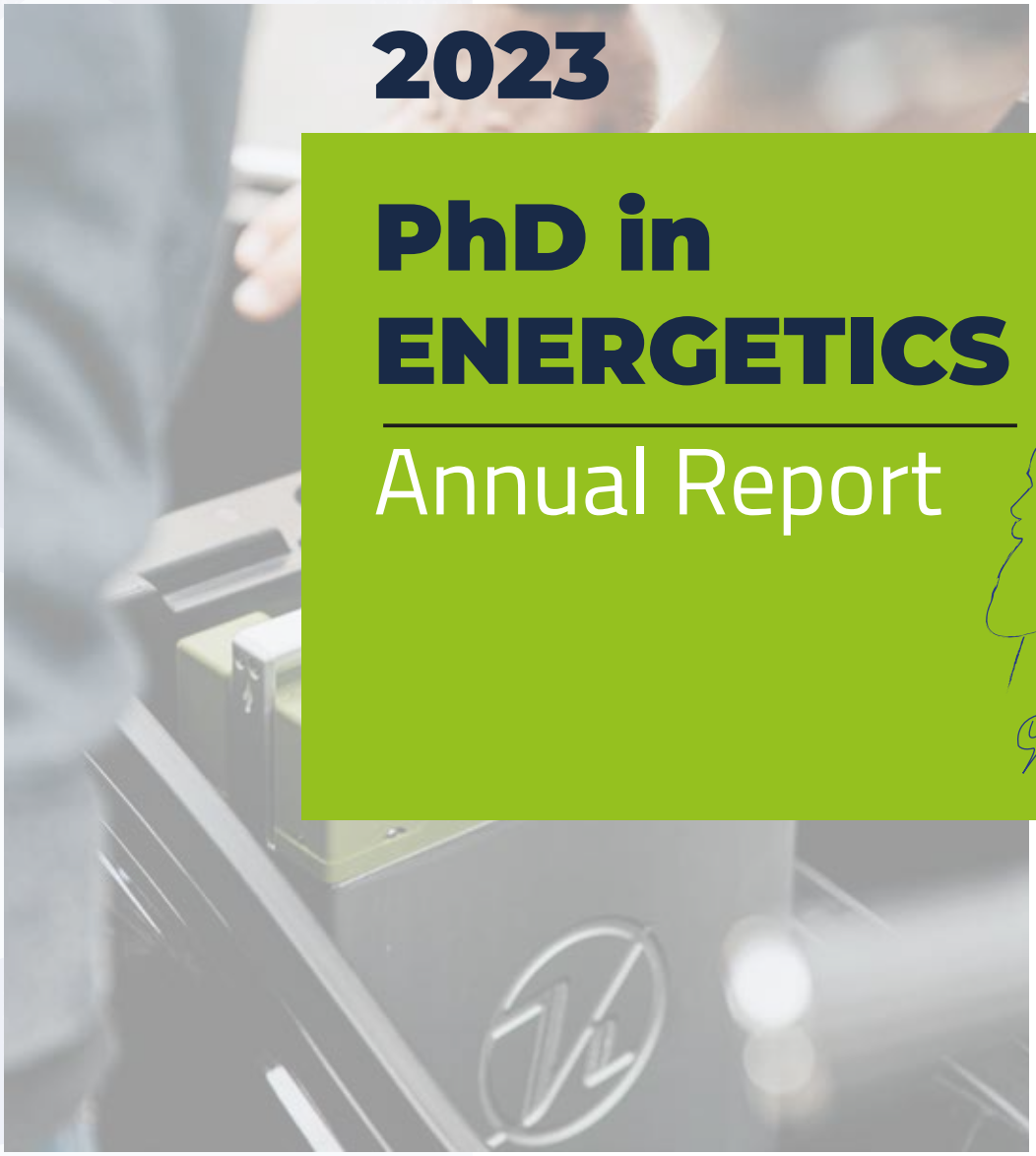
Politecnico di Torino

Department of Energy "G.Ferraris"



2023

PhD in ENERGETICS

Annual Report

Editors: Federico Millo & Laura Savoldi

Graphics: Mariapia Martino

December 2023

CONTENT

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 2023. The previous editions of the Annual Report can be downloaded from http://dottorato.polito.it/ene/en/documents_and_awards

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Acknowledgements

The following Companies are gratefully acknowledged for supporting the research activities of Energetics PhD students by granting academic licenses of their softwares:

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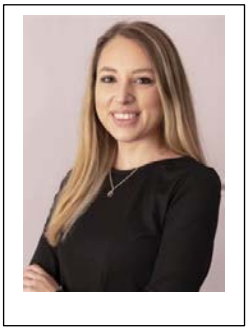
Sustainable propulsion and energy systems



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

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

Course year: 2nd **Tutor(s)**: Ezio SPESSA, Giovanni DOTELLI

Academic context

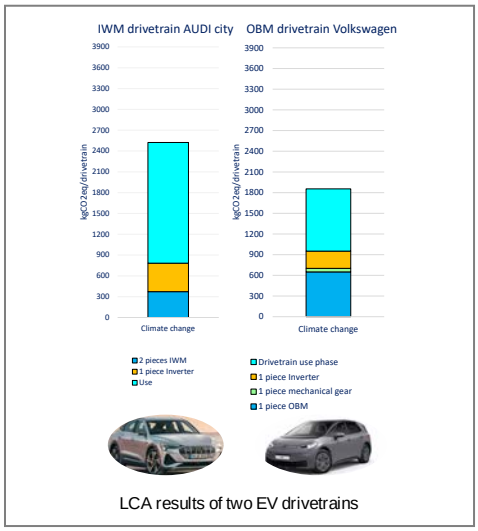
[1] Accardo, A.; Dotelli, G.; Musa, M.L.; Spessa, E. Life Cycle Assessment of an NMC Battery for Application to Electric Light-Duty Commercial Vehicles and Comparison with a Sodium-Nickel-Chloride Battery. Appl. Sci. 2021, 11, 1160. https://doi.org/10.3390/app11031160.
[2] A Accardo, G Dotelli, F Miretti, E Spessa. End-of-Life Impact on the Cradle-to-Grave LCA of Light-Duty Commercial Vehicles in Europe. Appl. Sci. 2023, 13 (3), 1494. https://doi.org/10.3390/app13031494.
[3] A Accardo, G Dotelli, E Spessa. Impact of different LCI Modelling Scenarios on the LCA Results. A Case Study for the Automotive Sector. SAE Technical Paper, 2023. https://doi.org/10.4271/2023-01-0884.

External collaborations

- POLIMI
- IVECO Group
- Stellantis

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, a significant part of the PhD activity is focused on critical Electric Vehicle (EV) components, namely the EV motor and the EV battery. The second year of the PhD course saw the data collection campaign and the assessment of the environmental impacts of two electric drivetrains in the framework of the EU-funded project "EM-TECH". One In-Wheel Motor (IWM) drivetrain and one On-Board Motor (OBM) drivetrain were chosen to be representative of the state-of-the-art and were assessed through LCA and Life Cycle Costing (LCC). The IWM drivetrain comprises two rear in-wheel motors and a dual IGBT inverter while the OBM drivetrain comprises one radial-flux electric motor, an IGBT inverter and a mechanical gearbox. The IWM drivetrain is mounted on a JAC iEV7 that was tested on a real driving mission, while the OBM drivetrain is representative of the MEB platform of the Volkswagen iD3 Pro performance.The carbon footprints of the IWM and OBM drivetrains are reported in the graph below. In the next months the state-of-the-art IWM and OBM drivetrains just assessed will serve as baseline for the comparison with two novel electric drivetrains.



LCA results of two EV drivetrains

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

Topic: Energy management of hybrid electric vehicles

Course year: 1st **Tutor(s)**: Daniela Anna MISUL

Academic context

[1] J. Zhou, S. Xue, Y. Xue, Y. Liao, J. Liu, and W. Zhao, "A novel energy management strategy of hybrid electric vehicle via an improved td3 deep reinforcement learning," Energy, vol. 224, p. 120118, 2021.
[2] H. Tan, H. Zhang, J. Peng, Z. Jiang, and Y. Wu, "Energy management of hybrid electric bus based on deep reinforcement learning in continuous state and action space," Energy Conversion and Management, vol. 195, pp. 548–560, 2019.
[3] G. Dulac-Arnold, N. Levine, D. J. Mankowitz, J. Li, C. Paduraru, S. Gowal, and T. Hester, "Challenges of real-world reinforcement learning: definitions, benchmarks and analysis," Machine Learning, vol. 110, no. 9, pp. 2419–2468, Sep 2021.

External collaborations

- Stanford University

Highlights of the research activity

During this first year of PhD, I mainly focus on the application of Reinforcement Learning (RL) to the smart mobility field. RL is one of the most promising branches of Machine Learning and has been applied in different research fields. In my work I tried to apply RL techniques to the energy management of Hybrid Electric Vehicles and to the Cooperative Adaptive Cruise Control applications.
In my first work, i.e., 'Influence of the reward function on the selection of Reinforcement Learning agents for Hybrid Electric Vehicles real-time control', I investigated the effects produced by a variation of the reward function and the real potentials of adopting a given RL agent under different testing conditions. In particular, the performances of different agents, specifically Q-learning, Deep Q-Network (DQN) and Double Deep Q-Network (DDQN), are investigated considering a full Hybrid Electric Vehicle in case of multiple driving missions and two distinct reward functions. The first function primarily aims at charge sustaining while the second on the minimization of fuel consumption (FC). The results surprisingly prove the incapability of DQN and DDQN to outperform traditional Q-learning when a SOC-oriented reward is considered, while confirming the results obtained in literature that DQN and DDQN outperform Q-learning with a FC-oriented reward.

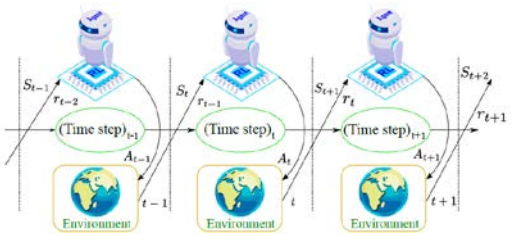


Fig. Scheme of sequential decision-making Reinforcement Learning process

In a second work, a recently developed reinforcement learning algorithm, called Twin Delayed Deep Deterministic Policy Gradient is applied to the control of the power-split to a high fidelity and real-time vehicle model developed in Simulink to reproduce as close as possible the conditions of a hybrid Toyota Prius. The focus of this work is to directly address the problem of infeasible control actions for RL applications in a continuous action space. A new physically guided exploration strategy is implemented, helping the RL controller to learn faster during the training phase.

First name: Filippo **LAST NAME**: AGLIETTI

Topic: Physics informed neural networks

Course year: 1st **Tutor(s)**: Federico MILLO, Andrea PIANO

Academic context

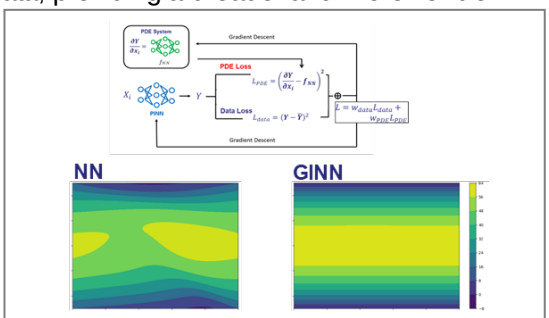
[1] Podina, Lena, Brydon Eastman, and Mohammad Kohandel. "Universal Physics-Informed Neural Networks: Symbolic Differential Operator Discovery with Sparse Data." In Proceedings of the 40th International Conference on Machine Learning, Honolulu, Hawaii, USA, 2023. PMLR 202.
[2] Chen, Z., Liu, Y. & Sun, H. Physics-informed learning of governing equations from scarce data. *Nat Commun* **12**, 6136 (2021). https://doi.org/10.1038/s41467-021-26434-1
[3] Udrescu, Silviu-Marian, and Max Tegmark. "AI Feynman: A physics-inspired method for symbolic regression." Science Advances 6, no. eaay2631 (2020). doi:10.1126/sciadv.aay2631.

External collaborations

- Punch Torino S. p. A.

Highlights of the research activity

As emission limits continuously tighten, the complexity of modern Diesel engines increases, making the calibration process ever more challenging. Recognizing the potential of virtualization in this field, the research activity was directed efforts towards leveraging Physics Informed Neural Networks (PINNs) to model diesel engine emissions. The key feature involves developing a new neural network architecture, named 'Gradient Informed Neural Network' (GINN). This represents a generalization of traditional Physics Informed Neural Networks (PINNs). Whereas PINNs generally require a full understanding of a system's differential equations, the GINN model extends their use to situations where such complete knowledge is not available.
This approach was partly inspired by a method outlined in [1], which employs a surrogate network to infer unknown parts of a system's differential equation. This method primarily focuses on the time derivative of the system. GINN builds on this by considering not just the time aspect but also gradients across all dimensions of the problem. It learns these gradient relationships directly from data, providing a broader and more flexible approach.
The GINN model's effectiveness hinges on a specialized loss function, denoted as $L(\Theta Y, \Theta F)$. This function is a composite of two components: LY (ΘY) and LF $(\Theta F, \Theta Y)$. The first component, LY (ΘY), minimizes the difference between predicted and actual data points, ensuring model accuracy with observed data. The second, LF $(\Theta F, \Theta Y)$, focuses on gradient alignment in all dimensions, facilitating adherence to system dynamics and derivative behavior.
To validate the effectiveness of the developed method, we conducted tests on synthetic datasets. A key demonstration of the method's capabilities is illustrated in a comparative analysis, presented in a figure within the study. This analysis shows the accuracy of a standard neural network versus a GINN in predicting the velocity field of a laminar viscous fluid in a tube
By incorporating the concept of surrogate networks into the GINN framework, the neural network becomes capable of effectively handling systems with only partial information as for in scenarios like emission formation, where a comprehensive understanding of all dynamics might not be available and data can be sparse.



Schematic architecture of the proposed gradient informed neural network.

Below accuracy test over laminar velocity field in straight pipe. NN vs GINN.

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

Topic: Innovative solutions for sustainable mobility

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

Academic context

[1] 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.
[2] 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
[3] Matteo Acquarone, Angelo Borneo, Daniela Anna Misul, "Acceleration control strategy for Battery Electric Vehicle based on Deep Reinforcement Learning in V2V driving", 2022 IEEE Transportation Electrification Conference & Expo (ITEC)

External collaborations

- MCA Engineering

Highlights of the research activity

The research acrivity carried out during the 2nd year involves further development of ADASs

Centralized controller for vehicular platooning

This activity consists in the comparison of two control strategies to realize a centralized controller for a platoon of vehicles. The compared control architectures are linear quadratic control (LQC), hence an optimal control, and deep reinforcement learning (DRL) as innovative solution to such a problem.
The comparative analysis of the two controllers evaluates: the ability to track inter-vehicle distance and vehicle speed references during a standard driving cycle, the string stability, and the transient response when an unexpected obstacle occurs. Promising results are achieved since the two controllers present similar value for most of some defined performance indices. Other than that RL-based controller shows great performance also on cycles different than the training one, assessing its potential for real time and real-world applications.

Localized controller for vehicular platooning

This second work aims at developing a controller on each vehicle along the platoon. Such a choice is dictated by the fact that from the commercialization point of view such a solution could spread wider. The DRL agent is once again the DDPG agent. The latter has no restrictions on the structure of its reward function. The chosen one is a multi-objective function, composed by 3 terms each multiplied by varying weights: a term dependent on the time headway, one dependent on the time to collision and one on the acceleration. The agent is trained in a car following scenario, and then deployed on each vehicle, hence tested in a platoon scenario. Moreover, maps containing the drag coefficient reduction as a function of the intervehicle distance have been integrated in the model, in order to assess energy savings. Results show great opportunity to achieve energy efficiency, safety and comfort, furthermore attenuation of speed perturbations along the platoon are quite evident. To further develop this control technique v2v errors and delays will be included in future works.

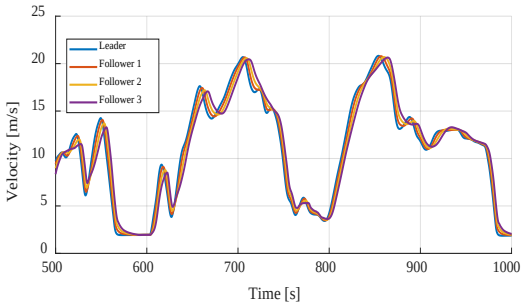


Fig. velocities of leader vehicle and followers

First name: Salvatore **LAST NAME**: CARUSOTTO

Topic: Fuel-flexible gas turbines for decarbonization

Course year: 1st **Tutor(s)**: Daniela Anna MISUL, Simone SALVADORI, Mirko BARATTA

Academic context

[1] 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

[2] Douglas, C. M., Shaw, S. L., Martz, T. D., Steele, R. C., Noble, D. R., Emerson, B. L., and Lieuwen, T. C. (July 28, 2022). "Pollutant Emissions Reporting and Performance Considerations for Hydrogen–Hydrocarbon Fuels in Gas Turbines." ASME. *J. Eng. Gas Turbines Power*. September 2022; 144(9): 091003

[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

External collaborations

- Ethos Energy Italia S.p.A.

Highlights of the research activity

During the first year of PhD the research activity focused mainly the combustion modelling both for premixed and non-premixed gas turbine combustors for low NOx emissions applications. Diffusive combustors in case of hydrogen blending have been extensively studied, focusing on two different study-cases provided by EthosEnergy Italia SpA (sponsor of the scholarship). The two burners have been characterized using 3D CFD RANS simulations. The analysis has been conducted by using the Flamelet Generated Manifold (FGM) combustion model. In the first machine the complete characterization in terms of pressure drops, air split and temperature profiles has been carried out, while in the second case-study, the computational domain has been simplified removing the casing, since the air split for the compressor flow was already known from a previous study. In this case, also the NOx emissions have been assessed by using a post-processing procedure. This work was presented at ASME Turbo Expo 2023 in Boston and published in Journal for Gas Turbine and Power [1]. The use of hydrogen can help in reducing the carbon dioxide emissions associated to the combustion process in the gas turbine burner. However, it is well known that the use of hydrogen can lead to higher NOx emission due to higher combustion temperatures and due to the presence of additional formation paths. Figure 1 reports the estimated NOx emissions increase with respect to the natural gas case in case of hydrogen blending for a diffusive burner. It is worth noticing that the use of a standard metric such as the concentration in ppmvd could lead to an overestimation of the increase for blending [1][2] and it is hence necessary a modification in the current metrics and regulations for the sector.

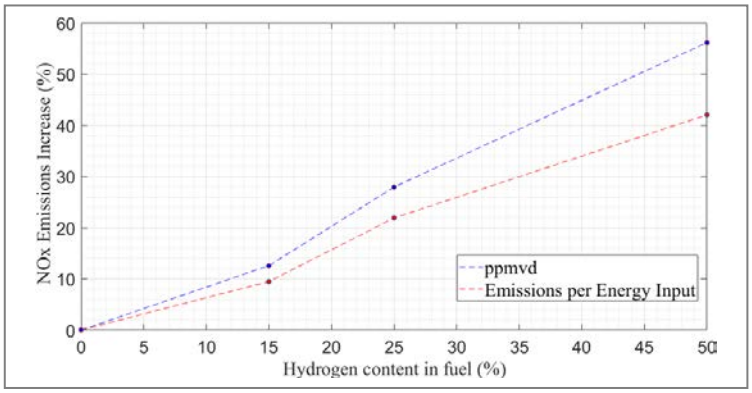


Fig. NOx emissions increase in case of hydrogen blending – ppmvd Vs Emissions per Energy Input, diffusive gas turbine combustor

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

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

Course year: 2nd **Tutor(s)**: Federico MILLO, Luciano ROLANDO

Academic context

[1] Scarcelli, R., Matthias, N., and Wallner, T., "Numerical Investigation of Combustion in a Lean Burn Gasoline Engine," SAE Technical Paper 2013-24-0029, 2013, https://doi.org/10.4271/2013-24-0029.
[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] Li, T., Gao, Y., Wang, J. and Chen, Z., "The Miller cycle effects on improvement of fuel economy in a highly boosted, high compression ratio, direct-injection gasoline engine: EIVC vs. LIVC," Energy Convers Manag 79:59–65, 2014, https://doi.org/10.1016/j.enconman.2013.12.022.

External collaborations

- FEV Italia
- Centro Ricerche Fiat
- IFP Energies Nouvelles

Highlights of the research activity

Many governments today have set legislative targets for the complete electrification of new light-duty vehicle fleets by 2035 in an attempt to reduce the carbon footprint and pollutant emissions of the transportation sector. Nevertheless, recent studies have shown that an approach based on a single technological scenario will not be sufficient to ensure that sustainability goals, like reaching carbon neutrality by 2050, are met. Thus, it is essential to continue to develop innovative hybrid-oriented Internal Combustion Engines (ICEs) as part of the environmentally friendly mix of solutions to achieve full decarbonization of on-road mobility.
In this context, my research activity is focused on assessing the benefits in terms of efficiency gains and emissions reduction of a set of innovative technologies applied to a state-of-the-art Spark-Ignited ICE as part of the EU-funded PHOENICE project. This prototype engine is characterized by a novel combustion system featuring a dual-diluted combustion based on the use of a lean mixture in combination with cooled long-route Exhaust Gas Recirculation (EGR). Additionally, the engine boasts a high compression ratio of 13.6 and redesigned intake ports to ensure strong in-cylinder turbulence. It also takes advantage of aggressive cycle Millerization through the full control over the intake valves timing and lift together with an electrified turbocharger to maximize the synergies with the hybrid architecture. On the exhaust aftertreatment side, an EU7-ready system with electrical heating and fit for lean combustion exhaust gases is found. To date, my Ph.D. activity has focused on assessing the potential of these technologies using 1D-CFD models as well as experimental testing at the dynamic engine test rig located inside the DENERG department of PoliTO. The developed fully physical 1D-CFD model of the PHOENICE engine served for virtual calibration purposes in terms of optimal intake valves actuation as well as best λ and EGR combinations. Currently, all the efforts are concentrated on experimental testing to further evolve the engine controls calibration under both steady-state and transient operations, such as driving cycles.

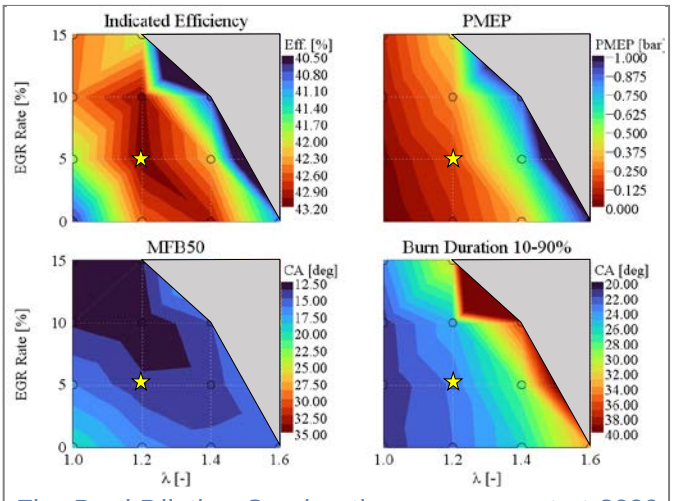


Fig. Dual Dilution Combustion assessment at 3000 RPM and 13 bar BMEP: effect of λ and EGR on indicated efficiency, pumping losses and combustion.

