Laboratories [2]. Several methodological efforts were invested, also regarding the development of methodologies to replicate experimental OH* chemiluminescence data and soot natural luminosity, thus ensuring a proper investigation of the in-cylinder soot formation and oxidation phenomena. Results from model validation were very promising, with the main combustion phenomena well described by the 3D-CFD model, as well as the main trend between CDC and DFI. The developed model was subsequently utilized for mixing analysis to verify whether the primary soot mitigation mechanisms associated with DFI are also valid in this application. Analysis of air entrainment within the spray, lift-off length (LOL) visualization, and equivalence ratio values at LOL confirmed DFI's ability to enhance air intake in the spray region, lower the equivalence ratio, and increase the LOL. Finally, the model has been employed to conduct preliminary simulations exploring multi-injection strategies combined with DFI, analyzing the effects of dwell time and mass distribution in different injection events. These preliminary results are very promising. The next steps will involve further simulations to expand this analysis, aiming to accelerate the market introduction of this technology.



Top: Experimental and 3D-CFD pressure and burn rates for both CDC and DFI.
Bottom: Computed cumulative air entrainment for both CDC and DFI configurations, along with their respective LOL at 5 deg aTDCf.

External collaborations

- Sandia National Laboratories
- GammaTech Engineering S.r.l.

Academic context

[1] Millo, F., Piano, A., Peiretti Paradisi, B., Postrioti, L. et al., "*Ducted Fuel Injection: Experimental and Numerical Investigation on Fuel Spray Characteristics, Air/Fuel Mixing and Soot Mitigation Potential*," Fuel (2021), doi:10.1016/j.fuel.2020.119835.
[2] Nyrenstedt, G. et al., "*Ducted fuel injection with Low-Net-Carbon fuels as a solution for meeting future emissions regulations*," Fuel (2023).

First name: Simone **LAST NAME**: RAGNATELLA

Topic: Development of Enabling Technologies for Rotating Detonation Engines for a Greener Propulsion

Course year: 1st **Tutor(s)**: Simone SALVADORI, Daniela Anna MISUL

Highlights of the research activity

Pressure Gain Combustion (PGC) is a promising approach to improving efficiency and reducing emissions in aviation. Among the various PGC technologies, Rotating Detonation Engines (RDEs) stand out as the most viable option due to their ability to replace traditional deflagration-based combustion with continuously rotating detonations. RDEs replace traditional combustion with continuous detonations, reducing entropy and enhancing thermodynamic efficiency. However, integrating RDEs with turbines poses challenges due to pulsating flows that can jeopardize the efficiency gain of the entire engine. My research is focused on addressing this key aspect by investigating and optimizing two primary components:

- **Transition Ducts** to dampen pulsating flows and reduce losses.
- **First Stage of the High-Pressure Turbine** for pulsating flow conditions.

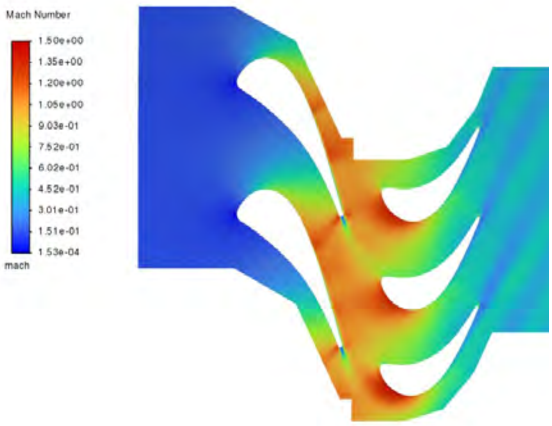


Figure 1: Mach number contour from a single time step in a URANS stator-rotor simulation

Initial efforts involved coupling the in-house solver *HybFlow* with ANSYS Fluent for combined 3D simulation of the transition duct and quasi-3D simulation of the Rotating Detonation Combustor (RDC), in collaboration with Università degli Studi di Firenze. The focus has since shifted to coupled simulations within ANSYS Fluent. My research also involves the performance analysis and optimization of a first-stage high-pressure turbine designed for inlet Mach numbers of 0.6. The turbine geometry is based on the CT3 test rig, extensively documented in the literature. Previous optimization efforts have improved the airfoil and endwall designs of the Nozzle Guide Vane (NGV) for enhanced performance. To evaluate the efficiency impact of coupling the turbine with an RDC, comparative studies are being conducted for the nominal configuration and an optimized configuration. These studies aim to quantify efficiency degradation caused by pulsating exhaust flow with respect to uniform inflow. The computational methodology relies on 3D Computational Fluid Dynamics (CFD) simulations using RANS equations for steady-state analyses and URANS for transient effects. The study initially analyzed stator-rotor interactions under steady conditions using a mixing-plane interface and has progressed to fully transient, pitch-scale simulations

External collaborations

- Università degli studi di Firenze

Academic context

[1] Braun, James, and Guillermo Paniagua. "Rotating detonation combustor operability and aero-thermal performance with an integrated diverging nozzle." Applied Thermal Engineering 249 (2024): 123126
[2] Grasa, Sergio, and Guillermo Paniagua. "Design, Multi-Point Optimization and Analysis of Diffusive Stator Vanes to Enable Turbine Integration Into Rotating Detonation Engines." Turbo Expo: Power for Land, Sea, and Air. Vol. 86984. American Society of Mechanical Engineers, 2023

First name: Alessio **LAST NAME**: RIORDA

Topic: Defossilization of hard-to-abate industries: The role of bio-based production routes

Course year: 1st **Tutors**: David CHIARAMONTI, Viviana NEGRO

Highlights of the research activity

During the first year of my PhD, I mainly worked on two European projects, namely BIORECAST and H2STEEL, both of which aim to defossilize the steel industry by promoting the transition from fossil fuels to sustainable alternatives. As part of the BIORECAST project, my research focused on the use of organic waste to produce biocoal and pyrogases as substitutes for traditional fossil fuels. A significant part of my activities involved the design of an integrated pyrolysis/ Electric Arc Furnace plant. This entailed identifying waste-heat sources within steel plants to support the pyrolysis process and exploring the integration of pyrogas into various stages of steel production to enhance energy efficiency and sustainability. In addition to technical research,. In parallel, my involvement in the H2STEEL project focused on developing sustainable hydrogen and biocoal production from biowaste. Specifically, I worked on the modeling of a biomethane pyrolysis reactor, assessing its energy efficiency and scalability for industrial applications. Complementing this, I carried out a preliminary techno-economic assessment to evaluate the feasibility of implementing biomethane pyrolysis at a commercial scale. In addiiton, as part of the EIC Green Hydrogen portfolio activities related to H2STEEL project, I performed a comaprative analysys of different processes aimend at the production of green hydrogen from biomass, resulting in the draft of a manuscript currently under revision. Amongo the activites of the above mentioned protfolio, , I contributed to a report for, that summarizes the findings and provides recommendations for future research and policy initiatives in the transition to green hydrogen.

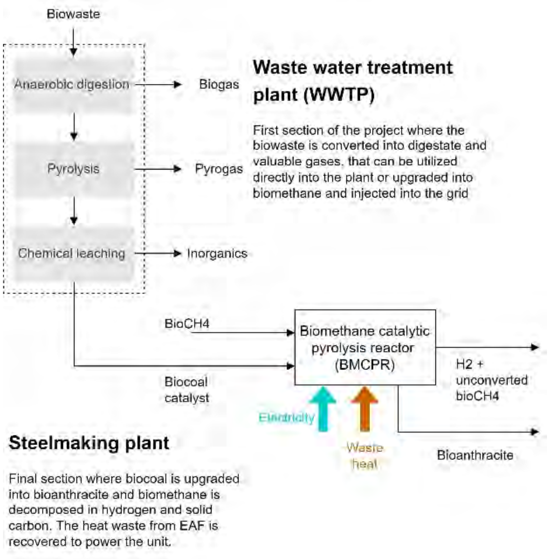


Figure 1 Process scheme of H2STEEL project, with the simultaneous production of green hydrogen and bioanthracite from biowaste streams.