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

Topic: Hydrogen efficient use in small size spark ignition engine

Course year: 2nd **Tutor(s)**: Federico MILLO, Luciano ROLANDO

Academic context

[1] Oamjee A., S. Rajesh, Suitability of helium gas as surrogate fuel for hydrogen in H2-Air non-reactive supersonic mixing studies, International Journal of Hydrogen Energy, Volume 47, Issue 15, 2022, Pages 9408-9421, ISSN 0360-3199, https://doi.org/10.1016/j.ijhydene.2022.01.022.

[2] Gevorkyan, L., Shoji, T., Peng, W., & Karagozian, A. (2018). Influence of the velocity field on scalar transport in gaseous transverse jets. Journal of Fluid Mechanics, 834, 173-219. https://doi:10.1017/jfm.2017.621.

External collaborations

- CNR - Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili (STEMS), Napoli (IT).
- Chalmers University of Technology, Gothenburg (SE).

Highlights of the research activity

The analysis of velocity and flow-field structure of helium through the use particle image velocimetry (PIV) technique was carried out. The experimental test campaign involved the acquisition of 24 operating conditions during which the pressure ratio (PR) ranged from 2.0 to 20. It was used a dual cavity Nd:YAG laser and an optically accessible spray chamber inside which was positioned a customized light-duty automotive sized gas injector that allowed the use of three geometry nozzles characterized by different holes surface size/shape. A cross-correlation algorithm was applied to evaluate the raw images. Using this tool, it was possible to divide the post processing of the scattered images in various steps aimed to the enhancement of the main image properties and the definition of an "useful area" with related coordinate. The first geometry turned out to have low mixing capacities if compared to the second, in fact for the latter it was observed that before reaching the steady-state conditions between the two jets take place a low velocity area, and it becomes more evident by decreasing the PR. This phenomenon can be explained by addressing to the increased backpressure of air, which acts mainly in the side regions of the jets, where the velocity streamlines are slower than in the inner area. The same considerations can be drawn out for the third geometry; indeed, it is clearly possible to distinguish the side and central jets. The main results follow:

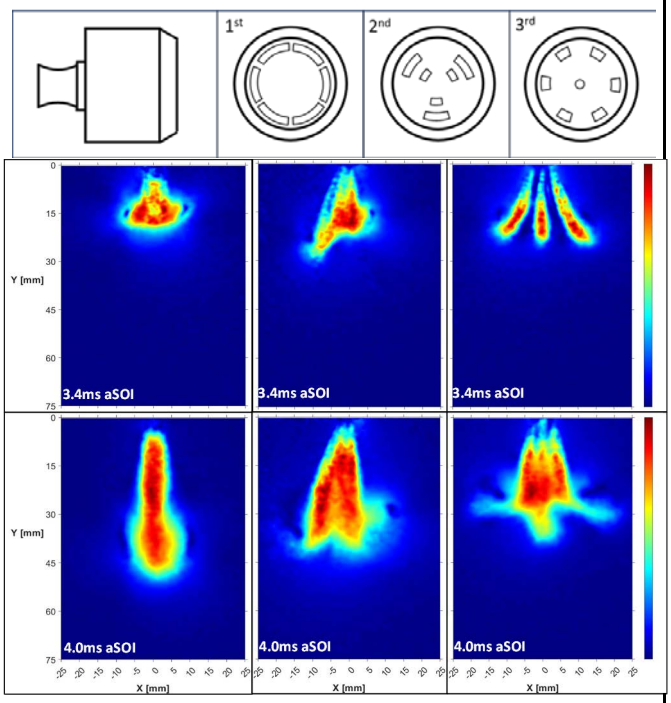


Fig. *Nozzle patterns (top), helium jet structure at 3.0, 3.4 and 4.0ms aSOI. frames, PR5 (bottom).*

- The use of nozzle patterns with a low "orientation" degree, like first geometry, lead to the generation of jet structures able to keep momentum, thus faster and with an improved penetration capacity. On the other hand, the tendency of the single jets to immediately "fall" on the injector axis suggests a reduced mixing properties limiting the entertainment of air to the side regions of the jet.
- The second and third geometries, both characterized by a higher degree of divergence with reference to the injector axis, showed how a more oriented solution improve the mixing capacity by expanding the jet-air area of contact, ensuring an extended "survival" of the jet structures although limiting the penetration.
- The PR variation turned out to have a greater influence on the velocity magnitude, which in steady state regime increased from around of 100 m/s to more than 300 m/s rather than vorticity that moved from 135000 1/s to slightly less than 250000 1/s, while velocity and vorticity distributions are minorly affected.

First name: Trentalessandro **LAST NAME**: COSTANTINO

Topic: Sustainability assessment of advanced propulsion systems and fuel pathways for Commercial Vehicles

Course year: 1st **Tutor(s)**: Ezio SPESSA, David CHIARAMONTI, Giovanni DOTELLI

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.

External collaborations

- IFP Energies Nouvelles

Highlights of the research activity

I conducted an in-depth analysis of alternative fuels, encompassing biofuels, advanced biofuels, and e-fuels. This involved an extensive literature review, focusing on the 'well-to-tank' impacts. I critically examined the Renewable Energy Directive II (REDII) and its amendments, as well as proposed modifications within the EU. My primary focus was on mandatory CO2 reduction targets for fuel production in Europe, offering a comprehensive overview of challenges and opportunities.

Additionally, I served as a course collaborator for 'Energy Management in Hybrid Electric Vehicles,' a course part of the Automotive Engineering MSc program. In conjunction with my teaching role, I delved into the electrification of commercial vehicles, emphasizing the potential benefits of applying Electrified Road Systems (ERS) along highways. I presented my findings at the "16th International Conference on Engines & Vehicles", September 2023 (DOI: https://doi.org/10.4271/2023-24-0161), showcasing potential environmental and economic benefits through the possibility of reducing battery capacity and, consequently, costs for fleet operators.

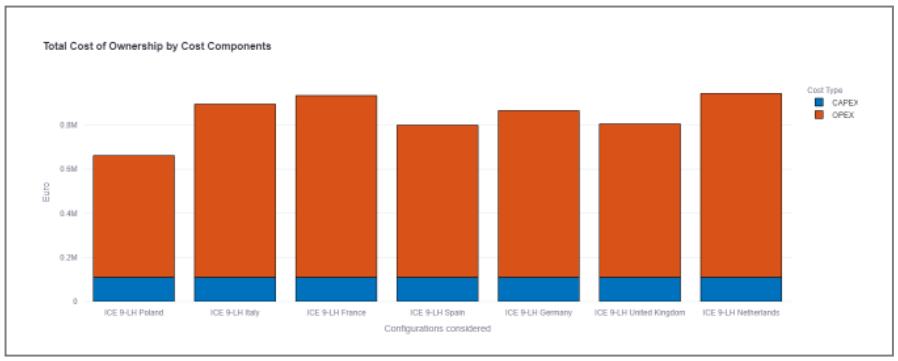


Fig. Total Cost of Ownership of Rigid Truck

During a three-month stint at IFP Energies Nouvelle, since September 2023, I honed economic analysis skills, specifically Total Cost of Ownership (TCO). These skills contributed to develop a model evaluating total costs associated with commercial vehicles. In this period, I focused on the assessment of two baselines Diesel powered, one for regional and the other for long haul application. The model aimed to assess various technologies, including BEV, FCEV, and alternative fuels.

In conclusion, these research endeavors provided valuable insights into alternative fuels, Electrified Road Systems for commercial vehicles, and economic considerations in Total Cost of Ownership analysis for commercial vehicles. I look forward to further exploring and analyzing these aspects over the next two years.

First name: Cosimo **LAST NAME**: DI DIO

Topic: Development and assessment of innovative controllers for the integrated optimization of the combustion process and ATS system in heavy-duty diesel vehicles

Course year: 3rd **Tutor(s)**: Roberto FINESSO, Ezio SPESSA

Academic context

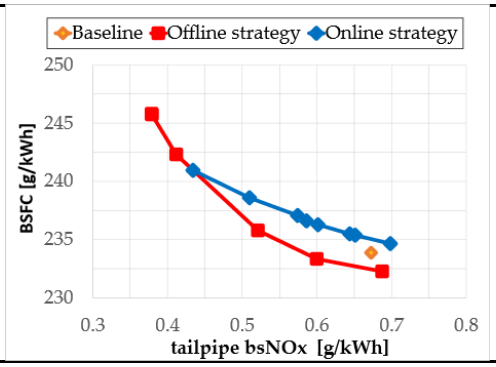
[1] David D., Randall et al. “Selective Catalytic Reduction”. Research Triangle Park, NC 27709 (2019): Chap.2
[2] Culbertson, David et al. “The Study of Exhaust Heating to Improve SCR Cold Start Performance”. SAE Int. J. Engines 8 [3] (2015): 1186-1195
[3] Finesso, R.; Hardy, G. et al. “Real-Time Simulation of Torque and Nitrogen Oxide Emissions in an 11.0 L Heavy-Duty Diesel Engine for Model-Based Combustion Control” Energies (2019), 12, 460, doi:10.3390/en12030460

External collaborations

- FPT Industrial
- Iveco

Highlights of the research activity

This PhD project involved the development of a scalable powertrain controller for combustion engines. The controller was evaluated using simulation data and showed the ability to meet the main homologation cycles in terms of brake-specific fuel consumption (BSFC) and NOx emissions. The research involved three main phases: vehicle model development, combustion controller model development, and coupled vehicle-and-controller model validation. A vehicle model of an FPT F1C EURO VI diesel engine was modified to include a Diesel Oxidation Catalyst (DOC), Diesel Particulate Filter (DPF), and Selective Catalytic Reduction (SCR) system. The DOC model was designed to reproduce the phenomenological trends of NO/NO2 conversion of similar models found in the literature as these curves are of big importance for the accuracy of the reduction efficiency curves of the SCR system. The DPF model accounted for the average pressure drop of a half-filled DPF with pressure drop curves taken also from literature. The SCR system model was based on equivalent performance data from the literature. Since no experimental data for the entire system was available, a general model validation was performed by comparing the model's performance to that of equivalent powertrains from the literature. The combustion controller was developed using two strategies: online and offline. The online strategy dynamically adjusts the engine to meet NOx tailpipe emissions, while the offline strategy optimizes fuel and AdBlue consumption and it’s based on the definition of an objective function. Both strategies demonstrated promising results in simulation experiments and will be further tested on an actual vehicle. The research team plans to merge the two strategies to explore the benefits of dynamic powertrain calibration in real-world powertrain operation. This will involve extensive experiments on an actual vehicle to evaluate the performance and robustness of the merged strategy.



Performances of both strategies showed in the form of break-specific fuel consumption-NOx emissions trade-off. The baseline point is presented in yellow.

First name: Giuseppe **LAST NAME**: DI LUCA

Topic: Advanced Battery Management System Solutions for a Smart and Connected Electrified Mobility

Course year: 1st **Tutor(s)**: Daniela Anna MISUL

Academic context

[1] Hannan, M.A.; Lipu, M.S.H.; Hussain, A.; Mohamed, A. A review of lithium-ion battery state of charge estimation and management system in electric vehicle applications: Challenges and recommendations, Renewable and Sustainable Energy Reviews, Volume 78, 2017, Pages 834-854, ISSN 1364-0321, https://doi.org/10.1016/j.rser.2017.05.001.
[2] Wang, Y.; Tian, J.; Sun, Z.; Wang, L.; Xu, R.; Li, M.; Chen, Z. A comprehensive review of battery modeling and state estimation approaches for advanced battery management systems, Renewable and Sustainable Energy Reviews, Volume 131, 2020, 110015, ISSN 1364-0321, https://doi.org/10.1016/j.rser.2020.110015
[3] Tran, M.-K.; Panchal, S.; Khang, T.D.; Panchal, K.; Fraser, R.; Fowler, M. Concept Review of a Cloud-Based Smart Battery Management System for Lithium-Ion Batteries: Feasibility, Logistics, and Functionality. Batteries 2022, 8, 19. https://doi.org/10.3390/batteries8020019

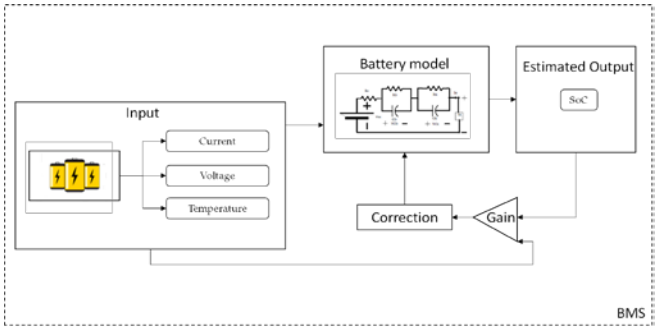
External collaborations

- CNR-STEMS
- Center for Automotive Research (CAR)-Ohio State University
- Teoresi SPA

Highlights of the research activity

The reference research period has been devoted to an extensive literature review of estimation methods for the battery state of charge (SoC) and state of health (SoH). The estimation of these latter is fundamental for the battery management system to ensure a proper charge/discharge phase and correct thermal management, thus avoiding battery degradation. The considered methods, characterized by different levels of detail and complexity, can be divided into different categories depending on the estimation approach: direct, model-based, and data-driven methods. Since direct methods are only for laboratory purposes, these methods are not suitable to be implemented online. SoC model-based estimation approach, particularly the Kalman filter and its extensions, represents the right trade-off between complexity and estimation accuracy due to their self-correcting nature and acceptable computational burden for online implementation. Conversely, model-based SoH estimation is more challenging due to the complex nonlinear aging mechanism of the battery. A growing trend is represented by the use of machine learning techniques for SoH prediction. Notwithstanding, the computational effort is another non-negligible aspect to consider. In a real scenario, as the number of batteries increases, the amount of computing and data storage required by BMS grows exponentially. Therefore, the advancements of in-cloud solutions for battery state estimation through more detailed data-driven algorithms is expected.

Model based approach for battery state estimation.



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

Academic context

[1] Perkins, H. Douglas, and Daniel E. Paxson. "Summary of pressure gain combustion research at NASA." (2018).
[2] LIU, Zhe; BRAUN, James; PANIAGUA, Guillermo. Integration of a transonic high-pressure turbine with a rotating detonation combustor and a diffuser. *International Journal of Turbo & Jet-Engines*, 2020.
[3] Insinna M., Salvadori S., Martelli F., 2014. Simulation of Combustor/NGV Interaction Using Coupled RANS Solvers: Validation and Application to a Realistic Test Case. Proc. of the ASME Turbo Expo 2014, Dusseldorf, Germany, June 16-20, Volume 2D: Turbomachinery, pp. V02CT38A010 (12 pages), doi: 10.1115/GT2014-25433, Paper No. GT2014-25433 (978-0-7918-4562-2).

External collaborations

- Pprime Institute, ENSMA, Poitiers, France
- University of Purdue (UP), West Lafayette, U.S.A
- Technical University of Berlin (TUB), Berlin, Germany

Highlights of the research activity

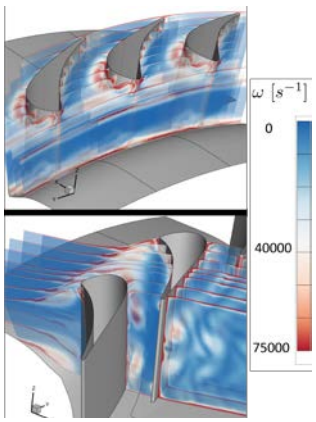


Fig. Secondary Flow Footprints in a HPT Vane after RDE

Nowadays, the Gas Turbine community focuses efforts on pioneer propulsion systems. One of the promising solutions is the Pressure Gain Combustors (PGC), in which stagnation pressure increases during combustion leading to a larger inlet turbine temperature and higher theoretical cycle efficiency. The advantages of PGC are accompanied by significant produced unsteadiness of the flow field which is guided inside the first stages of turbine. The current doctoral study focuses on the analysis of High-Pressure Turbine (HPT) stage under highly pulsating inflow using unsteady 3D CFD methods.

The first PGC, which is under investigation, is the Constant Volume Combustor (CVC). First, a 0D/1D model of the ensemble test rig is created to retrieve the highly unsteady outlet stagnation conditions of the chamber's exhaust valves. These transient signals are employed as spatial-average transient inlet Boundary Conditions (BCs) to the exhaust flow domain, which is consisted of a converging – diverging nozzle, and the Unsteady Reynolds - Average Navier – Stokes (URANS) equations are calculated. In addition, an optimization method leads to a transition duct after the CVC that couples the chamber with a HPT vane. Similarly, the unsteady flow field of the new exhaust domain is obtained. In the end, this part of the activity will be concluded with a 2-month secondment at the premises of ENSMA for the experimental test of the optimized transition duct.

The other analyzed PGC is the Rotating Detonation Engine (RDE). TUB developed a RDE experimental test rig. A 2-month secondment at TUB was spent focusing on the creation of a transition duct after the RDE by numerical means, which will attenuate the exhaust flow field before entering to a subsequent HPT stage. In parallel, a HPT vane with highly – diffusive endwalls is designed to serve the peculiar case of RDE. The endwalls intensively enlarge the secondary flows through the vane's passage, as it can be observed in Figure 1. Hence, a novel flow control system by blowing cool air through the endwalls of the vane will be designed, in the three-month secondment period in UP.

First name: Tiziano Alberto **LAST NAME**: GIULIACCI

Topic: A.I. solutions in automotive sector for xEV's energy management

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

Marco FAINELLO

Academic context

[1] L. Zubieta and R. Bonert, "Characterization of double-layer capacitors for power electronics applications," in IEEE Transactions on Industry Applications, vol. 36, no. 1, pp. 199-205, Jan.-Feb. 2000, doi: 10.1109/28.821816.

[2] P. Kollmeyer et al., "Optimal performance of a full scale li-ion battery and li-ion capacitor hybrid energy storage system for a plug-in hybrid vehicle," 2017 IEEE Energy Conversion Congress and Exposition (ECCE), Cincinnati, OH, USA, 2017, pp. 572-577, doi: 10.1109/ECCE.2017.8095834.

[3] T.A. Giuliacci et al., "Artificial Intelligence Solutions for Time Latency Cancellation for Driving Simulator and Remote Simulator Subsystems Connection", in the proceedings of the Driving Simulation Conference Europe 2023 VR, Antibes, France, 6-8 September 2023.

External collaborations

- Add-For S.p.a.

Highlights of the research activity

Li-ion cell data collecting test bench development was covered earlier in the activity. Nevertheless, the project was not completed, and homemade cell data were not obtained. Thus, literature data were used to tune and validate the battery electro-thermal model, obtaining different cell models. In particular, three cylindrical cells 186500 were examined. Then, an automated tool for model tuning and identification of the electrical cell model have been developed.

After that, a Hybrid Energy Storage System (HESS) with supercapacitors was built using the final battery model. For the supercapacitors, a literature model has been used. This system incorporates simple BMS logics formerly designed. A dynamic-longitudinal vehicle model is then connected to HESS. The HESS power-split control is being implemented utilizing a Reinforcement Learning agent. The main goal of the strategy is to ensure the health and safety of the Li-Ion battery, while also optimizing its autonomy. The final results will be available in a few weeks.

Meanwhile, the concept of cloud BMS has been introduced. This involves conducting studies on signal communication and investigating the communication performances between devices in terms of delay and stability. An AI solution has been proposed for the signal latency canceling in a cloud BMS perspective. Currently, the software has only been validated in local environments, for delay compensation in automotive driving simulators.

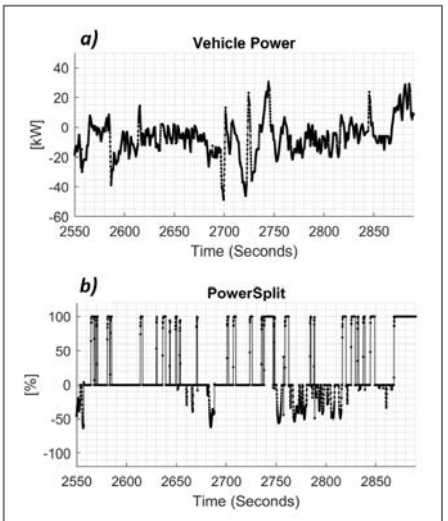


Fig. *Outputs from the HESS during a training episode of the Reinforcement Learning agent. In the figure* ***a.*** *the power required to the HESS, and in the figure* ***b.*** *the power-split between the two energy storage systems (100% means the whole power is provided by the supercapacitors, 0% the whole power is provided by the Li-Ion battery pack and negative values mean that the battery pack is also re-charging the supercapacitors).*

First name: Simona **LAST NAME**: GURRI'

Topic: New-generation of bi-modal freight electro-trains: engineering for hybrid ICEs powered with alternative fuels

Course year: 2nd **Tutor(s)**: Alessandro FERRARI, Bruno DALLA CHIARA

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

External collaborations

- Alstom Ferroviaria S.p.A.
- FPT Industrial
- Blue Engineering

Highlights of the research activity

In the domain of freight transportation, the imperative for sustainability has heightened, propelled by initiatives such as the European Green Deal and the Fit for 55 policies. Throughout 2023, my research delved into the analysis of ***sustainable freight transportation***. This endeavor encompassed collaborative engagements with industry partners, fostering advancements that not only exhibit economic viability but also align with the eco-friendly objectives mandated by EU policies.
The key aspects analyzed include:

- **F-EMU Monitoring System**; in collaboration with *Alstom Ferroviaria*, the development of an Integrated Monitoring System (*Fig 1*) for a new generation ***Freight Electric Multiple Unit (F-EMU)***, whose functional design was outlined last year, emerged as a pivotal project. In fact it enables the F-EMU to meet the requirements of high-speed rail operations. This system enhances the train's RAMS aspects, contributing to its efficiency and effectiveness in freight transport.

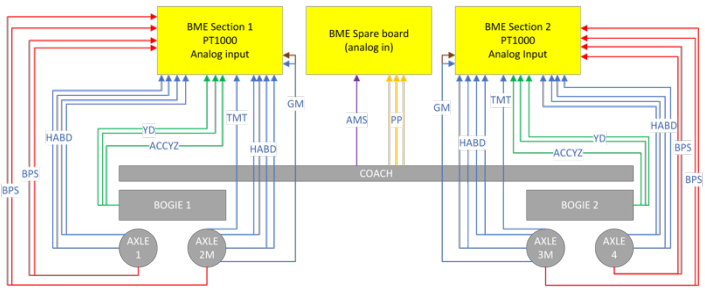


Fig. Monitoring system physical architecture: wiring layout

- **Yard Tractors Electrification Feasibility**; a focus was made on assessing the feasibility of electrifying yard tractors, applied to the case of the *PSA Sech terminal* in the port of Genoa. This study explored the ***economic viability*** and potential environmental benefits and limits associated with electrifying the fleet, providing insights for future port operations.
- **Software for Train Consumption Simulations**; a contribution involved the development of software tailored for ***simulating train consumption*** (kWh/pass·km). The aim is to optimize energy efficiency in freight train for various operational scenarios.
- **CFD for Heavy-Duty ICEs**; collaborating with *FPT*, CFD simulations have been initiated to explore the retrofitting of a heavy-duty spark ignition engine. This ongoing investigation aims at assessing the feasibility of ***alternative energy carriers*** - such as hydrogen or methanol - for freight transportation, taking into account new models for turbulence evaluation inside the cylinder and the combustion of these greener fuels. This work paves the way for the low-TCO bi-modal hybrid powertrain of the F-EMU.

First name: Mohammadjavad **LAST NAME**: JAFARI MAHMOUDABADI

Topic: Renewable fuels for ICE: analysis of GHG and pollutant emissions reduction potential

Course year: 3rd **Tutor(s)**: Federico MILLO, Andrea PIANO

Academic context

[1] G. Di Blasio, R. Ianniello, and C. Beatrice, "Hydrotreated vegetable oil as enabler for high-efficient and ultra-low emission vehicles in the view of 2030 targets," Fuel, vol. 310, Feb. 2022, doi: 10.1016/j.fuel.2021.122206.
[2] Jiaqiang E, Wanrong Xu, Yinjie Ma, Dongli Tan, Qingguo Peng, Yan Tan and Lehan Chen, "Soot formation mechanism of modern automobile engines and methods of reducing soot emissions: A review," Fuel Processing Technology, vol. 235. Elsevier B.V., Oct. 01, 2022. doi: 10.1016/j.fuproc.2022.107373.
[3 Wong, C.P. and Chan, T.L. and Leung, C.W., "Characterization of diesel exhaust particle number and size distributions using mini-dilution tunnel and ejector-diluter measurement techniques" Atmospheric Environment, vol.37, pp. 4435-4446, oct 2003, doi: 10.1016/S1352-2310(03)00571-5.

External collaborations

- ENI
- Punch Torino
- Università degli studi di Perugia

Highlights of the research activity

This research project was devoted to a comprehensive investigation into the utilization of neat Hydrotreated Vegetable Oil (HVO) as an alternative fuel in a light-duty engine. Following injection and spray tests, the experimental campaign encompassed diverse steady-state and transient operating conditions on a 1.6L, four-cylinder, turbocharged, Euro 6 diesel engine. The final phase of the research focused on characterizing HVO particulate matter (PM) under different load/speeds, injection pressures, and EGR levels using the Electrical Low-Pressure Impactor (ELPI). The results, consistent with those obtained from other measurement devices such as the smoke meter and Concentration Particle Counter (CPC), demonstrate a significant reduction in HVO particle mass at the engine-out sampling point. However, the distribution of particle number (PN) and mass (PM) concentrations revealed a higher number of particles in the nucleation mode region for HVO, exhibiting greater sensitivity to changes in load/speed compared to diesel (Figure 1-A1 and B1). Conversely, the number of particles in the agglomeration mode, which contributes most to total particle mass, was dramatically lower for HVO (Figure 1-A2 and B2). This difference is likely due to the absence of Poly-cyclic Aromatic Hydrocarbons (PAH) in the HVO structure.

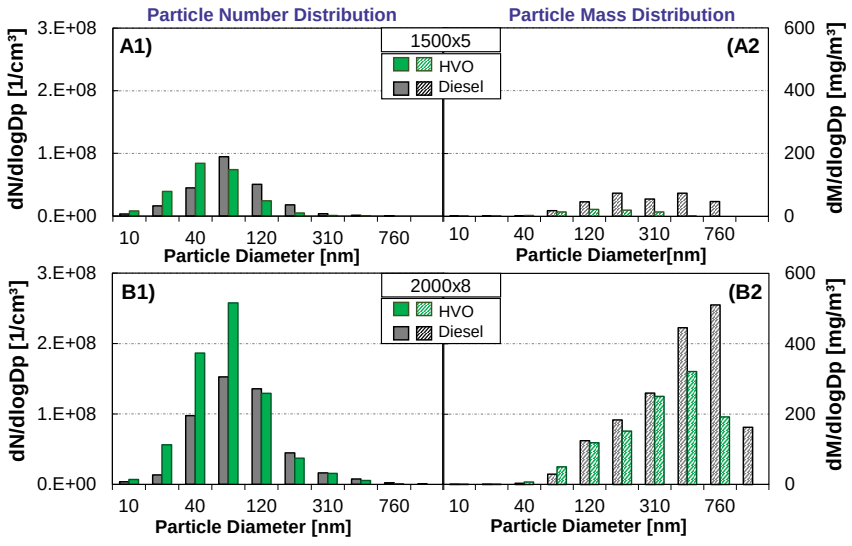


Fig. Distribution of particle number and mass concentrations for HVO and diesel fuels at 1500 rpm and 5 bar BMEP (A1-2) and at 2000 rpm and 8 bar BMEP engine operating condition.

First name: Meng **LAST NAME**: JI

Topic: Modeling and experimental analysis of combustion, fuel spray and turbulence in combustion engines

Course year: 3rd **Tutor(s)**: Alessandro FERRARI

Academic context

[1] Ji M, Ferrari A, Shang Q, et al. Combustion and Emission Characteristics of Ammonia Jet Flames, Based on a Controllable Activated Thermal Atmosphere. No. 2023-01-1645. SAE Technical Paper, 2023.
[2] Shang Q, Ji M, Li L, et al. NOx Emission Characteristics of Active Pre-Chamber Jet Ignition Engine with Ammonia Hydrogen Blending Fuel. No. 2023-01-1629. SAE Technical Paper, 2023.
[3] Ji M, Wu Z, Ferrari A, et al. "Experimental Investigation on Gasoline—Water Mixture Fuel Impingement Preparation Method and Spray Characteristics with High Injection Temperatures and Pressures." Energies 16.16 (2023): 6026.

External collaborations

- Tongji University
- Tsinghua University

Highlights of the research activity

Ammonia, as a new type of zero-carbon fuel with low storage and transportation cost, has wide application prospects. There are still problems that should be solved: high self-ignition temperature and high NOx emission. Investigations on ammonia combustion stability and on ammonia flame enhancement for low emissions are therefore crucial for its application as a fuel for internal combustion engines.
In my research, the ammonia diffusion jet flame had been investigated in a high temperature co-flow and three different flame enhancement methods (ammonia/hydrogen, ammonia/methane and rich-oxygen combustion) had been evaluated. In particular, combustion jet flame morphology and stability had been examined, based on an extensive experimental campaign referring to different co-flow velocities, co-flow temperatures and jet pressures. The overall color of the ammonia jet diffusion flame is orange with some red zones. With an increase in hydrogen ratio, the flame brightness, area and length increase. Moreover, the influence of co-flow temperature on the lift height and ignition delay of ammonia and ammonia mixtures flames had been analyzed. Under the conditions of higher co-flow velocities and injection pressures, forming a stable ammonia jet lift flame requires a higher co-flow temperature. These exist a critical temperature of pure ammonia at around 1170K beyond which the effect of co-flow temperature on lift height dramatically reduces, but around 1070K in ammonia with hydrogen mixture. The ignition delay of the ammonia jet decreases with an increase in the co-flow temperature. Based on the experimentally measured ignition delay of pure ammonia fuel at a temperature from 1150 to 1220K, the popular combustion mechanisms had been selected in the CHEMKIN simulation tool. The close-to-homogenous transient-model had been chosen to validate different chemical reaction mechanisms and analyze the ammonia emissions at different pressures and temperatures. The simulations show that with the increase in the equivalence ratio, an overall reduction in NO_x occurs. With the augment in temperature, NO_x species grow significantly and NO is the main pollutant. As the pressure increases, N_2O and NO_2 increase, while NO decreases. The water addition not only decreases the flame temperature to a sufficient degree to reduce appreciably the NO_x, but also enhances the DeNOx reactions.

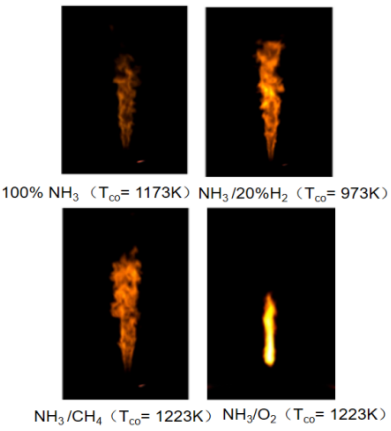


Fig. NH_3 mixture fuels auto-ignition flame in high temperature

First name: Salvatore **LAST NAME**: MAFRICI

Topic: Design of electric motor for circular economy

Course year: 2nd **Tutor(s)**: Alberto TENCONI, Giovanni Andrea BLENGINI, Luca SETTINERI

Academic context

[1] Ceschin, F., Gaziulusoy, I., "Evolution of design for sustainability: From product design to design for system innovations and transitions", 2016, https://doi.org/10.1016/j.destud.2016.09.002.
[2] Nordelöf, A., Grunditz, E., Lundmark, S., Tillman, A., Alatalo, M., Thiringer, T.," Life cycle assessment of permanent magnet electric traction motors", 2019, https://doi.org/10.1016/j.trd.2018.11.004
[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

External collaborations

- Punch Torino

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 and fits within the international context related to Climate Change and Sustainability. 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 focused on Design for Circular Economy of Electric motor 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 impact will be evaluated through Life Cycle Assessment and together with other conventional key performance indicators, like performance and economic impact, will be part of a balanced review. First portion of the research has been dedicated to the different design for sustainability methodologies, trying to understand which could be the most suitable approach for the product object of this PhD and more in general for products developed in the company in which I'm working. Furthermore, has been established a first workflow indicating where the new additional phases could be added to transform a conventional design process. As mentioned, the necessity of evaluating the environmental impact of the product requires the development of an LCA model to be used as virtual platform to provide information on the various design configurations that will be proposed and implemented during the Design process. A first LCA model has been derived from literature and will be further exploited introducing additional phases like the End of life and all the circular scenarios. The LCA model developed so far is taking into account the stages from the material extraction to the in-use phase. During my PhD primary data related to an in-house developed electric motor will be considered in the model. In Figure are reported preliminary results adopting literature motor data, highlighting influence of the considered country on CO2 emission and on cycle phases breakdown.

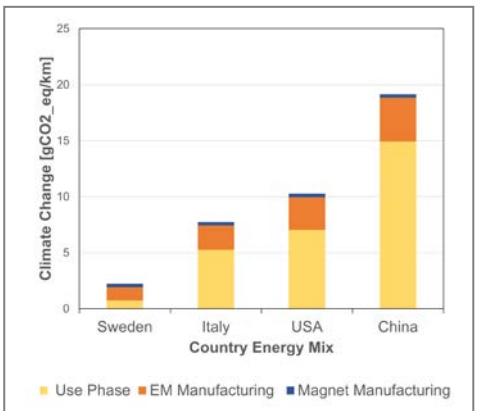


Fig. LCA of a PMSM produced and used in different countries.

First name: Giancarlo **LAST NAME**: MONTANARO

Topic: Hydrogen-Fueled High-Performance Powertrains

Course year: 1st **Tutor(s)**: Luciano ROLANDO

Academic context

[1]. Winklhofer, E., Jocham, B., Philipp, H., Kapus, P. et al., "Hydrogen ICE Combustion Challenges," SAE Technical Paper 2023-24-0077, 2023.
[2]. Grabner, P., Schneider, M., and Gschiel, K., "Formation Mechanisms and Characterization of abnormal Combustion Phenomena of Hydrogen Engines," SAE Technical Paper 2023-32-0168, 2023

External collaborations

- Ferrari Powertrain Simulation & Know-How, www.ferrari.com

Highlights of the research activity

This research activity sponsored by Ferrari S.p.a aims to develop, through both experimental and numerical simulations, a reliable and innovative combustion system for a high-performance internal combustion engine operating with hydrogen.

The starting point of the 1st year's activity has been an extensive literature review to collect information about the current state of the art about hydrogen combustion. After that, some time was spent getting experience with the Ferrari approach to developing innovative technology and their modelling techniques.
The experimental campaign performed on a spark-ignition single-cylinder engine fueled with hydrogen represents the core activity of the 1st PhD year. A huge amount of experimental data was collected to preliminary assess the potential of hydrogen and to support the development of a digital twin of the tested engine within the commercial software GT-Suite.
After an extensive validation process, the engine model was exploited to select the most promising technologies (e.g., Miller Cycle) and the best combination of operating conditions (e.g., lean operation) for engine performance maximisation. Moreover, focusing on the knock likelihood, additional analyses were performed to assess the benefits of a Port Water Injection (PWI) system.

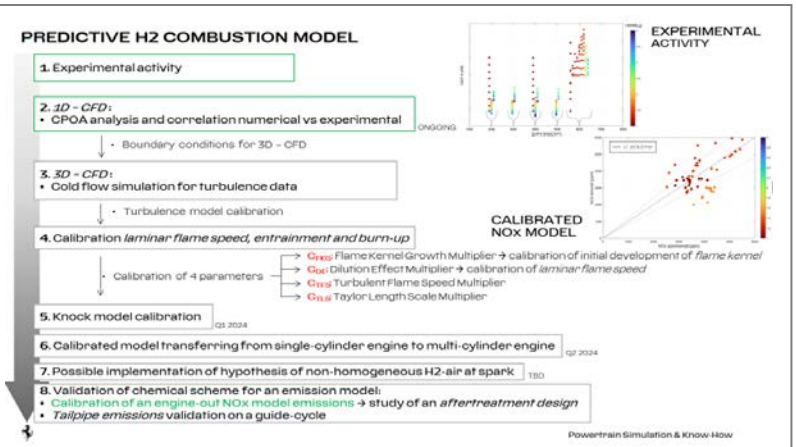


Fig. Development of H_2 predictive combustion model (*SITurb*) with highlighted in green the task performed during 1st year

Since a critical aspect of hydrogen engines could be represented by the production of NO_x emissions, an extended Zeldovich reaction mechanism was also integrated in the virtual test rig. The calibrated model can now predict NO_x emissions with an error of about 20% which represents a satisfactory result according to similar studies in literature. Proceeding with the advancement of the research, the aim is to reduce the error percentage below 20% increasing the set of data for NO_x model calibration. The availability of this emission model paved the way for a comparison between the effectiveness of lean mixtures and Exhaust Gas Recirculation (EGR) to minimize NO_x production.
The first step of the 2nd year's activity will be the cold flow simulations in some representative engine operating points that will enable the calibration process of the predictive combustion model.

First name: Alessia **LAST NAME**: MUSA

Topic: Enabling sustainable and intelligent mobility: control approaches for enhancing energy savings, safety, and comfort in electrified and ADAS-integrated vehicles

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

Academic context

[1] Musa, A.; Miretti, F.; Misul, D. (2023) "MPC-Based Cooperative Longitudinal Control for Vehicle Strings in a Realistic Driving Environment". In: WCX SAE World Congress Experience. ISSN 0148-7191
[2] Steinstraeter, M.; Heinrich, T.; Lienkamp, M. Effect of Low Temperature on Electric Vehicle Range. World Electr. Veh. J. 2021, 12, 115. https://doi.org/10.3390/wevj12030115
[3] Lelli, E.; Musa, A.; Batista, E.; Misul, D.A.; Belingardi, G. On-Road Experimental Campaign for Machine Learning Based State of Health Estimation of High-Voltage Batteries in Electric Vehicles. Energies 2023, 16, 4639. https://doi.org/10.3390/en16124639.

External collaborations

- KTH Royal Institute of Technology
- Hyundai Motor Europe Technical Center
- Teoresi S.P.A.

Highlights of the research activity

This research activity, carried out through the 2022-2023 academic year in partnership with PoliTO, CARS, KTH, and several industrial partners, was dedicated to developing predictive control solutions for enhancing energy savings, safety, and comfort in electrified and ADAS-integrated vehicles, covering four primary areas. The first area was the energy management in Hybrid Electric Vehicles (HEV), where we implemented a reinforcement learning (RL)-based approach, incorporating aspects like comfort and engine performance into the reward function. In the second area of Cooperative Adaptive Cruise Control (CACC), we developed a real-time CACC system using a model predictive control (MPC)-based approach combined with vehicle communication technology, and this work was showcased at the SAE 2023 WCX™ World Congress Experience. We extended this work to address challenges in CACC systems, such as communication delays and sensor uncertainties. In collaboration with a MSc thesis student, we developed a decentralized MPC control strategy for a string of five vehicles. This strategy was then compared against an RL-based algorithm. The third focus area, in partnership with KTH, delved into the effect of ambient temperature on the electric range of Battery Electric Trucks (BETs). Our research explored energy consumption across different climate conditions and battery sizes, paying close attention to the roles of HVAC (heating, ventilation, and air conditioning) and BTM (battery thermal management) systems. Additionally, in a side project, we supervised a master thesis project in collaboration with an industrial partner for the development of an AI-based method to predict the state-of-health of high-voltage batteries, which involved evaluating and comparing six machine learning algorithms: linear regression, k-nearest neighbors, support vector machine, random forest, classification and regression tree, and neural network.

	WLTP	CYCLE#1	CYCLE#2	CYCLE#3
Ego II	-13,46	-24,97	-20,56	-24,27
Ego I	-7,7	-17,6	-13,99	-16,39

Fig. Percentage reduction in RMS of vehicle acceleration as a passenger comfort index compared to the lead vehicle [1].

First name: Teodosio **LAST NAME**: NACCI

Topic: Robust Design of High Temperature Components for Innovative Gas Turbine Cycles

Course year: 1st **Tutor(s)**: Daniela Anna MISUL, Simone SALVADORI

Academic context

[1] Paniagua , G., De´nos , R., and Almeida, S. (December 29, 2004). "Effect of the Hub Endwall Cavity Flow on the Flow-Field of a Transonic High-Pressure Turbine ." ASME. *J. Turbomach*. October 2004
[2] Wang, H. P., Olson, S. J., Goldstein, R. J., and Eckert, E. R. G. (January 1, 1997). "Flow Visualization in a Linear Turbine Cascade of High Performance Turbine Blades." ASME. *J. Turbomach*. January 1997

External collaborations

- Technical University of Berlin

Highlights of the research activity

The research activity carried out during my first year of Ph.D. studies focused on the analysis of high-pressure turbine stages and related thermo-fluid-dynamic phenomena by carrying out two projects in parallel. In particular, the topic of refrigeration of components aimed at avoiding thermal stress and allowing components to last longer has been addressed.

The characterization of the geometry of a two-stage HP turbine with reproduction of Film cooling on the first stator blade

The study is in the context of protecting turbine blades from thermal stresses due to high combustor outlet temperatures in turbogas plants. Specifically in this case there is an RDC upstream of the turbine, which, despite the benefits of its use, causes even higher temperatures. The solution to this problem is blade cooling, in this case that of the high-pressure stator. The activity has involved the realization of 3D-CFD simulations through the use of Ansys CFX 2022R2 software. Refrigeration of the first stator was reproduced on the software by implementing the continuity source method, which introduces a source term representative of the Cooling flow entering the system, within the classical continuity equation. Unsteady simulations were carried out using the Profile Transformation method that allows for simulating uneven blade counts by imposing periodic boundary conditions and scaling the solution at the interface.

The analysis of the impact of Cavity Flows within a Transonic single-stage geometry of a HP turbine

This project is concerned with the simulation of a turbine stage with an attached internal cavity deputed to handle part of the cooling flow that enters the main flow under the name of Purge flow and analysis of its fluid dynamic impact. The activity has involved conducting 3D-CFD simulations, validated by experimental data obtained at Von Karman Institute (VKI) of Brussels, using Ansys CFX 2022R2 software. The idea was to use the CFD data to go into more detail about the thermo-fluid dynamic performance of the turbine and to analyze how the variation of the rotor angular velocity and the purge flow rate affected the results. Three main types of simulations were performed, one with injection into the cavity and the others with positive Purge flow entering the main flow. The geometry used to perform the Unsteady simulations, obtained through the Domain Scaling technique, is composed of two stators and three rotors and a cavity with two inlets, one radial and the other axial. In addition to an analysis of the results apt for comparison with experimental data, the influence of Purge flow on Secondary Flows has been defined.

Fig. Trailing Edge shock on a Transonic High Pressure Stage

First name: Rosario **LAST NAME**: NASTASI

Topic: Green - Tecnologie innovative per la gestione termica e soluzioni per una aviazione pulita

Course year: 2nd **Tutor(s)**: Daniela Anna MISUL, Simone SALVADORI

Academic context

[1] Adjoint optimization of film cooling hole geometry (Jones, Oliver, Bogard)
[2] Identification of fluctuation modes for a cylindrical film cooling hole using the spectral proper orthogonal decomposition method (Rosafio, De Cosmo, Salvadori, Carnevale, Misul)
[3] Optimization of a fan-shaped hole to improve film cooling performance by RBF neural network and genetic algorithm (Wang, Zhang, Zhou)

External collaborations

- Avio Aero

Highlights of the research activity

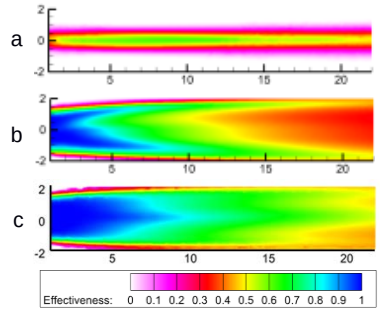


Fig. Film cooling effectiveness maps:
a) Cylindrical hole
b) Adjoint-optimized hole
c) ANN-optimized hole

The research activity is focused on the application of innovative optimization techniques in the design process of cooling systems for gas turbines. More specifically, film cooling is nowadays considered a crucial technology to prevent high metal temperatures caused by the blade exposure to hot gas and it is constantly subject to improvements aimed at increasing its efficiency. The selected test case consists of a cylindrical film cooling hole that operates at realistic working conditions. The optimization started with the application of a gradient-based approach (Adjoint method) combined with results from RANS CFD simulations. The entire hole length was thus parametrized with a set of morphing points whose position was iteratively deformed to improve the area-averaged cooling effectiveness on a flat surface downstream from the hole exit. An impressive improvement of film coverage was obtained with remarkable deformations from the original cylindrical shape. Despite the promising results, the use of gradient-based approaches is strongly limited by the possibility of the optimizer to stop at a local minimum/maximum. To disprove this possibility, the idea was to combine the benefits that emerged from the adjoint optimization (in particular the complexity of the geometry obtained), with the advantages of a global optimization technique. The hole was thus parametrized, and this permitted us to emphasize even more the geometrical features individuated by the adjoint optimization. The design space of each variable was explored with RANS CFD simulations, creating a robust database that was later used to train an Artificial Neural Network (ANN). The network hyperparameters (number of neurons, optimizer, dropout rate, batch size etc..) were tuned through a random search technique and the model performance was improved minimizing the Root mean square error (RMSE) obtained comparing predictions with observed (from CFD) data. Finally, the optimized model was used to find the maximum value of effectiveness within the design space, obtaining a further +20% increase in the objective function with respect to the previous optimization technique.

Another important topic of the research activity concerns the application of high-fidelity numerical approaches to accurately describe the complex physical phenomena that characterize film cooling. More specifically, the coolant mixing with hot gas is strongly underestimated by traditional RANS simulations. In this activity, Stress Blended Eddy Simulation (SBES) was used to test the same film cooling hole selected as the baseline test case for optimization. The idea behind this approach is to use a blending function to switch between RANS and LES, thus modeling only the boundary layer and solving the rest of the domain. This approach was also used to study the turbulence phenomena through POD (Proper orthogonal decomposition) and SPOD (spectral proper orthogonal decomposition). With this analysis it is possible to find the major sources of fluctuations in the flow field and analyze complex mechanisms such as the coolant attachment with the wall or the jet penetration into the main flow.