External collaborations

- RE-CORD

Academic context

[1] Savankumar Patel, “Production of hydrogen by catalytic methane decomposition using biochar and activated char produced from biosolids pyrolysis”, 2020, https://doi.org/10.1016/j.ijhydene.2020.08.036.
[2] Schneider, S., Bajohr, S., Graf, F. and Kolb, T. (2020), State of the Art of Hydrogen Production via Pyrolysis of Natural Gas† . ChemBioEng Reviews, 7: 150-158. https://doi.org/10.1002/cben.202000014
[3] Elsayed Mousa, Chuan Wang, Johan Riesbeck, Mikael Larsson,
Biomass applications in iron and steel industry: An overview of challenges and opportunities, 2016, https://doi.org/10.1016/j.rser.2016.07.061.

First name: Guglielmo **LAST NAME**: ROSSI

Topic: Model-based design for future ICE fuels

Course year: 1st **Tutor(s)**: Andrea PIANO, Federico MILLO

Highlights of the research activity

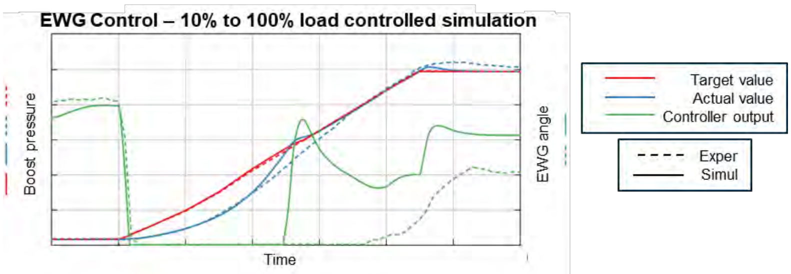


Figure 1 - Exhaust wastegate control, 10% to 100% transient load simulation

The more severe emissions targets and always more challenging fuel economy market demands are driving Wärtsilä to exploit future fuels, such as natural gas, hydrogen, ammonia, and methanol in order to comply with the targets imposed by the International Maritime Organization (IMO) regulations.
In this framework, the possibility to integrate a model-based approach (i.e., X-in-the-Loop simulations) into the product development process would be a breakthrough solution for reducing prototype costs and speeding up testing and product validation by achieving early assessment of system behavior. The current activity target is the development of a Model-in-the-Loop (MiL) platform capable of coupling an engine, represented by a physical based 0D-1D CFD model, with its control unit by the creation of a virtual simulation environment.
The original GT-SUITE detailed engine model was improved in terms of computational time in order to achieve a satisfactory performance for this MiL application. Despite the structure simplifications needed, its accuracy was preserved by keeping thermal and volumetric efficency into a ±3% error band with respect to the original model. Moreover, a predictive combustion and emissions model was integrated using a previously validated model from earlier PhD research [1]. The model accurately reflects engine performance by being sensitive to engine calibration parameters and geometry, thereby ensuring a high degree of realism of the simulation.
After that, several control strategies were implemented in Simulink and coupled with the engine model. These strategies span from basic engine controls, such as injection timing and duration, spark timing and exhaust wastegate control (Figure 1), to more complex controls which are based on combustion characteristics and emissions amount.
As a result, the developed MiL platform can accurately reproduce multiple real engine control strategies, thus becoming a valuable "test rig" for ECU development. Controls can be tested one by one or even together, making the platform useful for finer adjustments of already available controls or for the development of new ones too. In addition, the integration of a predictive combustion and emissions model permits to proper assess the behaviour of controls that influence combustion. Moreover, GT-SUITE model can be adapted to operate with alternative fuels in order to investigate their potentialities.
The MiL platform developed in this project could help into accelerate testing and validation of the product by reducing the need of experimental campaigns for ECU calibration or for main engine modifications, such as geometry and fuel type. Experimental testing is not only expensive in terms of time and financial resources but is also a source of CO2 emissions. Therefore, this simulation platform offers a sustainable alternative, enabling the company to reduce its carbon footprint while streamlining development processes.