First name: Francesco **LAST NAME**: PUCILLO

Topic: H2-HD: Hydrogen as a fuel for internal combustion engines for heavy-duty applications

Course year: 2nd **Tutor(s)**: Federico MILLO, Andrea PIANO

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

External collaborations

- FPT Industrial S.p.A.
- Garrett Motion Inc.
- Robert Bosch GmbH

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), seems to be particularly promising for its combustion properties, characterized by near-zero harmful emissions and fast flame propagation. However, notably for direct injection applications, more calibration efforts are required to optimize the mixture preparation and the combustion processes. In this context, the research activity, sponsored by FPT Industrial, focuses on the evaluation, through numerical simulation, of the potential of hydrogen as a fuel for internal combustion engines for heavy-duty applications, supporting the development of future combustion concepts.
Complete optimization of critical components and operating parameters is performed to achieve targets in terms of torque, power, efficiency, and emissions.

A 1D-CFD model developed in GT-SUITE, employed as a virtual test rig, has allowed the analysis of the air required to provide the target power output complying with functional limitations, in different ambient conditions. This process involved the investigation and optimization of the turbocharger size and architecture and the intake valve profiles.

In this year, 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 emissions. The investigation of the hydrogen injection process through 3D-CFD numerical simulation is currently ongoing, aiming to optimize the mixture stratification for different operating conditions. This synergetic approach among 1D and 3D-CFD simulations will allow the setup of a 1D-CFD predictive combustion model (SITurb). In addition, the analysis of the abnormal combustion phenomena (knock, pre-ignition) and cyclic combustion variability will extend the predictiveness of the 1D model, providing further insight into the main limitations of hydrogen combustion in internal combustion engines.

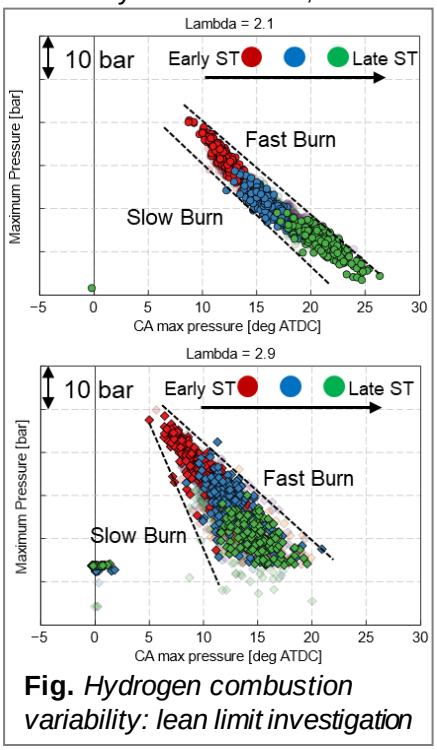


Fig. *Hydrogen combustion variability: lean limit investigation*

First name: Gianpaolo **LAST NAME**: QUATTRONE

Topic: Optimization of H2 fuelled ICE from fuel injection to exhaust aftertreatment

Course year: 2nd **Tutor(s)**: Federico MILLO, Andrea PIANO

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 HPDI™ Fuel System to a Demonstration Truck", Vienna Motor Simposium, 2023

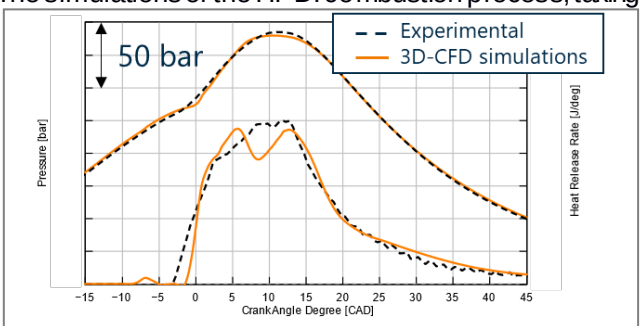
External collaborations

- PUNCH Torino
- Westport Fuel Systems
- Cornaglia Group

Highlights of the research activity

The main scope of the research activity, carried out in collaboration with PUNCH 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 technology, 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 combustion. 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 CRs and thermal efficiencies, and has proven its benefits on heavy-duty applications [3]. However, the literature lacks light-duty applications running with H2-HPDI.

One of the primary aims of this research activity is the development of a 3D-CFD predictive combustion model for the simulation of the H2-HPDI combustion for a heavy-duty application. Since the gas ignition strongly depends on the interactions between the gaseous jet and the high-temperature zone resulting from the Diesel pilot combustion, a proper modelling of the gaseous jet is of paramount importance to simulate the HPDI system. For this reason, the 3D-CFD gaseous jet model was validated basing on non-reactive CNG sprays experimental data. Then, a setup of an engine sector containing both a Diesel and a gas nozzle of the HPDI injector was built within the CONVERGE environment. The simulations of the HPDI combustion process, taking into consideration both hydrogen and compressed natural gas scenarios, facilitated the identification of the key combustion phases: the pilot combustion phase, the hydrogen ignition phase, the free-jet combustion phase, the jet-wall impingement phase, the global-mixing combustion phase, and the termination phase. Several assessments were conducted employing a detailed kinetic chemistry scheme to calculate the combustion rate, finding that the gaseous combustion is not strongly affected by the pilot Diesel spray model parameters.



Comparison of CFD H2-HPDI combustion model results and experimental traces (peak power point).

The 3D-CFD HPDI combustion model has revealed its strong predictive capabilities ranging from different engine speeds and loads and will be used to assess the potential of the usage of the H2-HPDI technology on a light-duty application, allowing a direct comparison between the H2-PFI and the H2-HPDI technologies on the same engine.

First name: Nicola **LAST NAME**: ROSAFIO

Topic: Development of a High Order Finite-Volume Solver for Turbomachinery Applications

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

Academic context

[1] Okada M., Simonassi L., Lopes G., and Lavagnoli, S. "Particle Image Velocimetry Measurements in a High-Speed Low-Reynolds Low-Pressure Turbine Cascade." ASME. J. Turbomach. March 2024; 146(3): 031010. https://doi.org/10.1115/1.4063674
[2] Lopes G., Simonassi L., and Lavagnoli S. "Impact of Unsteady Wakes on the Secondary Flows of a High-Speed Low-Pressure Turbine Cascade". International Journal of Turbomachinery, Propulsion and Power. 2023; 8(4):36. https://doi.org/10.3390/ijtpp8040036

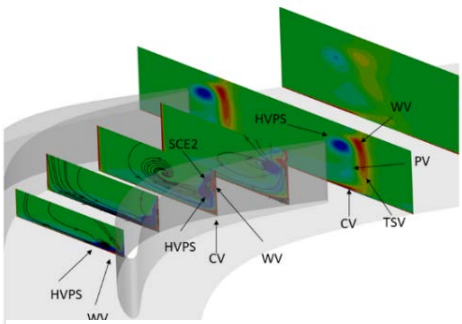
External collaborations

- Von Karmann Institute for Fluid Dynamics

Highlights of the research activity

The research activity was devoted to the analysis of the newly designed SpleenC1 high-speed low pressure turbine blade, experimentally investigated at the Von Karmann Institute for Fluid Dynamics. An initial sensitivity analysis to the turbulence model was performed via 2D simulations of the blade mid-span flow. Various correlation-based and physics-based turbulence models were tested for the blade nominal and off-design conditions. This allowed to select the proper modelling approach for the test case.

Subsequently, the research was devoted to the study of the three-dimensional cascade to assess the impact of secondary flow on the blade performance. To this end, spanwise averaged experimental total pressure and angle profiles were imposed as inlet conditions to the numerical domain, to correctly represent of the incoming boundary layer. Moreover the impact of the inlet turbulence profile specification was analyzed and its effect on the redistribution of inlet vorticity throughout the cascade was assessed. The numerical analysis allowed to underline how the specification of turbulence quantities in 3D simulations of low-pressure turbines can greatly impact the flow field, both in terms of secondary flows, loss generation mechanism and endwall losses. The analysis was conducted both at design and off-design operating conditions for the cascade.



Secondary flows development

Eventually, the unsteady flow field occurring in the cascade under incoming wakes was analyzed. A first set of simulations was run imposing the experimentally measured wake profiles as inlet conditions to the blade domain. This allowed to assess turbulence models performance in predicting wake induced boundary layer transition and re-laminarization. A second set of simulations was run introducing a rotating domain for the simulation of the bars generating the wake. The coupling between the moving bar domain and the stationary blade domain was achieved by means of a sliding interface treatment which was implemented in the code during the period of stay at VKI. The procedure is based on finding the intersections between the faces of the elements across the interface, while a procedure based on 2nd order interpolation of face values allows to correctly compute the viscous and inviscid fluxes between the rotating and stationary domains. The results with the sliding interface showed great sensitivity to the prescribed boundary conditions and relative speed between the inlet flow and the moving bar because of the formation of strong shocks in the bar domain, which affect the flow field upstream of the low pressure turbine blade.

First name: Andrea **LAST NAME**: SCALAMBRO

Topic: H2GT - Hydrogen as a ICE fuel for Ground Transportation

Course year: 2nd **Tutor(s)**: Federico MILLO, Luciano ROLANDO, Andrea PIANO

Academic context

[1] White, C. M., R. R. Steeper, and A. E. Lutz., "The hydrogen-fueled internal combustion engine: a technical review." International journal of hydrogen energy 31.10 (2006): 1292-1305.
[2] Addepalli, Srinivasa Krishna, et al. "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] Maio, G., et al. "Experimental and numerical investigation of a direct injection spark ignition hydrogen engine for heavy-duty applications." International Journal of Hydrogen Energy 47.67 (2022): 29069-29084.

External collaborations

- FEV
- CNR STEMS
- POWERTECH Engineering S.r.l.

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, the research work carried out during the second year of PhD activity was focused on the study and optimization of the mixture formation process in a DI H2-ICE (retrofitted from a diesel engine) through 3D-CFD simulations. Simulations were carried out in the rated power point, since the high engine speed increases the injection duration and reduces the time that hydrogen has to properly spread into the combustion chamber, making this operating condition particularly challenging from a mixture homogenization perspective. First, a sweep of injection timing was performed, considering three different starts of injection (SOI). From this first analysis, an optimum SOI was found, leading to the best mixture homogeneity, with a negligible reduction of the volumetric efficiency. This injection timing was then used for the next part of the analysis. Different boundary conditions, in terms of intake/exhaust pressure, and intake/exhaust valve lift profiles and timings were tested. These factors showed a non-negligible influence on the in-cylinder motion patterns whose optimization is crucial for favoring a homogeneous spread of the gaseous fuel within a short time. Afterward, six injector spray caps (small chambers positioned downstream of the injector valve exploited to guide the high-speed injected hydrogen) were tested. Even though the spray were effective in providing to the injected gas the desired direction, none of them led to a large improvement in the H2 distribution. Therefore, the swirl intensity was varied, by acting on the intake valve seat eccentricity, as a final step of the optimization. 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.

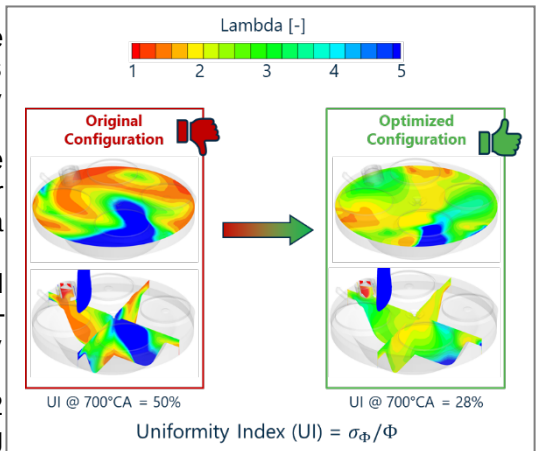


Fig. Lambda distribution 20 CAD before TDC firing for the original and the optimized engine configuration

First name: Cristiano **LAST NAME**: SEGATORI

Topic: Study of a new mixing-enhancement strategy for zero-soot future diesel engine applications

Course year: 3rd **Tutors**: Federico MILLO, Andrea PIANO

Academic context

[1] Gehmlich, R.K., Mueller, C.J., Ruth, D.J., Nilsen, C.W. et al., "Using Ducted Fuel Injection to Attenuate or Prevent Soot Formation in Mixing-Controlled Combustion Strategies for Engine Applications," *Applied Energy* (2018), doi:10.1016/j.apenergy.2018.05.078.
[2] 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.
[3] Segatori, C., Piano, A., Peiretti Paradisi, B., Bianco, A. and Millo, F., "Exploiting the potential of large eddy simulations (LES) for ducted fuel injection investigation in non-reacting conditions," *International Journal of Multiphase Flow* (2023), doi:10.1016/j.ijmultiphaseflow.2023.104686.

External collaborations

- PUNCH Torino S.p.A.
- POWERTECH Engineering S.r.l.
- Università degli Studi di Perugia

Highlights of the research activity

Soot (or black carbon) emissions are toxic for the human health and are recognized as climate-forcing species, second only to carbon dioxide. Diesel engines are within the most contributors to the atmospheric pollution by soot in the transportation sector. Nonetheless, diesel engine characteristics are desirable for many applications in which the electrification is not an easily viable route (e.g., ships, trucks).

In this context, ducted fuel injection (DFI) is one of the most promising technologies to attenuate the emission of soot in diesel combustion. DFI concept, developed by researchers from Sandia National Laboratories [1], is based on the idea of injecting the fuel spray along the axis of a small duct positioned within the combustion chamber some distance downstream of the injector orifice exit. Although several experiments showed its impressive effectiveness, many questions remain unanswered about the mechanisms through which DFI suppresses soot formation and its real feasibility on the whole engine operating map. In light of this, the present research activity aims to cover key knowledge gaps for the complete success of this new concept.

For this purpose, a spray model was developed in the 3D computational fluid dynamics environment, validated against data from an extensive experimental campaign in constant-volume non-reacting conditions [2]. Given the high turbulence level expected, the very accurate but computationally expensive large eddy simulation (LES) turbulence model was adopted as a mean to investigate the DFI-related physics. LES combined with statistical analysis allowed the computation of vortices formation and turbulent kinetic energy, showing that DFI intensifies and spatially advances the air-to-fuel mixing, first driver of soot formation mitigation [3]. However, despite the knowledge deepening provided by the LES approach, an increased need of more simplified and less expensive models (i.e., RANS) for optimization purposes is expected if DFI is going to succeed in series production. Therefore, the high-fidelity LES data were finally exploited to assess the performance of several RANS turbulence models (Fig.1), with the final goal of defining best practices in DFI modelling to obtain reliable results at an affordable computational cost.

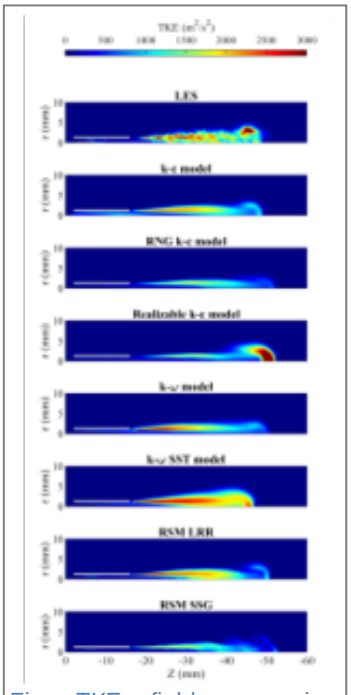


Fig. TKE field comparison among LES and several RANS turbulence models for DFI under non-reacting conditions.

First name: Gerardo **LAST NAME**: STANZIONE

Topic: H_2 ICE – H_2 as an ICE fuel for marine & industrial

Course year: 1st **Tutor(s)**: Federico MILLO, Andrea PIANO

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.

External collaborations

- YANMAR
- Gamma Technologies LLC

Highlights of the research activity

In this research activity, sponsored by YANMAR, the conversion of a medium-speed diesel engine into an H2-Diesel dual-fuel engine was explored. In this system, the Port Fuel Injection (PFI) system provides the hydrogen while the diesel is directly injected during the compression stroke, and the autoignition of the pilot diesel triggers the hydrogen pre-mixed combustion.
In the first year of PhD, the activity was divided into three parts, in the first part, a pre-ignition analysis was carried out to determine the operating condition characterized by the autoignition of the hydrogen. The analysis was based on the experimental pressure cycles and led to the differentiation between pre-ignition, ringing, and knocking cycles.
Lastly, the analysis was focused on the development of a 0-1D-CFD predictive combustion model that takes account of the two combustion modes, diesel spray combustion and turbulence flame propagation of the hydrogen.
Different steps were needed:

- A 3D-CFD cold flow model was calibrated to replicate the turbulence condition inside the combustion chamber.
- The 1D-CFD turbulence model was calibrated against the 3D-CFD results to replicate the in-cylinder turbulence conditions; This model was calibrated to reduce the error on the turbulence kinetic energy (TKE) and the length scale at TDC compared with 3D results.
- A preliminary dual-fuel combustion model was calibrated against the experimental data.
- To improve the accuracy of the dual-fuel combustion model, a dedicated ignition delay model correlation that replicated the inhibition effect of the hydrogen was developed. The ignition delay was computed by means of the 0D-CFD detailed chemistry considering the in-cylinder conditions at Diesel SOI.

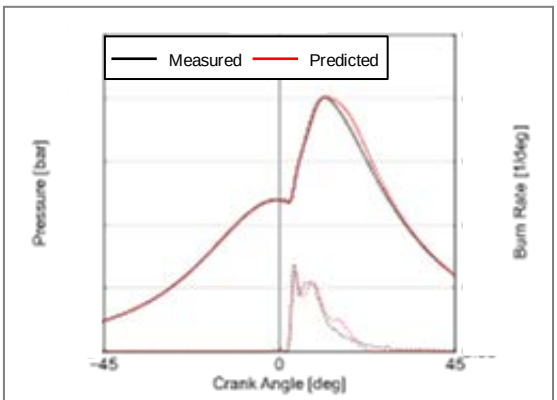


Fig. Comparison of measured and predicted pressure and HRR with 83.5% of hydrogen

Once assessed these steps, the dual-fuel combustion model will be calibrated by considering a wide range of engine parameters to increase its predictive ability.
Lastly, the 1D-CFD model will be simplified for Real-Time application.

First name: Lorenzo **LAST NAME**: TESTA

Topic: Towards Sustainable Biofuel Production for Aviation and Maritime

Course year: 3rd **Tutors**: David CHIARAMONTI, Samir BENSAID

Academic context

[1] Chiaramonti D, Goumas T. Impacts on industrial-scale market deployment of advanced biofuels and recycled carbon fuels from the EU Renewable Energy Directive REDII. Applied Energy, 251 (2019) 113351, https://doi.org/10.1016/j.apenergy.2019.113351

[2] Chiaramonti D, Panoutsou C. Policy measures for sustainable sunflower cropping in EU-MED marginal lands amended by biochar: Case study in Tuscany, Italy. Biomass and Bioenergy 126 (2019) 199–210, https://doi.org/10.1016/j.biombioe.2019.04.021

External collaborations

- Renewable Energy Consortium for Research and Demonstration (RECORD)
- Food and Agriculture Organization of the United Nations (FAO)

Highlights of the research activity

The primary focus of the research is the European project *"Biofuels Production at Low ILUC Risk for European Sustainable Bioeconomy" - BIKE*, aimed at supporting the implementation of the Renewable Energy Directive II, particularly addressing the ILUC risk associated with biofuels. The study centers on a value chain on increased productivity through improved agricultural practices, specifically the Biogas Done Right (BDR) model for aviation and maritime biofuels. Framed within the European context, with Italy as a case study due to its recent incentivization scheme supporting sustainable biomethane production, the research aims to secure a renewable raw material with a guarantee of origin for producing advanced liquid biofuels. The strategy involves a combined centralized and decentralized approach, integrating farm-level biomethane production, injection into the natural gas grid, and centralized production of liquid biofuels in a Gas-to-Liquids (GTL) plant. This process utilizes advanced technologies like Fischer-Tropsch synthesis (GTL-FT), methanol synthesis (GTL-MeOH), and syngas fermentation to ethanol, coupled with the alcohol-to-jet process (GTL-F_ATJ). The study analyzes these three routes and compares two biomethane reforming technologies, namely steam methane reforming (SMR) and partial oxidation of methane (POX), alongside insights into investment costs. The research employs a model developed using commercial simulation software and data from an extensive literature review of industrial references. This model provides key insights into process yields and energy balances, facilitating a data-driven approach to simulate biofuel production. The findings suggest that within the European context, the GTL-FT route could potentially fulfill approximately 9% of the demand for kerosene-based jet fuel using SAF produced from this pathway with POX technology. If SMR technology is used, it could cover 4% of the demand. Alternatively, the GTL-F_ATJ route might cover around 10% of the jet fuel demand. Concerning methanol as maritime fuel, the GTL-MeOH route, with POX reforming technology, could potentially meet approximately 54% of the demand, while utilizing SMR technology could cover around 24%. Additional assessments, including a Technology Innovation Assessment (TIS), demonstrate the promising state of development in the case study. The established biomethane supply chain, sustainable and scalable agronomic models, and the Italian incentive scheme contribute to the feasibility of implementing the value chain. However, the study highlights the need for a more structured, long-term, and clear policy framework at both national and EU levels. Furthermore, the sustainability analysis, developed in collaboration with the Food and Agriculture Organization of the United Nations (FAO), reveals exceptional environmental performance, positive social impacts in job creation and income improvement, and promising economic sustainability within the value chain.

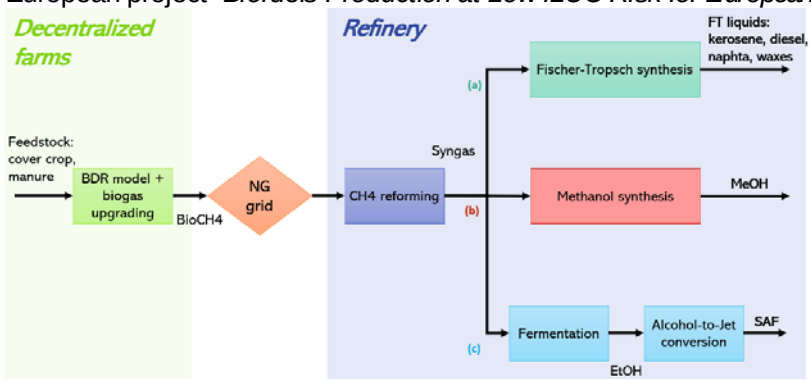


Fig. Liquid biofuels production chain scheme

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: 1st **Tutor(s)**: Luciano ROLANDO, Andrea PIANO

Academic context

[1] L. Pulvirenti, L. Tresca, L. Rolando, and F. Millo, "Eco-Driving Optimization Based on Variable Grid Dynamic Programming and Vehicle Connectivity in a Real-World Scenario," Energies 2023, Vol. 16, Page 4121, vol. 16, no. 10, p. 4121, May 2023, doi: 10.3390/EN16104121.
[2] F. Millo, L. Rolando, L. Tresca, and L. Pulvirenti, "Development of a neural network-based energy management system for a plug-in hybrid electric vehicle," Transportation Engineering, vol. 11, Mar. 2023, doi: 10.1016/j.treng.2022.100156.
[3] B. Xu, F. Malmir, D. Rathod, and Z. Filipi, "Real-Time reinforcement learning optimized energy management for a 48V mild hybrid electric vehicle," in SAE Technical Papers, SAE International, Apr. 2019. doi: 10.4271/2019-01-1208.

External collaborations

Highlights of the research activity

Reducing the carbon footprint of the transportation sector is essential for reaching carbon neutrality by 2050, as set by the regulations. The Greenhouse Gas (GHG) emissions of the current vehicle fleets can be strongly reduced by the synergistic exploitation of eco-driving algorithms, that optimize the vehicle speed in a connected environment, along with electrified mobility solutions. In this context, powertrain hybridization can represent, at least in the short term, a viable solution to improve powertrain efficiency, and, at the same time, curb the current disadvantages of Battery Electric Vehicles (BEVs). However, the introduction of an auxiliary energy source on board must be properly managed to fully exploit the benefits of powertrain electrification. Recently, the application Machine Learning (ML) techniques has become widely adopted in the automotive sector, in particular in the powersplit control framework for Hybrid Electric Vehicles (HEV).
The first PhD year was mainly dedicated to the study of innovative techniques to be used on HEVss, focusing on Deep Neural Networks training, vehicle speed optimization and RL agents development.
A first activity regards the development of an innovative deep learning-based EMS able to efficiently handle the energy management of a PHEV. The supervised learning model has been trained off-line by providing the optimal solutions given by the Dynamic Programming (DP) over a wide range of driving and traffic scenarios. Addtionally, the vehicle control process employs a deep learning model based on Recurrent Neural Networks (RNNs), since they can deal with past temporal and sequential information.
A second activity regarded the development of an optimization tools able to globally optimize the vehicle speed profile given a starting and a target location while operating in a connected environment. The optimized speed profile was compared against a Real Driving Emissions (RDE) compliant route, highlighting that introducing a smart infrastructure along with optimizing the vehicle speed in a real-world urban route can potentially reduce the required energy by 54% while shortening the travel time by 38%.
The last activity, which is still on-going, regards the evaluation of the potentiality of RL agent integration into the EMS of hybrid electric vehicles. A sensitivity analisys to the reward function of a Deep Q-Learning (DQL) agent was performed by training the agent on the Worldwide harmonized Light-duty vehicles Test Cycle (WLTC). The proposed rewards are then compared based on the vehicle fuel economy and on the battery charge sustainability at the end of the driving cycle, and in terms of training performance. Finally, the best reward was tested on different driving scenarios from the training one to assess the robustness of the methodology.

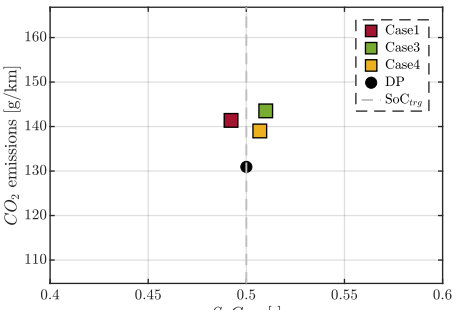


Fig. Trade-off between CO_2 emissions and final battery state of charge value for the three rewards compared

First name: Afanasie **LAST NAME**: VINOGRADOV

Topic: A Comprehensive Methodology for the Development of Electrified Powertrain Solutions for off-road Applications

Course year: 2nd **Tutor(s)**: Federico MILLO, Luciano ROLANDO

Academic context

[1] Lajunen, A.; Sainio, P.; Laurila, L.; Pippuri-Mäkeläinen, J.; Tammi, K. Overview of Powertrain Electrification and Future Scenarios for Non-Road Mobile Machinery. Energies 2018, 11, 1184. https://doi.org/10.3390/en11051184
[2] D. Troncon, L. Alberti, S. Bolognani, F. Bettella and A. Gatto, "Electrification of agricultural machinery: a feasibility evaluation," 2019 Fourteenth International Conference on Ecological Vehicles and Renewable Energies (EVER), 2019, pp. 1-7, doi: 10.1109/EVER.2019.8813518.
[3] Federico Millo, Jianning Zhao, Luciano Rolando, Claudio Cubito & Rocco Fuso (2015) Optimizing the design of a plug-in hybrid electric vehicle from the early phase: an advanced sizing methodology, Computer-Aided Design and Applications, 12:sup1, 22-32, DOI: 10.1080/16864360.2015.1077072

External collaborations

- Lombardini - Kohler Engines

Highlights of the research activity

Concerning the climate issue, electrification of the vehicles is a solution that helps with the CO2 reduction request. The electrifican is becoming interesting even for the off road sector since it could improve both efficiency and performance ensuring, at the same time, the compliance with the strigent emissions standards. In this context the activity of the first year was focused on the investigation of an Hybrid Power Unit: a 56 kW internal combustion engine (ICE) coupled with a 16 kW electric motor. The investigation was performed to evaluate achievable performance and limiting the overall emissions.
The PhD project, globally aims at developing a comprehensive methodology to design off road hybrid powertrains starting from the architecture definition moving to the component sizing and up to the optimization of the Energy Management Strategy (EMS). The activity of the second year focused on a specific application: a Skid Steer Loader (SSL). Different powertrains architecture models were developed and coupled with a component database and with a Dynamic Programming (DP) optimizer for the EMS. The DP guarantees the optimal control for every architecture and thus not introducing further bias in the assessment process. The analysis evidenced how for the specific application different architecture enables diverse engine control logics. For example, for an electric traction architecture, the engine could operate at lower speeds during an important part of the duty cycle of the SSL, thus guarantying a relevant improvement in fuel consumption. Another important impact, enabled by each hybridized architectures was the possibility of engine downsizing that from initial analysis allows fuel consumption reduction and some performance boosting thanks to the electric unit. Overall, the proposed methodology demonstrated to be effective in assisting the design of this traction system. More in detail, it defined the minimum component size highlighting the critical aspects of each configuration and its potential. On a typical duty cycle of a SSL, the simplest architecture showed a 10% reduction in fuel consumption and up to 30% if a stronger electrification is considered, but complexity and cost would be probably higher.

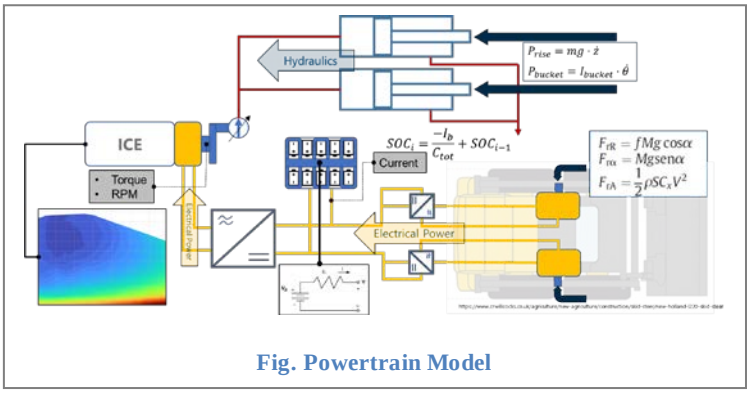


Fig. Powertrain Model

First name: Massimiliano **LAST NAME**: ZANATTA

Topic: Combustion system development for alternative low and net zero carbon fuels

Course year: 1st **Tutor(s)**: Federico MILLO, Luciano ROLANDO, Andrea PIANO

Academic context

[1] Eicheldinger, S., Nguyen, H., et al, 2018, "Mitteldruck 30 bar bei Gasmotoren", Hrsg.: Forschungsvereinigung Verbrennungskraftmaschinen e.V.. Nummer 1201
[2] Peng Zhang et al., "Comparison of methane combustion mechanisms using laminar burning velocity measurements", Combustion and Flame, 111867 ,ISSN 0010-2180

External collaborations

- PUNCH Torino

Highlights of the research activity

The research activity, sponsored and assisted by PUNCH Torino, was focused on exploring the potential of low carbon fuels such as methane and investigating related innovative combustion systems, in particular prechamber-ignition.
Therefore, the PhD activity was focused on the research and development of a high efficiency large bore (~4L/cyl) methane engine. The research project began with the development of a 3D-CFD model in CONVERGE CFD, having as a test case the engine equipped with a passive prechamber (pPC) system. Before modelling combustion in a multi-dimensional environment, the research focused on the investigation of the most suitable methane reaction mechanism for this application [2].

The combustion model is based on SAGE detailed chemical kinetic solver which was proven to be capable of reproducing combustion phenomena of both premixed and partially premixed mixtures, even in lean conditions. Different sensitivity analyses have been carried out accounting for different parameters such as grid, spark energy, spark position, and geometry of the pPC. In particular, several different pPC geometries have been tested in which number of holes, holes diameter, orientation, volume and spark plug position varied. Different combustion indicators were employed to assess the performance of each pPC geometry. Then, the most promising one was chosen to define the optimal range of combustion start and mixture dilution in two working conditions (i.e., high and low load).

Future developments of the work consist of the numerical investigation of an active prechamber system mounted on the same engine in order to compare the performance of these innovative combustion systems and to identify each optimal operating range.

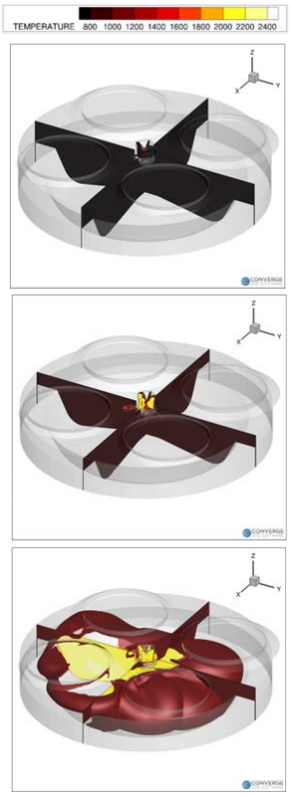


Fig. Top. Spark ignition inside the passive prechamber.
Center. Hot flames exiting from the pPC and igniting the mixture in the main chamber.
Bottom. Flame propagation in the main

Industrial energy systems, technologies and materials for the energy transition

First name: Salvatore Francesco **LAST NAME**: CANNONE

Topic: Carbon capture utilization and storage (CCUS)

Course year: 3rd

Tutor(s): Andrea LANZINI, Massimo SANTARELLI

Academic context

[1] Walawender, W. P., & Stern, S. A. (1972). Analysis of Membrane Separation Parameters. II. Counter-current and Cocurrent Flow in a Single Permeation Stage. Separation Science, 7(5), 553–584. https://doi.org/10.1080/00372367208056054

External collaborations

- Università di Torino
- Università di Bologna
- Istituto Italiano di Tecnologia (IIT)

Highlights of the research activity

The overarching objective of the PhD research is to develop innovative strategies for decarbonizing hard-to-abate industries by either removing carbon dioxide from flue gas or providing a carbon-neutral fuel. The primary focus is on characterizing innovative materials for CO2 capture using membrane technology and liquid absorption, along with the development of simulation models to assess the capabilities of these technologies and system efficiencies. Key activities include:

Membrane characterization: Three innovative dense polymer membranes (Matrimid, PEEK, PES) were characterized through experimental activities. Testing involved maintaining a constant temperature, varying working pressures, and using different gas mixtures to obtain permeability and selectivity values under diverse process conditions. Results for Matrimid, synthesized by the University of Bologna, are illustrated on the left side of Figure 1.

Membrane model development: The theoretical model of a counter-current single membrane module is based on the work done by Walawender [1]. The steady-state model was developed assuming isothermal conditions, negligible pressure drops and constant permeability and selectivity. Additional components such as heat exchangers, compressors, and vacuum pumps were incorporated into the code, and diverse separation systems were designed by integrating various separation stages and additional components. Finally, a multi-objective optimization system, capable of maximizing separation efficiencies and minimizing the required surface area of the membrane, was coded, generating one Pareto curve for each analyzed configuration.

Ionic liquid characterization: A biobased ionic liquid solution comprising 25%wt of [Cho][Pro] diluted in DMSO was characterized. Density and viscosity of the innovative ionic liquid were evaluated using a Gay-Lussac pycnometer and a Cannon-Fenske viscometer, respectively. An experimental campaign was initiated to understand the absorption and desorption performance of this innovative solution. Tests were conducted at various temperatures and feed flow concentrations, and the material's cyclability performance was assessed through a stability test of 30 absorption/desorption cycles. The regeneration efficiency is presented on the right side of Figure.

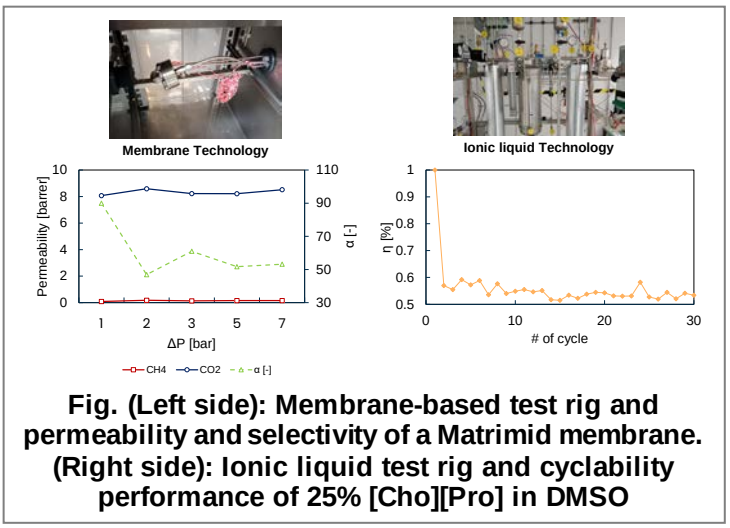


Fig. (Left side): Membrane-based test rig and permeability and selectivity of a Matrimid membrane. (Right side): Ionic liquid test rig and cyclability performance of 25% [Cho][Pro] in DMSO

First name: Roberta **LAST NAME**: CAPPABIANCA

Topic: Multi-scale modelling of advanced colloids for energy applications

Course year: 3rd **Tutor(s)**: Pietro ASINARI, Eliodoro CHIAVAZZO

Academic context

[1]Amici, J., et al., A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+, Advanced Energy Materials, 2022, DOI:10.1002/aenm.202102785
[2]Cappabianca, R., et al., Assembling Biocompatible Polymer on Gold Nanoparticles: Toward a Rational Design of Particle Shape by Molecular Dynamics, ACS omega, 2022, DOI:10.1021/acsomega.2c05218
[3]Cappabianca, R., et al., An Overview on Transport Phenomena within Solid Electrolyte Interphase and Their Import on the Performance and Durability of Lithium-Ion Batteries, Energies, 2023, DOI:10.3390/en16135003

External collaborations

- INRiM, National Institute of Metrology Research (Homepage | INRIM)
- KIT, Karlsruhe Institute of Technology (INT- Research Unit Wenzel (kit.edu))

Highlights of the research activity

This research aims to design advanced functional materials for energy storage applications using a multi-scale modelling approach. For thermal energy storage, the addition of nanoparticles (NPs) in fluids appears as a valid alternative due to the high thermal conductivity of solid NPs compared to conventional heat transfer fluids. Such phenomena are also key for electrochemical energy storage. Here, a crucial aspect is the optimal design of interfacial chemistry between electrode and electrolyte at the nanoscale for developing next-generation rechargeable batteries [1]. In both applications, the ability to manipulate material properties at the nanoscale provides significant opportunities for the development of innovative and more efficient energy solutions.

We have investigated nanoparticle aggregation and mass transport phenomena at the interface at the nanoscale. Nanoparticle aggregation phenomena in solution have a crucial role in energy storage applications. The stability of nanofluids is ensured by limiting self-aggregation between NPs, but meanwhile, such self-assembly can transform NPs in solution into crystalline and amorphous structures with specific properties [2]. In addition, mass transport phenomena at the electrode-electrolyte interface at the nanoscale play a crucial role in improving the performance of current electrochemical storage systems [3]. A passivation layer is formed at the anode-electrolyte interface due to the initial thermodynamic instability of the electrolyte, called solid electrolyte interphase (SEI). Its initial formation is desirable for the chemical stability of the battery, but its subsequent uncontrolled growth consumes the lithium ions and the electrolyte. The study of complex aggregation and transport phenomena within SEI is critical to understanding its formation and growth and its impact on battery performance and lifetime. SEI consists of organic and inorganic compounds. The inorganic compounds of SEI are typically composed of lithium salts and their decomposition products. The organic compounds of SEI are usually composed of polymeric materials formed by the reduction of the organic electrolyte solvent. We conducted reactive atomistic simulations to study the diffusion of lithium ions in an inorganic component of SEI. Then, we used classical atomistic simulations to study the aggregation of polymeric components leading to the formation of organic SEI. Finally, we worked on the realization of mesoscale models (such as kinetic Monte Carlo, implicit solvent models, etc.) to bridge the atomistic scale to a continuous scale.

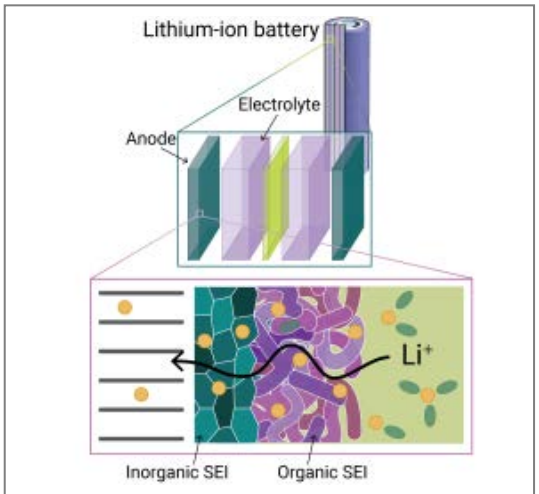


Fig. Looking at the image from top to bottom: LIB image, LIB internal scheme, and SEI illustration.

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

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

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

Academic context

[1] Chen, Chang-Hui, et al. "Development of experimental techniques for parameterization of multi-scale lithium-ion battery models." Journal of The Electrochemical Society 167.8 (2020): 080534.
[2] Kindermann, Frank M., et al. "A SEI modeling approach distinguishing between capacity and power fade." Journal of The Electrochemical Society 164.12 (2017): E287.
[3] Kabir, M M, and Dervis Emre Demirocak. "Degradation Mechanisms in Li-Ion Batteries: A State-of-the-Art Review." International journal of energy research 41.14 (2017): 1963–1986.

External collaborations

- Silk Sports Car Company S.r.l
- University of Ljubljana

Highlights of the research activity

Despite lithium-ion batteries increased performances and safety, a deep understanding of degradation mechanisms and their interplay remains a challenge. In this frame, this doctoral research aims to understand and numerically model the causes and mechanisms of battery degradation during normal usage.
An experimental campaign was planned based on the information obtained from the literature search. The aim was to isolate the three main degradation mechanisms: solid electrolyte interphase (SEI) growth, lithium plating for the anode and transition metal dissolution in the cathode. A reference performance test (RPT) was performed at the beginning and periodically during the life test. The RPT allows to obtain useful information on the degradation status of the battery such as resistance increase, impedance variation and capacity/power fade. To obtain the electrochemical parameters necessary for the model and compare them with the ones found in the literature for the previous version of the same cell (LGM50), one cylindrical cell was opened in controlled conditions. The two extracted electrodes were used to assemble coin cells and run different electrochemical tests. This allowed to obtain the equilibrium curves of the two materials as well as the diffusion coefficients and the Butler-Vomer current density. Moreover, FESEM was used to get other physical parameters used in the model. To analyze the results of the aging test, non-destructive electrochemical techniques were used. To get useful information about the electrochemical thermal behaviour of the battery a pseudo-4D (P4D) model was developed. It extends the original 1D geometry of the P2D model into a 3D geometry including both electrochemical and thermal physics. Voltage curves, as well as temperature profiles obtained with the model, were compared to the experimental results showing good agreement. Now the different degradation mechanisms are being implemented in the P4D model using the experimental data to get information about their kinetics.

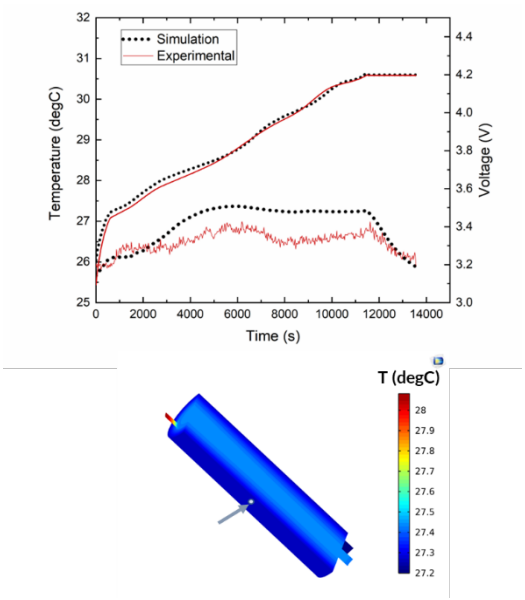


Fig. Comparison between the experimental and the model results during a charge at C/3 + CV and T=25.5°C (a). Temperature profile of the cell at 4.2V (13560 s). The arrow indicate the point used to get the temperature in the simulation and experimentally (b)

First name: Hossein **LAST NAME**: EBADI

Topic: Development of high-performance thermal receivers equipped with a porous metal matrix

Course year: 3rd **Tutor(s)**: Laura SAVOLDI, Antonio CAMMI

Academic context

[1] E.M. Moghaddam, E.A. Foumeny, A.I. Stankiewicz, J.T. Padding, Heat transfer from wall to dense packing structures of spheres, cylinders and Raschig rings, Chemical Engineering Journal 407, 2021.
[2] Z. Zheng, M. Li, Y. He. Thermal analysis of solar central receiver tube with porous inserts and non-uniform heat flux, Applied Energy 185, 2017.
[3] M. Jadidi, A. Revell, Y. Mahmoudi. Pore-scale large eddy simulation of turbulent flow and heat transfer over porous media, Applied Thermal Engineering 215, 2022.

External collaborations

- Politecnico di Milano, Italy
- Plataforma Solar de Almeria, CIEMAT, Spain
- Institute IMDEA Energy, Madrid, Spain

Highlights of the research activity

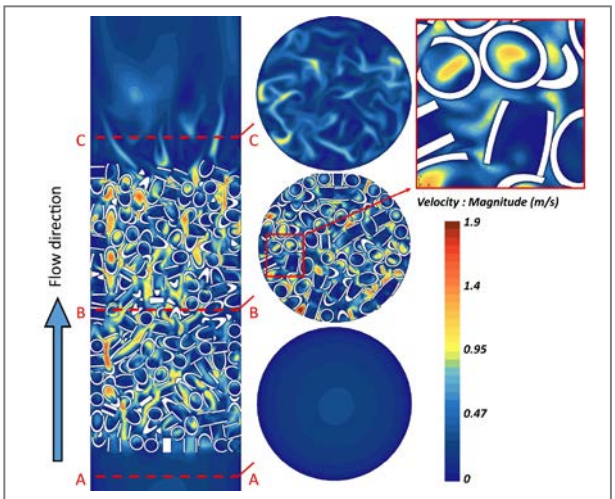


Fig. Velocity field with cross sectional views for fluid flow through the 40mm RR insert.