External collaborations

- Wärtsilä Italia S.p.A.
- Wärtsilä Finland

Academic context

[1] Accurso, F., Piano, A., Millo, F., Caputo, G., Cimarello, A., & Cafari, A. (2022). Numerical Simulation of a Prechamber-Ignited Lean-Burn Gas Engine by means of Predictive Combustion Models. *SAE International Journal of Engines*, *16*(03-16-05-0037), 623-641.

First name: Alex **LAST NAME**: SCOPELLITI

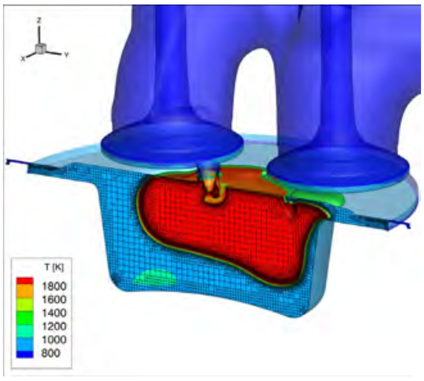
Topic: H2-based power units for zero-equivalent mobility solutions

Course year: 1st **Tutor(s)**: M. BARATTA, D. A. MISUL

Highlights of the research activity

Bibliographic research on H_2 ICEs (from H_2 production to injection, combustion, and challenges of 1D and 3D CFD), and on Free-piston engines, with particular attention to opposed piston configurations.

Publication of the journal paper "Feasibility and Performance Analysis of Cylinder Deactivation for a Heavy-Duty Compressed Natural Gas Engine", summing up the research activity carried out during the Master's thesis activity.



Lean H_2 combustion with Sage model, AMR active - T plot during combustion (20°CA after SA)

1D modelling, in GT-SUITE, of a prototype natural gas engine, converted to run on a lean hydrogen combustion mode. The results have been published in the paper "High-Performance Hydrogen-Fueled Internal Combustion Engines: Feasibility Study and Optimization via 1D-CFD Modeling". The study compares the full-load performance of the hydrogen-fuelled engine with the original NG configuration, focusing on the entire system, including the turbocharger. The aim was to assess the compatibility of the existing engine with hydrogen combustion and determine any necessary design modifications to optimize performance.

1D modelling for the FLEX-GEN project (FLEXi-fuel high-efficiency linear piston engine for future power GENerators). With reference to a possible range-extender application with direct injection, two kind of models have been studied. The first model is a pure free-piston engine, without any control system, analysed to fully characterise the peculiar characteristics of an engine without a crankshaft mechanism. The results show that the engine can be controlled to run with several CR, and particular attention has to be paid on the scavenging process in order to have the best volumetric efficiency. The second model employs a PID controller, to impose the position of TDC and BDC, thus controlling the CR.

3D-CFD modelling has been carried out on a 6-cylinders heavy-duty hydrogen PFI engine, with the objective of developing a predictive combustion model. Heat release rate has been studied to compare experimental and 3D simulations, by employing a model with heat capacity ratio dependent on burned and unburned species. The calibration of the model has shown good results in replicating the experimental data and the next steps are improving the combustion model and then move to the Direct Injection version of the engine.

External collaborations

- CNR STEMS
- PoliMI
- FPT Industrial

Academic context

[1] Wang J, Feng H, Zhang Z, et al. Development of a coupling model and parametric analysis of an opposed free-piston engine linear generator. Appl Therm Eng 2023; 219:119205.

[2] Mogi Y, Oikawa M, Kichima T, Horiguchi M, Goma K, Takagi Y, et al. Effect of high compression ratio on improving thermal efficiency and NOx formation in jet plume controlled direct-injection near-zero emission hydrogen engines. Int J Hydrogen Energ 2022;47:31459–67.