The Ph.D. project focuses on the application of porous technology with gaseous solar absorbers, targeting performance enhancements in the current CSP (concentrating solar power) technologies. Raschig Rings (RR) porous media as one of the emerging materials are used in different sizes and for a wide range of applications from chemical to environmental industries. Thus, after the recognition of the best RR porous application in the CSP field during the first year, an experimental campaign was made in the second year to assess the performance of a tubular absorber enhanced with RR porous inserts in a solar furnace. Reaching an ample amount of experimental data, in the next phase a numerical investigation was performed on a 3D model to simulate porous inserts with random packing of metallic RR at pore-scale. The effects of several influential parameters, such as the fluid turbulence model, the effective thermal conductivity of the porous material, and the randomness of the RR in the porous structure, were studied to assess the accuracy and repeatability of the model in predicting thermal and fluidic characteristics of air inside the absorber pipes under different working conditions. A detailed thermo-hydraulic analysis revealed an irregular flow pattern inside the porous zone, while the air recirculation at the porous entrance and exit provides an uneven pressure drop distribution in the azimuthal direction (Fig.). Moreover, fluid turbulence is enhanced downstream of the porous insert thanks to several stream jets formed by uneven flow discharge at the insert outlet face, which improves heat transfer in that area. The analyses demonstrated a significant improvement in heat transfer, with a maximum enhancement factor of 10 - 15 than the smooth tube. Additionally, in the evaluation of thermo-hydraulic performance, the enhanced absorbers exhibit Performance Evaluation Criteria up to 2, compared to the tube without RR inserts.

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

Topic: Artificial Intelligence for Energy Efficiency

Course year: 2nd **Tutor(s)**: Andrea LANZINI, Lorenzo BOTTACCIOLI

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.

External collaborations

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

Highlights of the research activity

Energy efficiency oriented measures, including retrofit actions, optimal control of the buildings HVAC system and reduction of abnormal events, require deep understanding of the buildings thermal behaviour, benchmarking of building stock, analysis regarding the cooling system and many other task. To this purpose, non-intrusive analysis, extracting useful information by the data collected by smart meters, is a promising research activity. To these purposes, we focus out research activity in the application of Machine Learning techniques to 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 behaviour
- Estimation of the benefits associated to retrofit actions

To these purposes, hourly electrical energy consumption data from about 2000 buildings were employed. With respect to the activity developed in the previous year, which mainly focused on the pre-processing step and on benchmarking, during the last year we focused our attention on the energy audit of buildings. To this extent, we designed specific Machine Learning-based tools, capable of providing reference thermal behaviour 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 CuSum one, enhanced detection of changes in operative conditions of the buildings and other deviation from reference behaviour. Finally, such charts allow the ex-post estimation of the savings related to a certain retrofit measure.
Future work shall focus on the estimation of ex-ante energy savings, to support decision making in adoption of energy efficiency measures. Besides, another fundamental research area to investigate shall be the optimal control strategy of cooling systems.

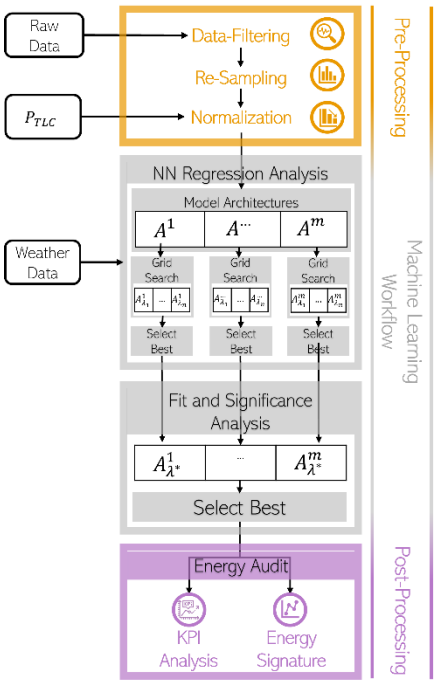


Fig. Outlook of a Neural Network-based approach for energy audit of buildings

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

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

Course year: 1st **Tutors**: Massimo SANTARELLI, Giuliana MATTIAZZO

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.

External collaborations

Highlights of the research activity

The initial approach was to conduct a literature review on the state of the art of offshore hydrogen production assessment. From this resulted the identification of 4 different main steps to proceed in the aim of the research:

1) **Maritime Area Eligibility Assessment (GIS-based)**
2) **Producibility Assessment**
3) **Data clustering and nodes modelling**
4) **Matching with the onshore energy model grid & scenarios simulation**

From a second literature review about step1 was determined that:

- Among the existing criteria to perform GIS analysis, those necessary for the energy assessments for the development of spatially solved energy models are *"exclusion"* criteria.
- GIS-based tools are mainly commercial or non-user-friendly.
- There is not a unique reference list of exclusion criteria nor for the legislations driving their determination to which refer.
- There is not a unique reference list for the sources of GIS data.

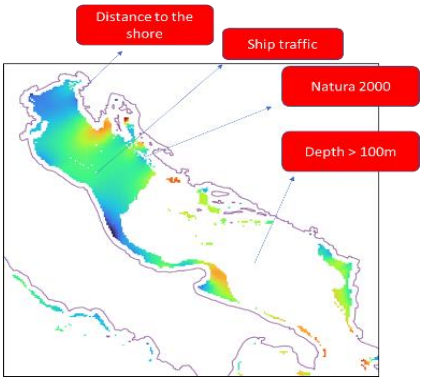


Fig. Example of an Eligibility Layer for mean wind speed thematic layer with the indication of the origin of the exclusion choices

Downstream, it was decided to provide a solution to fill the gaps identified: **(1)** The collection of information necessary to the production of a reference schematic map for the sources is in course; **(2)** It is under development a proposal of offshore exclusion criteria taxonomy. This will reflect the existing normative on the maritime spatial planning and the practices developed with reference to specific EEZs or geographical areas, relating to different RES technologies; **(3)** An open access (QGIS) and flexible tool for the GIS-based spatial assessment was developed. This allows the user to provide as input different georeferenced data file extensions and satisfies 3 different requirements of a GIS-based area assessment process:

a. **Generate the "exclusion layer**": this is a map accounting only for the ineligible areas of the studied zone.
b. **The "eligibility layers" and "eligibility database core" generation:** the "*eligibility layers"* are thematic maps deprived of the exclusion areas via the application of the exclusion layer. They can be produced in the preferred georeferenced file format and one of them can constitute the core of the eligibility database.
c. **The updating of the eligibility database:** the eligibility database can contain whatever kind of GIS information desired by the user that can be added to the database by the user itself, taking in account only the eligible areas.

The novelty of this tool allows to do preliminary producibility assessment studies by using the information stored in the eligibility GIS database. The preliminary selection of only the eligible areas data will lead to a reduction in computational cost for the energy model solving. The tool was presented in July 2023 to OSESS conference in Malta. The activities planned for next year will involve the development of steps 2 and 3.

First name: Daniele **LAST NAME**: FERRARIO

Topic: Decarbonization of Industrial Plants

Course year: 3rd **Tutor(s)**: Andrea LANZINI, Vittorio VERDA, Stefano STENDARDO

Academic context

[1] "Carbon footprint of a calcium looping carbon capture process in steel production system", 2023 International Journal of Greenhouse Gas Control, C. Carbone, D. Ferrario, A. Lanzini, V. Verda, A. Agostini, S. Stendardo.
[2] "Solar-driven calcium looping system for carbon capture in cement plants: process modelling and energy analysis", 2023, Journal of Cleaner Production, D. Ferrario, S. Stendardo, V. Verda, A. Lanzini.
[3] "Cost and environmentally efficient design of an absorption-based post-combustion carbon capture unit for industry applications", (under review), Chemical Engineering Journal, D. Ferrario, T. Pröll, A. Lanzini.

External collaborations

- Ente Nazionale Energia Ambiente (ENEA).
- International Energy Agency (IEA) – IEA IETS Task 21.
- University of Natural Resources and Life Sciences (BOKU - Wien, Austria).

Highlights of the research activity

Among the most energy-intensive and CO_2-emitting industries, the cement industry emits alone around 2.2 Gt_{CO2}/year (6-7% of the global anthropogenic GHG emissions). Furthermore, cement production is a hard-to-abate process where around 60% of the CO_2 produced comes from the calcination of the raw minerals. One of the most promising solutions for the mitigation of the CO_2 emissions of this sector is, therefore, the application of Carbon Capture and Storage technologies (CCS), such as Post-combustion Carbon Capture (PCCC) and Direct Air Carbon Capture (DAC). Furthermore, PCCC and DAC are considered key technologies to reach "net-zero" CO_2 emissions in cement production.
PCCC systems can greatly reduce the "direct" CO_2 emission of a state-of-the-art cement plant. Indeed, they can capture both combustion and process (i.e. calcination) CO_2 emissions. However, these technologies are very energy-intensive processes requiring large amounts of low enthalpy steam. DAC systems are even more energy-intensive processes, but they can play a critical role in reducing the "upstream" CO_2 emissions of the production process.
An in-depth analysis of several "net-zero" process configurations was performed considering some of the most promising and more technologically mature decarbonization and CO_2 emission mitigation strategies: (i) fuel shift; (ii) post-combustion carbon capture (PCCC), and (iii) direct air carbon capture (DAC).
To provide a broad overview of the entire production value chain we performed a multi-step analysis. The mass and energy balances of a reference state-of-the-art plant with and without the integration of PCCC was first estimated through a detailed process modeling. The results obtained were then used as input for a carbon footprint analysis, which was performed with a life cycle analysis approach and a cradle-to-gate system boundary. This approach allows for a detailed accounting of all the GHG emissions along the value chain and the estimation of the overall. The obtained results show how the integration of PCCC is usually not enough to reach net-zero CO_2 emissions and negative CO_2 emission technologies such as DAC are thus needed. The combination of a fuel shift to RDF and PCCC, instead, is a very promising solution that could potentially lead to a zero or even negative CO_2 process as shown in Figure 1.

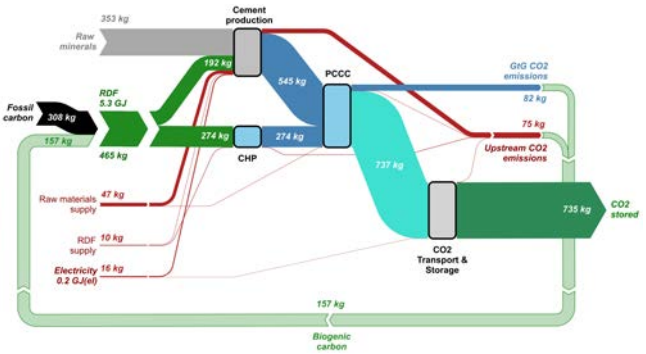


Fig. CO_2 Sankey diagram for PCCC integration into cement plant with RDF combustion.
Units [$kg_{CO2,eq}/t_{cem}$].

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

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; European Association of Development Research and Training Institutes (EADI). Vol. 32. Issue 4. pp. 1249-1287.

External collaborations

- ENI

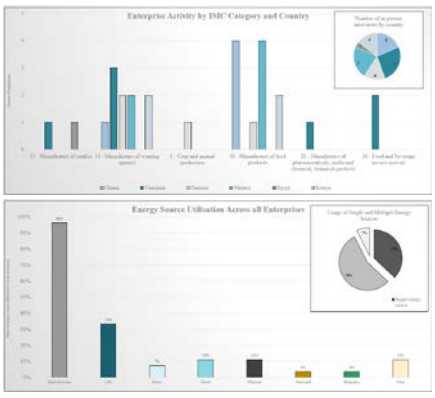
Highlights of the research activity

In the second year, significant strides were made in understanding the productive use of women-owned enterprises. To fill some research gaps in the field of energy, gender and entrepreneurship within the African context, the focus of the second year was put on gathering first-hand data through semi-guided interviews with micro-, small-, and medium-sized enterprise owners.

1. A comprehensive survey sourced data from women-owned micro, small, or medium-sized enterprises in targeted industries and countries. Out of 175 contacts, 49 responses were received, and 39 were deemed suitable for analysis. Key findings shed light on the prevalence of single-source energy dependence and highlighted concerns regarding enterprises' awareness of their energy usage and associated costs.

2. Energy audits: A series of in-depth interviews with 27 women entrepreneurs in the food and textile sectors across six focus countries generated crucial insights. The interviews covered enterprise specifics, technical data, and perspectives on renewable energy. These findings are pivotal for shaping the development of business models and renewable energy solutions planned for the upcoming research year.

Overview on energy audits conducted in 2nd year



3. Tanzanian case study: Explorations into converting slaughterhouse wastewater into biogas for textile manufacturing in Tanzania indicated potential CO_2 emission reductions. However, limitations in biogas production volume pose financial challenges that necessitate further exploration to ensure business viability.

In the third year, this accumulated knowledge will be translated into actionable strategies aimed at fostering sustainable practices, enhancing energy efficiency, and driving the adoption of renewable energy solutions within targeted enterprises. The ultimate aim is to catalyse the movement toward a greener, more sustainable future for the food and textile sectors across Africa.

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

Topic: Optimal energy management of hybrid grid-scale energy storage systems coupled with renewable energy sources

Course year: 2nd **Tutor(s)**: Andrea LANZINI, Francesco Demetrio MINUTO

Academic context

[1] N. DiOrio, P. Denholm, and W. B. Hobbs, "A model for evaluating the configuration and dispatch of PV plus battery power plants", Applied Energy 262, 2020.
[2] J. Cao, D. Harrold, Z. Fan, T. Morstyn, D. Healey, K. Li, Deep Reinforcement Learning Based Energy Storage Arbitrage With Accurate Lithium-ion Battery Degradation Model, IEEE Transactions on Smart Grid, Vol. 11, No. 5, (2020).
[3] A. V. Vykhodtsev, D. Jang, Q. Wang, W. Rosehart, and H. Zareipour, "A review of modelling approaches to characterize lithium-ion battery energy storage systems in techno-economic analyses of power systems", Renewable and Sustainable Energy Reviews. 166 112584, 2022.

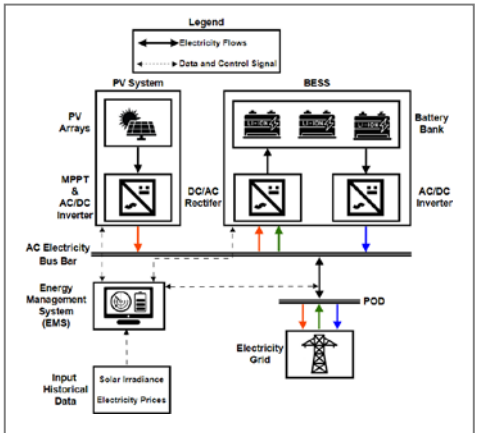
External collaborations

- Samueli School of Engineering, University of California Irvine (UCI), Irvine, California, USA.
- Officine Edison, Edison S.p.A., Energy Center, Turin, Italy.

Highlights of the research activity

The research activity conducted during my first year as PhD student (from November 2021 to November 2022), was addressed on techno-economic analysis of utility-scale grid-connected energy storage systems. Thanks to an industrial collaboration with Edison S.p.A., I had the possibility to elaborate real data provided by a Li-ion battery energy storage system currently in operation and managed by Edison. On March 23rd, 2023, I published, as first corresponding author on Elsevier's Journal of Energy Storage, my first scientific article entitled "*Ageing and energy performance analysis of a utility-scale lithium-ion battery for power grid applications through a data-driven empirical modelling approach*" (https://doi.org/10.1016/j.est.2023.107232).

During my second PhD year I have continued the research activity of the first year, passing from a data-driven modelling approach to a mixed-integer linear/non-linear modelling approach built in a simulation framework. The goal of my research is to demonstrate that energy storage technologies are crucial to successfully complete the energy transition path decarbonizing the power sector and supporting the renewable energy sources deployment on the electrical distribution network making it more flexible. In this perspective, during the 2nd PhD year spent at PoliTo (from November 2022 to December 2022, and from August 2023 to present) and at University of California Irvine (from January 2023 to July 2023), the main research topic is focused on linear (LP), mixed-integer linear (MILP), and mixed-integer non-linear (MINLP) optimization programming approaches applied on energy storage system models aimed at achieving the optimal energy dispatch management from a techno-economic point of view. Recently, I sent a conference paper in collaboration with UCI to participate at the IEEE Power & Energy Society General Meeting 2024 (https://pes-gm.org/). As illustrated in the scheme, the conference paper proposes an optimal scheduling for an energy management system (EMS) of a utility-scale photovoltaic power plant (PV) coupled with a battery energy storage system (BESS). The EMS model is based on a computationally efficient optimization logic formulated as a mixed-integer linear programming (MILP) problem. In the proposed case study, PV hourly generation data and historical electricity market prices from the CAISO electricity market in the United States, California, are used as input. The achievable profit from energy arbitrage of PV + BESS systems is determined considering the impact of battery degradation. Furthermore, in the next weeks, a further journal article always in collaboration with UCI will be published on Elsevier's Journal of Energy Storage.



Layout of PV + BESS System

First name: Azad **LAST NAME**: HAMZEHPOUR

Topic: Simulation and Experimental Analysis of Water Mist Systems for Shielded Fire Applications

Course year: 3rd **Tutor(s)**: Vittorio VERDA, Romano BORCHIELLINI

Academic context

[1] Hamzehpour, A.; Verda, V.; Borchiellini, R. Simulation Study on Suppressing Shielded Fires by Water Mist Systems. Fire. 2023, 6, 10.3390/fire6040129.
[2] Liu, Y.; Wang, X.; Liu, T.; Ma, J.; Li, G.; Zhao, Z. Preliminary study on extinguishing shielded fire with water mist. Process Saf. Environ. Prot. 2020, 141, 344–354
[3] Beihua, C.; Guangxuan, L.; Zhen, H. Extinction Limit of Diesel Pool Fires Suppressed by Water Mist. J. Fire Sci. 2009, 27, 5–26; 10.1177/0734904108095337.

External collaborations

- Imperial College
- NIST
- Technositaf

Highlights of the research activity

An extensive experimental campaign was conducted to analyze the performance of water mist systems (both low-pressure and high-pressure nozzles) in suppressing and controlling shielded fire scenarios in an enclosure (Figure1). Several cases with different shielding conditions, such as the obstruction size and its distance from the nozzle, diverse pool fire size, and two activation times were defined and the fire extinguishing time, the temperature distribution, the exhaust gas concentration, the water discharge rate, and the inlet air flow into the compartment were measured. The Heat Release Rate (HRR) values of two pool fires were also obtained by measuring the fuel mass loss rate during the dry tests. Furthermore, the characteristics of tested water mist nozzles were measured by a Phase Doppler Particle Analyzer (PDPA) system. These characteristics include the downward velocity of the nozzle and the droplet size distribution. The fire results showed that the fire suppression time increases by reducing the block ratio in cases with the same obstacle size. Also, the estimated plume-spray thrust ratios for successfully suppressed cases were below the critical value reported in the literature. It was seen that some droplets could bypass the obstruction and reach the fire zone and suppress the sheltered fire mainly through flame and fuel surface cooling and evaporation mechanisms. However, when the largest obstacle was placed closer to the fuel surface, mist nozzles failed to extinguish the fire, and fire intensification happened in some cases. Moreover, it was proved that the longer water discharge time leads to a longer duration of CO production due to incomplete combustion. Both lateral and flame temperatures inside the compartment were successfully controlled by the mist nozzle in suppressed cases. Moreover, the possibility of using additives like F500 encapsulator agent for shielded fire scenarios was assessed experimentally. The extinguishing time was reduced by 70% in some cases using the F500-water mist system.

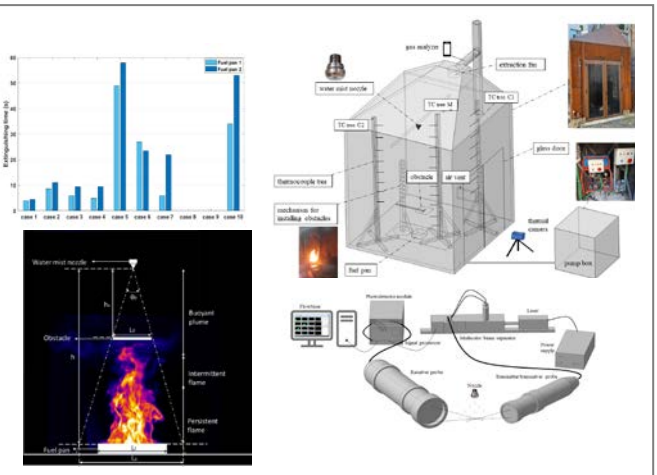


Fig.The experimental set-up for fire tests and PDPA system, the comparison of fire suppression time, and the schematic view of geometric projections in shielded fire scenarios

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

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

Course year: 1st **Tutor(s)**: Pierluigi LEONE

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] I. Pappis, M. Howells, V. Sridharan, W. Usher, A. Shivakumar, F. Gardumi, E. Ramos, Energy projections for African countries – Publication Office of the EU. 2019, doi: 10.2760/678700.
[3] P.M. Koshikwinja, M. Cavana, S. Sechi, R. Borchiellini, P. Leone, "A systematic review for hydrogen supply chain and domestic use in Africa", *in preparation (under internal review)*

External collaborations

Highlights of the research activity

The main goal of my Ph.D. work is to customize an existing energy modeling to the African socio-economical with the main objective of analyzing different pathways for green energy carriers production and utilization in the African continent. The model aims also to assess the role of productive uses of energy in the clean energy access process, both electricity and clean fuels such as hydrogen mainly for domestic industrial application in Africa in line with the AU Agenda 2063 and the joint vision for 2030 between Africa and Europe towards energy transition.

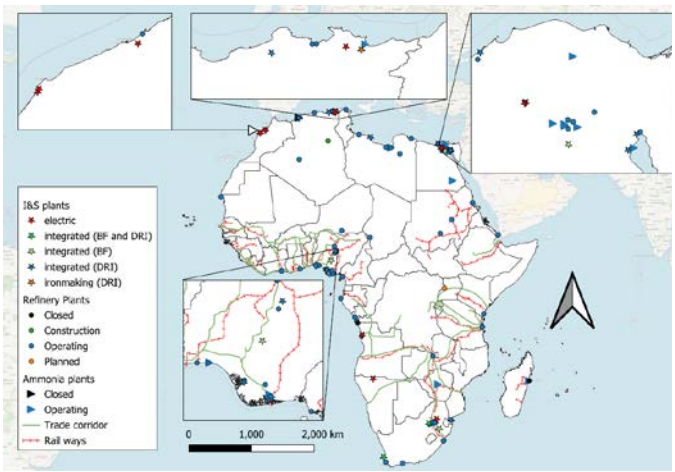


Fig. Map of selected African industry plants and main sub-Saharan trade corridor and railways.

During this first year of the Ph.D., a systematic literature review was performed; leading to both the analysis of the hydrogen value chain in Africa, and the identification and selection of energy system modeling tool 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.

Furthermore, an energy database for African countries including the industrial sector, power network, pipelines, ports, liquified natural gas terminals, etc. has been performed. The compilation of the energy database for African countries was mainly performed by screening and collecting relevant information in freely accessible online gray literature and databases including the International Energy Agency (IEA), International Renewable Energy Agency (IRENA), United Nations Framework Convention on Climate Change (UNFCCC), Desert Industrial Initiative (Dii), and World Bank databases, etc.

Based on gathered data, the first MUSE model for the power sector of the D.R. Congo is under development.

First name: Lorenzo **LAST NAME**: LAVENEZIANA

Topic: Clean energy transition of airport energy systems

Course year: 2nd **Tutor(s)**: David CHIARAMONTI, Matteo PRUSSI

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, M. Howells, M. Bazilian, J. F. DeCarolis, S. Hermann, and H. H. Rogner, *"Modelling elements of Smart Grids - Enhancing the OSeMOSYS (Open Source Energy Modelling System) code,"* Energy, vol. 46, no. 1, pp. 337–350, 2012.
[3] de Rubeis, T., Nardi, I., Paoletti, D., di Leonardo, A., Ambrosini, D., Poli, R., & Sfarra, S. (2016). Multi-year consumption analysis and innovative energy perspectives: The case study of Leonardo da Vinci International Airport of Rome. Energy Conversion and Management, 128, 261–272.