[3] Baratta M, Chiriches S, Goel P, Misul D. CFD modelling of natural gas combustion in IC engines under different EGR dilution and H2-doping conditions. Transport Eng 2020;2:100018

First name: Riccardo **LAST NAME**: SOLA

Topic: CFD 3D internal combustion engines

Course year: 2nd **Tutor(s)**: Mirko BARATTA, Daniela Anna MISUL

Highlights of the research activity

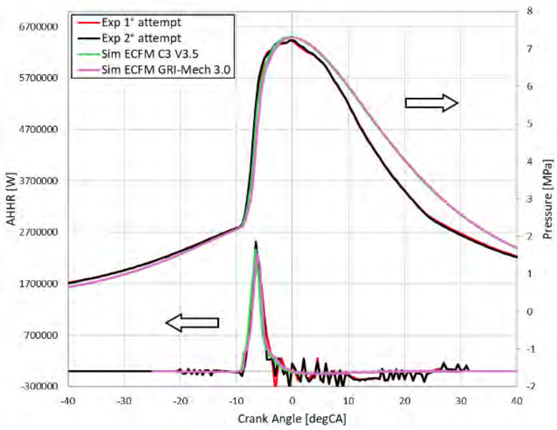
The present PhD project is focused on developing and applying advanced combustion models to internal combustion engines (ICEs) fueled by alternative fuels and their blends, with an emphasis on hydrogen and ammonia mixtures. A key experimental foundation is the Rapid Compression Expansion Machine (RCEM), used to analyze combustion processes for various hydrogen-methane blends at different equivalence ratios.
The study evaluates the predictive performance of detailed kinetic models (e.g., SAGE) and flamelet-based models (e.g., ECFM), with particular attention to pressure and flame propagation behavior. Optical imaging techniques validate the numerical results, ensuring accurate flame evolution and pressure curve predictions.

In parallel, the research investigates hydrogen combustion in two-stroke engines, comparing an opposed-piston layout to a traditional boxer design.

The analysis includes:

- Grid sensitivity assessments to evaluate scavenging efficiency.
- Port design optimizations to enhance scavenging under fixed conditions.
- High-pressure direct injection simulations to optimize charge stratification and mixing processes.

Insights from RCEM experiments inform the combustion simulations, emphasizing hydrogen's unique behavior under high turbulence and jet ignition conditions. Additional simulations based on the Sandia optical engine validate hydrogen injection processes, with results showing strong agreement with experimental data, despite minor limitations from RANS turbulence modeling.



Experimental - numerical correlation RCEM test case (Φ=1 - HR=0.75)

This research contributes to improving the understanding and predictive capabilities of combustion in hydrogen/ammonia engines, paving the way for optimized designs with alternative fuels.

External collaborations

- Convergent Science GmbH
- IFP-EN
- PRISME Laboratory

Academic context

[1] C. Lhuillier, P. Brequigny, F. Contino, and C. Mounaïm-Rousselle, "Experimental study on ammonia/hydrogen/air combustion in spark ignition engine conditions," *Fuel*, vol. 269, Jun. 2020, doi: 10.1016/j.fuel.2020.117448.
[2] S. Dong *et al.*, "A new detailed kinetic model for surrogate fuels: C3MechV3.3," *Applications in Energy and Combustion Science*, vol. 9, Mar. 2022, doi: 10.1016/j.jaecs.2021.100043.
[3] Baratta M, Chiriches S, Goel P, Misul D. "CFD modeling of natural gas combustion in IC engines under different EGR dilution and H2-doping conditions". Transportation Engineering, Vol. 2, 2020, 100018. https://doi.org/10.1016/j.treng.2020.100018

First name: Kaveh **LAST NAME**: ZAYER KABEH

Topic: Hydrogen-rich gas production via two-stage pyrolysis and catalytic steam reforming process

Course year: 1st **Tutor(s)**: David Chiaramonti, Matteo Prussi

Highlights of the research activity

Hydrogen production is one of the main sections of the hydrogen value chain, and a secure supply of green hydrogen is a significant challenge that should be addressed in the following years. Biomass resources can be used as feedstock to produce green hydrogen in thermochemical processes, such as pyrolysis. Although the pyrolysis process is a well-established technology with a high technology readiness level, hydrogen yield is not considerable in this process. The literature review demonstrates that reforming pyrolysis volatiles could considerably enhance hydrogen yield. Catalytic reforming of pyrolysis volatile including condensable and non-condensable components has some advantages compared to the pyrolysis, such as higher hydrogen production volume and more effective separate control of the processes conditions, e.g. temperature and steam input. However, most research studies were performed on a laboratory scale to evaluate this process. Considering the results of an extensive literature review that I performed during the first year of my PhD, my research goal is the techno-economic evaluation and life cycle assessment of this two-stage process on an industrial scale to produce hydrogen-rich gas. Also, it is worth mentioning that producing hydrogen-rich gas in this process will pave the way for producing clean alternative fuels such as bio-methanol and synthetic fuels.

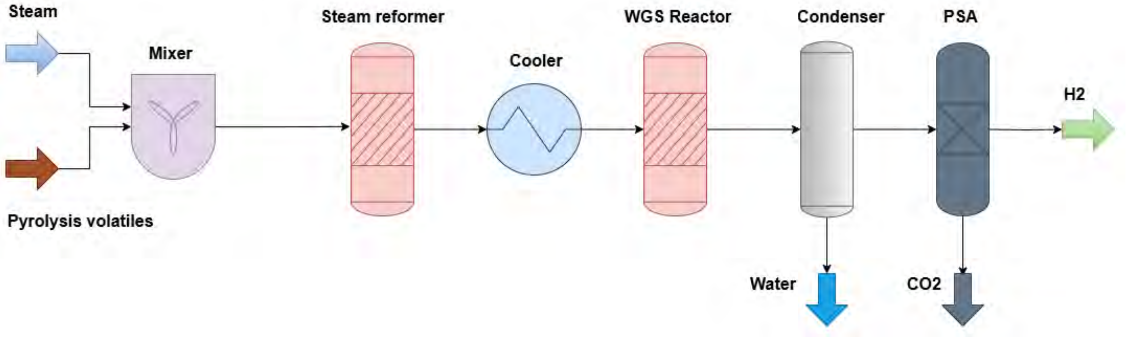


Figure. Catalytic reforming process of pyrolysis volatiles

It is necessary to assess different factors affecting hydrogen yield in this process, such as operational conditions, including reforming and pyrolysis temperatures and steam to carbon ratio and type of catalyst. In the first step of modeling this process, the process is modelled by using only non-condensable compositions of biomass pyrolysis volatiles. After that, condensable and non-condensable compositions will be used as a feedstock. The main challenge of this stage is some complex compositions of condensable materials that negatively affect the process, such as catalyst deactivation. Therefore, separating some compositions of pyrolysis volatiles before reforming could be beneficial to increase the efficiency of this process.

External collaborations

- RE-CORD- Renewable Energy Consortium for Research and Demonstration

Academic context

[1] Akubo K, Nahil MA, Williams PT, Pyrolysis-catalytic steam reforming of agricultural biomass wastes and biomass components for production of hydrogen/syngas, *Journal of the Energy Institute* 92 (2019) 1987-1996

[2] Zaini IN, Sophonrat N, Sjöblom K, Yang W. Creating Values from Biomass Pyrolysis in Sweden: Co-Production of H2, Biocarbon and Bio-Oil. *Processes 2021, Vol 9, Page 415.*

[3] Arregi A, Amutio M, Lopez G, Bilbao J, Olazar M. Evaluation of thermochemical routes for hydrogen production from biomass: A review, *Energy Conversion and Management 165(2018) 696-719*

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During the Phd Days our Energetics PhD students will have the chance to present and discuss their research activities.
Furthermore the workshop "Which energy sources (and which energy vectors) for final uses?" will provide a unique opportunity to gain insights from four distinguished international experts who have made significant contributions to the field of decarbonization.

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