External collaborations

SAGAT S.p.A. Società Azionaria Gestione Aeroporto Torino

Highlights of the research activity

The objective of my research project is the analysis and modelling of the energy system of Turin airport, aimed at the realisation of a long-term decarbonisation strategy in line with the ambitious environmental goals set for the following decades. Building on the setup of the model configured during the first year, the second year saw the application of the model to the study of the potential development of the airport under different scenarios. Several analyses were conducted. One example is reported in the figure below, which shows the results of a study aimed at develping a set of reccomendations to inform the airport on the optimal development pathways

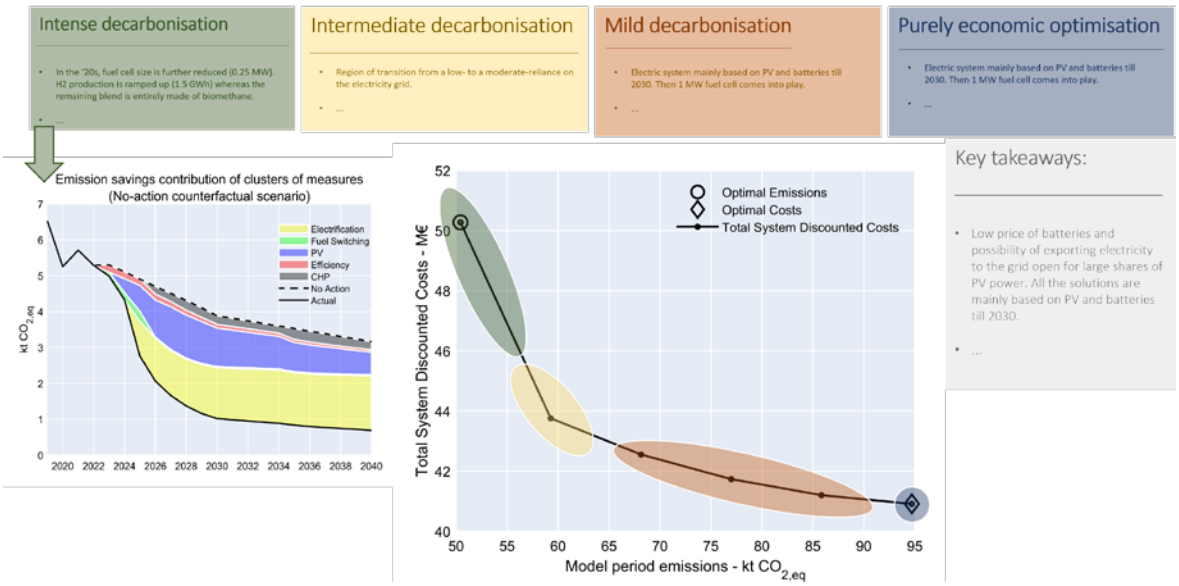
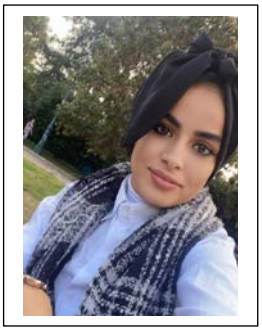


Fig. Example of the analysis carried out during the second year of the PhD: determination of the optimal development pathway of the airport for environmental targets with growing ambition.

under different levels of environmental ambition. The economic aspects of each pathway were evalauted in terms of necessary CAPEX and OPEX and the contribution of each basket of measure to the decarbonisation objectives was quantified. Further analyses are still in course. The possibility of adopting a hydrogen-based economy, also taking advantage of the foreseen role of Hydrogen Valleys in the Piedmont region, is being examined. Beside on-site hydrogen production, the possibility of interacting with local partners to provide a stream of green hydrogen to the airport is being explored. Moreover, the uncertainties concerning the future development of the national and international energy systems have been characterised (e.g., energy prices), and their impact on the development of the airport is being studied through a scenario-approach.



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

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

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

Academic context

[1] 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, Volume 267, 2024, 112236, ISSN 0038-092X, https://doi.org/10.1016/j.solener.2023.112236
[2] Hossein Ebadi, Antonio Cammi, Rosa Difonzo, José Rodríguez, Laura Savoldi, Experimental investigation on an air tubular absorber enhanced with Raschig Rings porous medium in a solar furnace, Applied Energy, Volume 342, 2023, 121189, ISSN 0306-2619, https://doi.org/10.1016/j.apenergy.2023.121189
[3] Hossein Ebadi, Andrea Allio, Antonio Cammi, Laura Savoldi. "First Numerical Evaluation of the Thermal Performance of a Tubular Receiver Equipped With Raschig Rings for CSP Applications." Proceedings of the ASME 2021 Power Conference. ASME 2021 Power Conference. Virtual, Online. July 20–22, 2021. V001T04A005. ASME. https://doi.org/10.1115/POWER2021-65714

External collaborations

- M2EM Research Unit, university of Gabes, Tunisia.

Highlights of the research activity

In the first PhD year, the research focused on the study and optimization of novel tubular absorbers for parabolic trough solar collectors (PTSC), achieving a significant milestone through experimental investigations of various absorber configurations such as the conventional simple absorber, the sinusoidal absorber, and the spiral absorber at the University of Gabes, Tunisia.

Fig. Photo of the parabolic trough solar collector of the experimental setup.

Through meticulous experimentation conducted, a wealth of data was gathered, offering insights into the performance nuances of each configuration. This comprehensive dataset sets the stage for advanced numerical analyses, aligning with the overarching goal of optimizing solar concentrators and advancing the field towards more sustainable and efficient solar energy utilization.

As the PhD progresses, the groundwork has been laid for rigorous optical simulations, in-depth CFD analysis, and the ultimate optimization of solar receivers for parabolic trough solar collectors. These efforts not only consolidate the findings from experimental studies but also pave the way for a comprehensive understanding of the complex interactions within the solar collector system. This approach sets a promising trajectory for the coming years, marked by advancements in both experimental and numerical methodologies, thereby contributing significantly to the field of solar energy research and technology.

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

Topic: Advanced management for resilient and sustainable multi-energy systems

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

Academic context

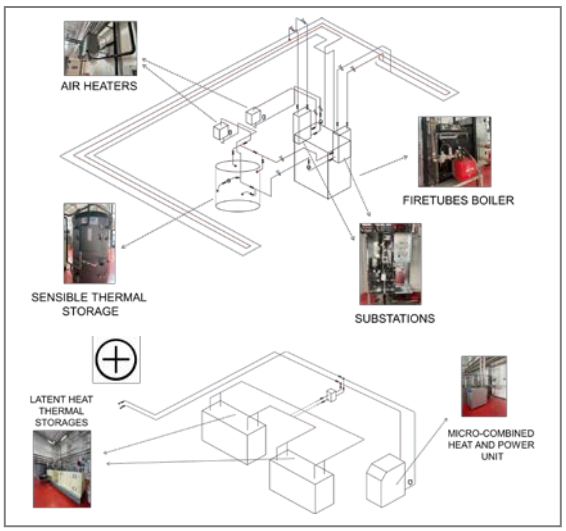
[1] Mancarella P. MES (multi-energy systems): An overview of concepts and evaluation models. Energy 2014, Vol 65, Pages 1-17.
[2] Guelpa E., Bachi A., Verda V., Chetco M., Lund H. Towards future infrastructures for sustainable multi-energy systems: A review. Energy 2019, Vol 184, Pages 2-21.
[3] Capone M., Guelpa E., Mancò G., Verda V. Integration of storage and thermal demand response to unlock flexibility in district multi-energy systems. Energy, 2021, Vol.237, Pages 121601.

External collaborations

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

Highlights of the research activity

In the context of Multi-Energy Systems (MES) operation optimisation some of the challenges still to be faced are: a) the characterisation of the uncertainties affecting these systems; b) the operation of the district heating network which is rapidly changing due to flexibility measures, prosumers integration, operation at different temperature levels etc.; c) the need for experimental validation to prove the accuracy of the mathematical models and the competitiveness of the proposed MES strategy with respect to existing management strategies. In general, 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. Special emphasis is placed on modelling the district heating network and its integration with other system components. The experimental testing of the proposed mathematical models and optimisation strategies will be carried out using a laboratory scale system installed at the Energy Centre (Turin). The lab-scale system is composed of a small-scale district heating network (with a firetubes boiler, a primary circuit, two substations, two secondary circuits, and two air-heaters) and a sensible thermal storage. Recently, a micro cogeneration unit and two latent heat thermal storages have been included in the multi-energy system. During the last year, my research has developed in two directions. On one hand, the analysis of different heat prosumer district heating connections and how the type of configuration can influence the network operation, with a specific investigation of the role of the sensible storage system at the prosumer side. On the other hand, the development of a digital twin capable of simulating the behaviour of the laboratory scale system. This analysis involves modelling each component of the lab-scale MES. First, a mathematical model for the district heating system was adapted to the laboratory-scale system to accurately characterise the thermal transient of the network. Then, a 1D multi-layered stratified model was used to characterise the storage system. Simplified models were incorporated to describe the heat flux at the substations and air heaters. Finally, an iterative procedure was employed to integrate the various models, determining mass flow rates in each branch and temperatures at each node in the network. Over the last few months, my research has been focused on converting the iterative procedure into an optimisation process. This is a challenging task, given the inherently non-linear nature of the problem. The aim is to obtain the optimal schedule for managing the system, defining charging and discharge timings for the thermal storage.



The district heating laboratory-scale system at the Energy Center Thermal Lab.

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

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

Course year: 2nd **Tutor(s)**: Francesco LAVIANO, Debora FINO

Academic context

[1] S. Hou, H. Li, and Y. Rezgui, 'Ontology-based approach for structural design considering low embodied energy and carbon', *Energy Build*, vol. 102, pp. 75–90, Sep. 2015, doi: 10.1016/J.ENBUILD.2015.04.051.

[2] V. Rai, D. Liu, D. Xia, Y. Jayaraman, and J.-C. P. Gabriel, "Electrochemical Approaches for the Recovery of Metals from Electronic Waste: A Critical Review," *Recycling*, vol. 6, no. 3, p. 53, Aug. 2021, doi: 10.3390/recycling6030053.

[3] C. E. L. Latunussa, F. Ardente, G. A. Blengini, and L. Mancini, "Life Cycle Assessment of an innovative recycling process for crystalline silicon photovoltaic panels," Solar Energy Materials and Solar Cells, vol. 156, pp. 101–111, 2016, doi: 10.1016/j.solmat.2016.03.020.

External collaborations

- ENI S.p.A

Highlights of the research activity

In order to have an efficient and cost effect handling process of e-waste, it is important to determine precisely the possible gains from each type and component of e-waste handled. Such information enables the informed decision of what materials to target from each component and helps mitigate the hazardous impacts of e-waste and its handling by avoiding the mishandling or exposure to the toxic and hazardous materials found inside electronic components and following the right cost-effective processes. With this in sight, and while developing the ontology that would be used as the core for the decision support system, it was found that precise quantification of materials found in e-waste is not a topic widely spoken of in the literature. Therefore, an investigation of the quantities of materials found within a Printed Circuit Board (PCB), which is one of the widely found components in e-waste, was initiated. The investigation includes the analyzing of different types of PCBs, namely RAM, motherboard, CPU and integrated circuit. This investigation is still ongoing, and the data obtained would then be fed into the ontology. The analysis is carried out by means of ICP, SEM and XRF to detect the various materials included both metallic and organic as well as to quantify them. The initial data obtained for the RAM component using SEM and ICP shows their richness in copper, tin, and gold. In addition, the analysis shows high content of lead which is a hazardous material and requires special handling.

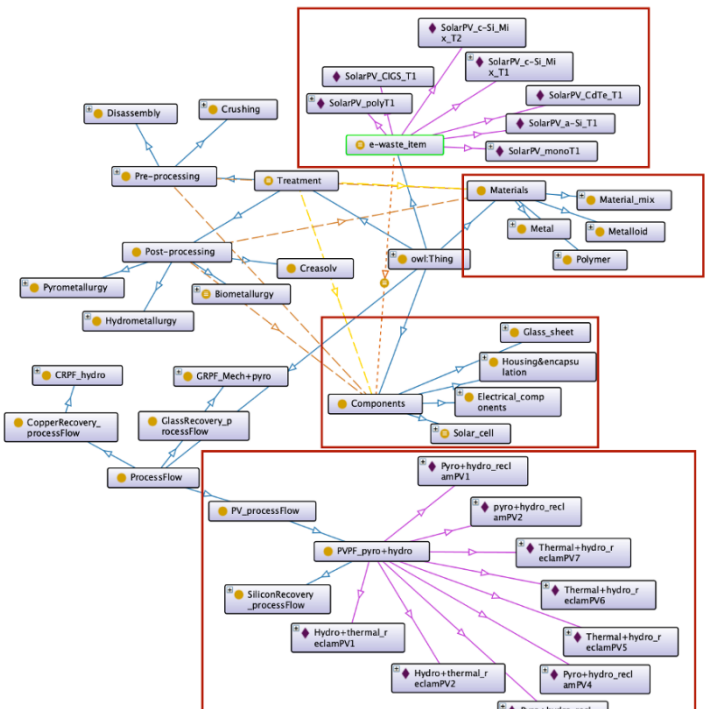


Fig. The ontology developed for the handling of e-waste with a focus on solar PVs.

First name: Chiara **LAST NAME**: MONZANI

Topic: Decarbonization of district heating systems

Course year: 2nd **Tutor(s)**: Alberto POGGIO

Academic context

[1] European Parliament and Council. (2023, May 16). Directive (EU) 2023/959 **[2]** European Parliament and Council. (2023, September 13). Directive (EU) 2023/1791 **[3]** Bersani, A. M., Falbo, P., & Mastroeni, L. (2022). Is the ETS an effective environmental policy? Undesired interaction between energy-mix, fuel-switch and electricity prices. Energy Economics, 110, 105981

External collaborations

- Iren Spa

Highlights of the research activity

As part of ongoing PhD research, a simulation tool is being developed to evaluate District Heating Systems (DHSs), offering a comprehensive analysis of their operational dynamics. This tool is capable of evaluating DHSs across diverse technological, service, and user configurations, focusing on their resilience, robustness, and assessing their environmental, economic, and energetic impacts. Beyond simulating operational performance, the model plays a pivotal role in assessing environmental and economic impacts, guiding towards rational decision-making in regulatory system evolution. A particular application of this model has been in analyzing the influence of emissions policies on the revamping investments in DHSs, crucial for aligning with European decarbonization processes. A spotlight is cast on the Emission Trading System (ETS), which, despite its wide coverage, presents loopholes allowing smaller units to bypass regulations [1]. The study examines an existing third-generation District Heating System, defining four revamping scenarios to avoid the current ETS regulations: two traditional natural gas cogeneration plants (FF, FFHP with heat pumps) and two partially renewable options using wood biomass (R1 with a biomass boiler, R2 with an ORC unit). Despite gas scenarios showing higher efficiency, only the renewable ones meet efficient heating standards [2], significantly cutting CO_2 emissions. Economic performances were evaluated up to 2040 under both *current regulation* and potential *ETS extension*, considering revenues and expenses (Fig.). Analysis occurred across three electricity market models: *Current Market* (CM), where electricity prices are correlated with gas costs; *Partial Decoupling* (PDC); and *Full Decoupling* (DC), each of which represents different levels of decoupling between electricity and gas pricing. Our findings indicate that environmental policy alone doesn't drive renewable investment. Fossil technology investments become risky and uneconomical with simultaneous ETS extension and energy market reform (indicated by the red box in the figure). For effective decarbonization, a dual strategy is necessary: revising the ETS directive and overhauling energy markets and pricing. This dual approach is vital to realize European decarbonization goals.

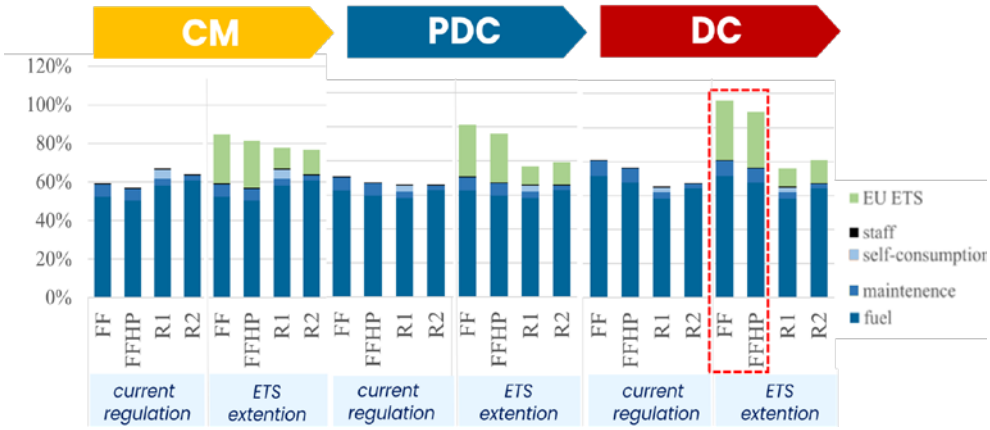


Fig. Economic performances: *Expenses* over *Total Revenues (%)*

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

Topic: Entropy generation minimization in high temperature concentrating solar power receivers equipped with TPMS

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

Academic context

[1] Bejan A., "Entropy generation minimization: The new thermodynamics of finite-size devices and finite-time processes," *J. of Applied Physics,* vol. 79, pp. 1191-1218, 1996.
[2] Flesch J., Marocco L., Fritsch A., Niedermeier K., Wetzel T., "Entropy Generation Minimization Analysis of Solar Salt, Sodium, and Lead–Bismuth Eutectic as High Temperature Heat Transfer," *J. of heat transfer,* vol. 142, no. 4, p. 120168, 2020.
[3] Liang D., Shi C., Li W., Chen W., Chyu M.K., "Design, flow characteristics and performance evaluation of bioinspired heat exchangers based on triply periodic minimal surfaces," *Int. J. of Heat and Mass Transfer,* vol. 201, p. 123620, 2023.

External collaborations

- Politecnico di Milano
- IMDEA Energy, Madrid, Spain

Highlights of the research activity

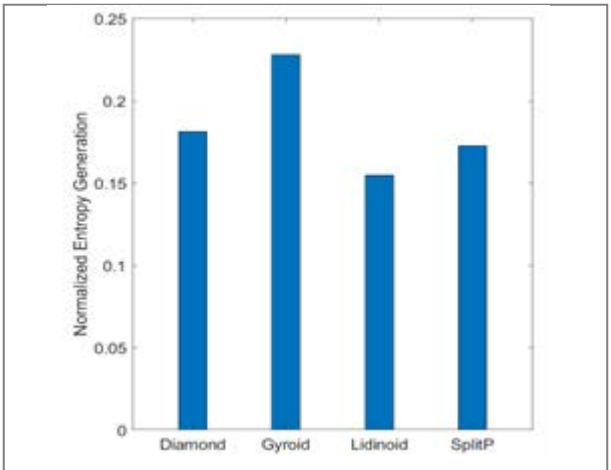


Fig. Entropy generation of an absorber (5.08 inner diameter and 10 cm length) equipped with different TPMS structures with unit cell size of 20mm×20mm×20mm under uniform circumferential heat flux of 1 MW/m^2 and mass flow rate of 1 kg/s

The research activity is focused on Entropy Generation Minimization (EGM) of high temperature concentrating solar power (CSP) receivers equipped with Triply Periodic Minimal Surfaces (TPMS) as the porous medium. TPMS is defined as a zero-mean curvature surface which is repeated periodically in three principal directions, with continuous and non-intersecting surfaces. This leads to lower frictional pressure drop and prevention of "dead zones" in which the flow is subjected to stagnation and poor mixing. A substantial part of the literature is mainly focused on thermal efficiency improvement, overlooking the unfavorable effects of the resultant pressure drop. Unlike thermal studies, entropy-based analyses consider both the positive aspect of thermal performance improvement and the consequent pressure drop combined inside the overall entropy generation amount.
Four different TPMS structures – namely: Diamond, Gyroid, SplitP and Lidinoid - were studied. These structures were simulated in STAR-CCM+ as a porous insert in a limited length of a CSP receiver and investigated from many different points of view such as uniform and non-uniform heat flux, different TPMS unit cell sizes and different mass flow rates with water as the working fluid. The total entropy generation (Fig.) and Thermal Enhancement Factor (TEF) of these cases were compared together; these two factors could bring interesting insight as KPIs in the design/improvement process. The participation to an experimental test campaign at IMDEA Energy studying the performance of two planar solar receivers equipped with Diamond and Split TPMS structures was also possible. From the results of the 1st years' studies, a structure and the working conditions are chosen to study for practical solar applications. Currently, the influence of TPMS inserts placed in different locations of a tubular CSP receiver with concentrated, non-uniform heat flux and the heat transfer fluid of Syltherm-800 is under study.

First name: Atta **LAST NAME**: MUHAMMAD

Topic: Atomistic Modelling and Experimental Characterization of Plastic crystals as Solid-Solid Phase-Change Material for Thermal Energy Storage

Course year: 3rd **Tutor(s)**: Matteo FASANO, Eliodoro CHIAVAZZO

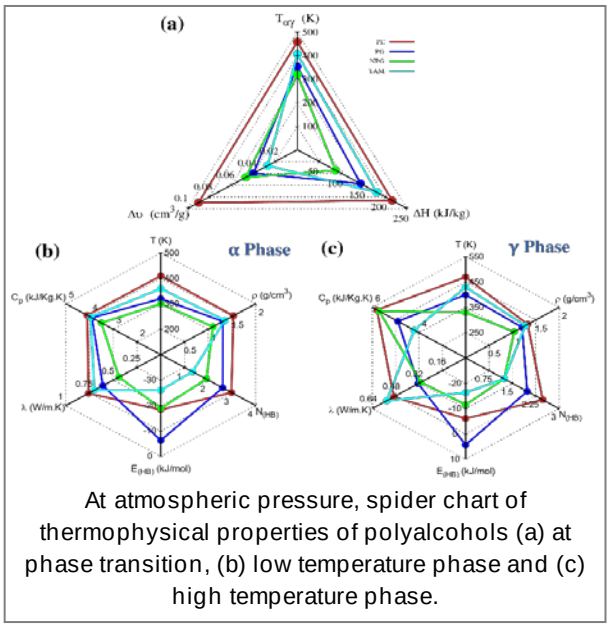
Academic context

[1] Ribezzo, et al. *Journal of Energy Storage* **53**, 105140 (2022).
[2] Lloveras, et al. *Nat Commun* **10**, 1803 (2019).
[3] Feng, et al. *International Journal of heat and mass transfer* **141**, 789-798 (2019).

External collaborations

- Department of Industrial Engineering, University of Rome Tor Vergata, Italy.
- Department of Physics, Universitat Politècnica de Catalunya, Spain.

Highlights of the research activity



At atmospheric pressure, spider chart of thermophysical properties of polyalcohols (a) at phase transition, (b) low temperature phase and (c) high temperature phase.

The study investigates Solid-Solid Phase Change Materials (SS-PCMs) pentaerythritol (PE), Pentaglycerine (PG), neopentylglycol (NPG), and trihydroxy methyl-aminomethane (TAM) for thermal energy storage (TES). These materials exhibit polymorphic behavior with high transition enthalpies, making them promising for TES applications. The inclusion of nanofillers such as carbon nanotubes enhances durability and addresses encapsulation concerns. Eutectic mixtures offer the ability to tune transition temperatures and latent heats. However, the low thermal conductivity of SS-PCMs presents challenges for charging and discharging rates, potentially causing thermal hysteresis. The study utilizes LAMMPS for Molecular Dynamics simulations with the GROMOS force field, focusing on PE, PG, NPG, and TAM. Various properties, including latent heat, density, hydrogen bonds, specific heat capacity, and thermal conductivity, were calculated. Latent heat was determined as the potential energy difference between the two phases. NPT simulations involved heating α phases to the phase transition temperature ($T_{\alpha\gamma}$) and cooling γ phases to $T_{\alpha\gamma}$. Multiple independent NPT simulations were conducted, equilibrating for 2 ns in α phases at atmospheric pressure. Temperature intervals varied (390 K for PE, 300 K for PG, 250 K for NPG, and 300 K for TAM), reaching $T_{\alpha\gamma}$ in 10 K intervals. Similar simulations were performed for γ phases under atmospheric pressure, covering temperatures from $T_{\alpha\gamma}$ to 530 K for PE, 420 K for PG, 400 K for NPG, and 500 K for TAM. Specific heat capacity in both phases was calculated from the enthalpy-temperature curve slope, and thermal conductivity was determined using the non-equilibrium MD method with the Muller-Plathe algorithm. The study highlighted the strong dependence of solid-phase thermal conductivity on system length, requiring a linear approximation for accurate predictions. Densities of plastic crystals in both phases exhibited a linear decrease with increasing temperature, resulting in an expansion of specific volume. Solid-solid phase transitions induced notable specific volume changes: ~0.09 cm³/g for PE, ~0.04 cm³/g for PG, ~0.047 cm³/g for NPG, and ~0.027 cm³/g for TAM, aligning with experimentally measured values. PE exhibits highest latent heat, followed by TAM, PG, and NPG. Predicted latent heat values (in kJ/mol) were 29.47 in PE, 21.72 in TAM, 17.37 in PG, and 9.06 in NPG. Heat capacities for non-transition phases (α and γ phases) were computed, revealing higher values in the γ phase under MD simulations, approximately 1.5-2 times larger than experimental literature values. This overestimation was attributed to the exclusion of quantum effects in MD simulations. Thermal conductivity gradually decreased with increasing temperature particularly during solid-solid phase transitions. For instance, the thermal conductivity of PE decreased from 1.01 W/mK to 0.70 W/mK (300 K to 455 K) and further dropped to 0.51 W/mK at 465 K during the α to γ phase transition. Similar trends were observed for PG, NPG, and TAM. The number and energy of intermolecular hydrogen bonds (HBs) were analyzed concerning temperature, revealing a significant decrease in PE, PG, and NPG after the phase transition, while TAM showed a slight decrease. This reduction in HBs was attributed to molecular vibration and rotation, causing disorder in the γ phase of plastic crystals. Extensive experimental characterizations, including differential scanning calorimetry were conducted on PE and PG materials. Both materials exhibited varying phase transition temperatures and latent heats during different scans. Mass loss measurements showed substantial mass loss in PE but none in PG. Tablets of both materials were fabricated, with PE tablets displaying mass loss and PG tablets remaining stable. PG tablets reinforced with Multi-Walled Carbon Nanotubes (MWCNTs) and Aluminum nanoparticles showed minimal changes in phase transition temperature but a decrease in latent heat with increasing MWCNT content. In summary, this work provides valuable insights into the molecular mechanisms of plastic crystals and suggests a potential approach to enhance their thermal conductivity by incorporating materials with higher thermal conductivities. Future work could benefit from combining atomistic MD simulations with experimental characterizations of composite plastic crystals.

First name: Manfredi **LAST NAME**: NERI

Topic: Strategic roadmap for district cooling development

Course year: 3rd **Tutor(s)**: Vittorio VERDA, Elisa GUELPA

Academic context

[1] M. Neri, E. Guelpa, V. Verda, Design and connection optimization of a district cooling network: Mixed integer programming and heuristic approach, Applied Energy, Volume 306, Part A, 2022, 117994
[2] R. Khir, M. Haouari, Optimization models for a single-plant District Cooling System, European Journal of Operational Research, Volume 247, Issue 2, 2015, Pages 648-658
[3] D.F. Dominković, K.A. Bin Abdul Rashid, A. Romagnoli, A.S. Pedersen, K.C. Leong, G. Krajačić, N. Duić, Potential of district cooling in hot and humid climates, Applied Energy, Volume 208, 2017, Pages 49-61

External collaborations

- ENEA
- Nanyang Technological University of Singapore

Highlights of the research activity

Demand for space cooling has more than tripled since 1990 and is continuing to increase, with an enviromental impact in terms of emissions. Moreover, especially during heat waves cooling is responsible for high shares of peak demand, causing grid instabilities. More efforts are therefore needed to increase the energy efficiency of cooling systems. In this context, district cooling represents a feasible alternative to conventional cooling technologies, especially in highly populated areas with large energy densities. However, due to the large capital costs, if district cooling networks are not properly designed and managed, the economic advantages with respect to other technologies could be limited or inexistent. With this regard, during the third year of my PhD I implemented a hierarchical approach for the design and operation of district cooling networks. The objective was to further improve a heuristic algorithm developed in the first two years to make it optimize a wide number of variables with only few input parameters, such as the cooling demand, and road structure of a neighbourhood. This tool optimizes the network topology, the position of the chillers, the buildings to be connected, the storage technology to be installed, the network supply temperature and the operation strategy. We applied the model to a Singaporean case study under eight different scenarios, varying the indoor set point temperature, waste heat availability, the cost of electricity during peak hours and the space occupancy costs. The results demonstrated that due to the large cost of space occupancy in Singapore, ice is the most suitable storage technology. In addition, it was shown that optimizing the network supply temperature allows to reduce operation costs from 1 to 3.7 %. The analysis showed also that the availability of waste heat can reduce payback time by up to 5 years and increase the net present value (NPV) by more than 3.5 times. In addition increasing the indoor set point temperature by 3°C can lead to a 3 years reduction of payback time and to a 43% increase of NPV. It was also shown that the cost of electricity has an impact on the network topology and on the operation strategy. Indeed, with a higher cost of electricity pumping cost increases and it may be necessary installing two separate networks to minimize these costs. Concerning the operation strategy, the tool showed that in the baseline scenario, it would be convenient to operate the chillers with almost constant load, while by increasing the peak electricity cost, it becomes convenient to install larger chillers and storages and to operate the chillers mainly during the night to exploit the lower tariffs.

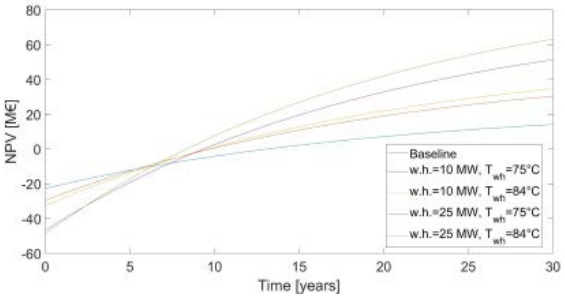


Fig. Impact of waste heat on NPV and payback time

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

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

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

Academic context

[1] Orsini et al., «Exsolution-enhanced reverse water-gas shift chemical looping activity of $Sr_2FeMo_{0.6}Ni_{0.4}O_{6-\delta}$ double perovskite», *Chem Eng Journal* **2023**. DOI: 10.1016/j.cej.2023.146083.
[2] Lidor et al., «Parametric investigation of a volumetric solar receiver-reactor», *Solar Energy* **2020**. DOI: 10.1016/j.solener.2020.04.045.

External collaborations

- University of Udine
- Massachusetts Institute of Technology

Highlights of the research activity

In the wide context of solar fuels production *via* CL, the research activity covered both the experimental and the modeling levels. On the experimental side, the investigations 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 successfully published [1]. Further experimental campaigns are ongoing, with the goal of disclosing the redox performance of SFMN in different operating conditions, as well as in alternative CL synfuels generation routes. The material is being investigated at the structural and morphological level by means of XRD and SEM, as well as at the redox performance level by means of TGA and reactor tests. Strong efforts were devoted on developing the experimental setup for water splitting tests (Environment Park laboratory), that is still currently being addressed. On the modeling side, mainly the solar thermochemical splitting is being explored, with redox cycles composed of high-temperature thermal reduction and following lower-temperature H_2O-driven oxidation for producing H_2. Cerium dioxide ($CeO_{2-\delta}$) is being considered as the active material at this purpose, being the SoA. Simplified geometries were addressed so far, with the main goal of ensuring the correct physics implementation. Considering a directly irradiated solar receiver-reactor [2], the ceria-based complete water splitting redox cycle is being simulated, with particular attention to the redox kinetics. For the reduction, kinetics from the literature was implemented.

$$(1)\quad \frac{\partial \delta_{red}}{\partial t} = (0.35-\delta)\, A_{red} e^{-\frac{E_{red}}{RT}} - \delta p_{O_2}^{n_{O_2}} A_{ox,O_2} e^{-\frac{E_{ox,O_2}}{RT}}$$

For the oxidation, an analytical expression was purposely derived, with α being the solid ceria conversion.

$$(2)\quad \frac{\partial \delta_{ox}}{\partial t} = f(T, p_{H_2O}, \alpha)$$

Nonstoichiometry δ is shown in Figure 1 for both the steps of the cycle – reduction (top) and oxidation (bottom). Redox kinetics is coupled to heat and mass transport using Comsol Multiphysics®. The approach developed for the kinetics implementation, though being analytically simple, can be extended to any solid-gas reaction involving nonstoichiometric oxides, and being a local approach, can be easily transposed in more complex reactor geometries.

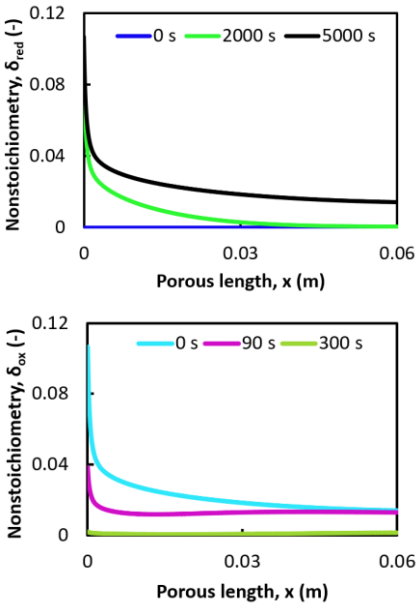


Fig. Nonstoichiometry field in the porous bed, during reduction (top) and following oxidation (bottom).

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

Topic: Analytical and Experimental Methods for Methane leak detection from the Natural Gas Distribution Grid

Course year: 2nd **Tutor(s)**: Andrea LANZINI, Romano BORCHIELLINI

Academic context

[1] MacMullin, S., & Rongère, F. X. (2023). Measurement-based emissions assessment and reduction through accelerated detection and repair of large leaks in a gas distribution network. *Atmospheric Environment: X*, *17*. https://doi.org/10.1016/J.AEAOA.2023.100201

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

[3] Zavala-Araiza, D., Lyon, D. R., Alvarez, R. A., Davis, K. J., Harriss, R., Herndon, S. C., Karion, A., Kort, E. A., Lamb, B. K., Lan, X., Marchese, A. J., Pacala, S. W., Robinson, A. L., Shepson, P. B., Sweeney, C., Talbot, R., Townsend-Small, A., Yacovitc, T. I., Zimmerle, D. J., & Hamburg, S. P. (2015). Reconciling divergent estimates of oil and gas methane emissions. Proceedings of the National Academy of Sciences of the United States of America, 112(51), 15597–15602. https://doi.org/10.1073/pnas.1522126112

External collaborations

- Italgas S.p.A.

Highlights of the research activity

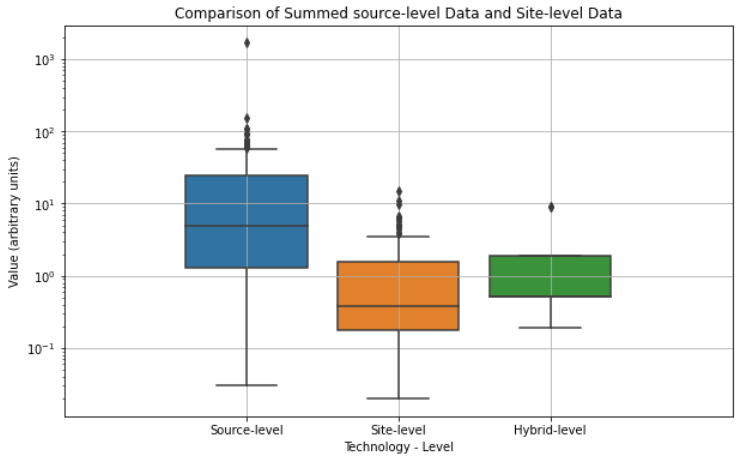


Fig. Methane emission estimates based on source-level technology data, site-level technology data, and hybrid-level (see ref. [1] in Academic context). A discrepancy is present between source and site levels, and it is partially compensated in the site-level transformation described in [1] (hybrid-level).

The research activity carreid out in 2023 has been focused on an experimental campaign in partnership with Italgas. The aim is the recnociliation between source-level estimates and site-level estimates of methane emissions from the distribution syste. We integrated of a new commercial device within standard leak detection, sampling, and repair practices to improve the direct measurement of methane emission rates from leak points. The experimental activity started of with a two-months period in which the sampling activity has been performed in 10 cities in two Italian regions. Moreover, after a formal training we provided to selected Italgas personnel crews, data have been gathered on national scale.

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

Topic: Lattice Boltzmann Method CFD techniques applied to multiphase flow

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

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] Mathias Krause et al., OpenLB—Open source lattice Boltzmann code, Computers and Mathematics with Applications, 2020, DOI:10.1016/j.camw.2020.04.033
[3] 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

External collaborations

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

Highlights of the research activity

This research topic, funded by ENI, is focused on the development of Lattice Boltzmann Method (LBM) apt for handling multiphase flows as found in bubble columns and stirred reactors. It is possible to simulate multiphase systems with the conventional CFD methods, but it is computationally cumbersome and not compatible with the industrial rhythms. The lattice Boltzmann equation regulating LBM turns simulations substantially faster due to the spatio-temporal locality of the computations [1]. This makes the method easily parallelizable, while Finite Volume based solvers need to communicate data from mutually distant nodes, because of the pressure-velocity coupling of iterative NS solvers. Hence, it is supposed to scale up better than usual CFD techniques in parallel hardware, with the challenge to obtain solutions in a time compatible with industrial needs. We have initially considered all the various open-source software that implement the studied numerical method, selecting OpenLB and Palabos. The first important result came with the validation of the two LBM codes by means of the classical 2D laminar lid-driven cavity benchmark. Another important achievement was the implementation of a scalability analysis of both identified LBM software with a workstation (SMaLL) from 1 to 16 cores on the lid-driven cavity case, underlining the advantages of OpenLB [2]. In the OpenLB school, together with professor Krause (LBRG), we modified the C++ code of a 2D multiphase example case, already implemented in OpenLB, making it more similar to a sectioned bubble column [3]. During my three-month staying at the ENI Research Center in San Donato Milanese, I worked with my company tutors to optimize GPU-enabled configurations for Lattice Boltzmann Method (LBM) simulations on the HPC4 cluster. Initially facing challenges with GPU parallelization, we collaborated with CINECA and LBRG to partially overcome issues. Two configurations are now available for parallelizing OpenLB on multiple GPUs, though NVLink Interconnect limitations still affect efficiency. This work also involves validating a 3D turbulent monophase case using OpenLB, comparing it with Ansys Fluent through Large Eddy Simulations (LES) and Reynolds Averaged Navier-Stokes (RANS) simulations. The goal is to evaluate turbulence models and performance differences between the two simulation tools. Ongoing challenges include optimizing parallelization on multiple GPUs and addressing system-side issues to make the most of computing node power. The study of how OpenLB models turbulence is important because typically a bubble column works with heterogeneous churn-turbulent flows.

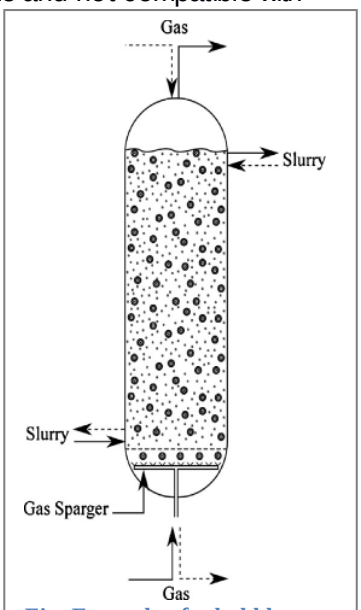


Fig. Example of a bubble column reactor (M. J. Angeles et al., "A review of experimental procedures for heavy oil hydrocracking with dispersed catalyst", 2013)

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

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

Course year: 1st **Tutor(s)**: Vittorio VERDA

External collaborations

- Iren Energia S.P.A.

Highlights of the research activity

District heating (DH) is a well-established technology, since the first networks date back to the end of the 19th century. Nowadays, it's possible to distinguish five generations of district heating systems, starting from the first generation in which the heat transfer medium was steam, and the supply temperature was around 200 °C, up to the latest systems in which the supply temperature is less than 50 °C. 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 etc… in the 2nd and 3rd generation of DH. This is a very difficult task, because to do this it's mandatory to decrease the supply temperature to operate the systems with a high efficiency. The decrease of the supply temperature, for sure, will bring the system to an increase of the mass flow rate, that can be translated into an increase of the pumping cost. One of the main topics of my PhD, is to make this transition as efficient as possible, from the point of view of the fluid-dynamics aspect. My PhD is co-funded by IREN S.p.A. which is the company who operates the DH Network in Turin.

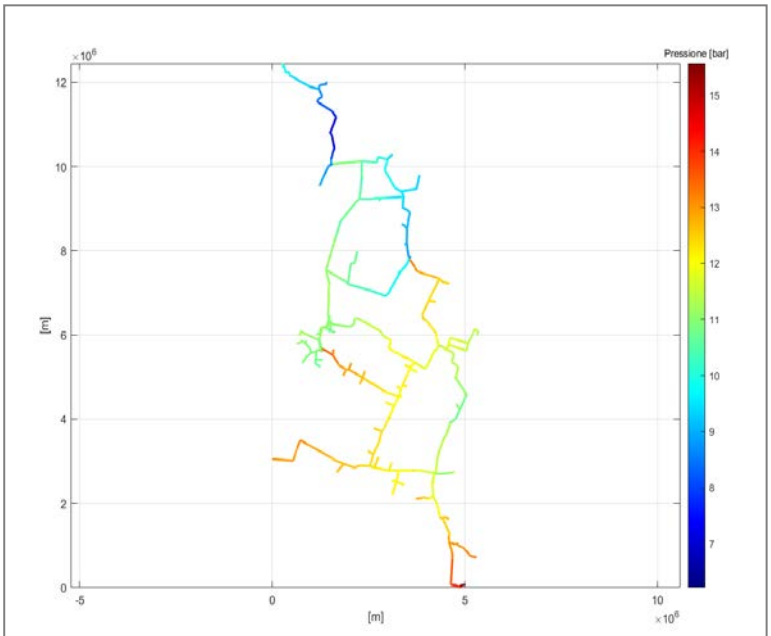


Fig. Turin DH Network - plot of the pressure values

After a very intense literature review about the available fluid-dynamic model, in the first period I tried to model the system using an open-source tool called OpenModelica, which is a Modelica language-based tool, and it uses a component-by-component approach. For a huge network such as the Turin one, this approach did not turn out to be a good methodology.

After this try, I've made a Gurobi-based model which is a very powerful optimization tool. This model is based on the main fluid-dynamic equations, such as the momentum equation and the conservation law. I have implemented all these equations using Julia, a new language which allows us to use Gurobi in a very simple way. This approach has revealed many advantages; an example is the cross-sectionality because I'm able to model the system with this code, but I'm able to optimize the network with the same code too. As an example, in Figure 1 it's possible to see the entire Turin DH Network, plotted with the pressure values. This is the result of an optimization with the aim to minimize the pressure alongside the network. This allowed me to discover a new methodology to minimize the pumping power used in the pumping stations in the main suppliers, and the pumping power utilized in the booster pumping station. Another activity that I've achieved by using this code, is the analysis of the dependence of the accuracy of the model from the friction factor. Up to now, all the model developed were based on a constant friction factor, obtained from the Moody diagram. Thanks to the transversality of this approach, it has been possible to obtain the friction factor through an iterative process by using the Coolebrok-White formula. The computational time has not increased heavily, and the main result of this analysis has been the improved accuracy of the model.

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

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

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

Academic context

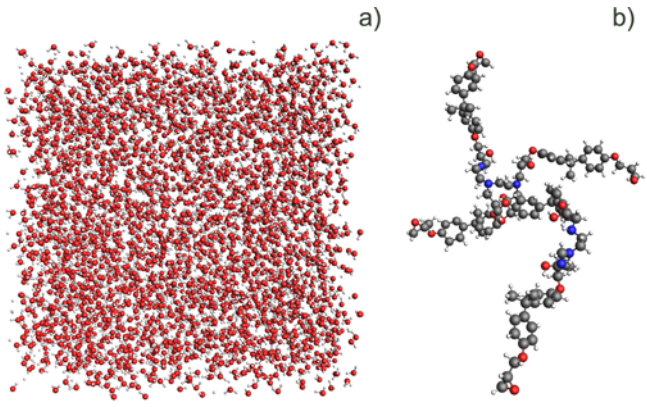
[1] Nejad, S. M., Srivastava, R., Bellussi, F. M., Thielemann, H. C., Asinari, P., & Fasano, M. (2021). Nanoscale thermal properties of carbon nanotubes/epoxy composites by atomistic simulations. *International Journal of Thermal Sciences*, *159*, 106588.
[2] Karalis, K., Ludwig, C., & Niceno, B. (2019). Supercritical water anomalies in the vicinity of the Widom line. Scientific reports, 9(1), 15731.
[3] Li, G., Hu, P., Luo, W., Zhang, J., Yu, H., Chen, F., & Zhang, F. (2021). Simulation of pyrolysis of crosslinked epoxy resin using ReaxFF molecular dynamics. Computational and Theoretical Chemistry, 1200, 113240.

External collaborations

- Technical University of Dresden
- National Technical University of Athens

Highlights of the research activity

During the first year of the Ph.D. program, my research activity focused on analyzing the use of molecular dynamics simulations to investigate the properties of materials involved in polymer composite recycling processes, with a special emphasis on supercritical water solvolysis. The application of new solvolysis methods for recycling carbon fiber-reinforced polymers is gaining increasing attention, primarily driven by the high environmental impact of composite materials used in various industries, such as wind energy. Nevertheless, solvolysis relies on the coupling of physicochemical and heat and mass transfer phenomena occurring over multiple scales, so a mechanistic understanding of the process has not yet been achieved. The research activity I am developing aims to create a suitable simulation protocol based on classical molecular dynamics (MD) that will help in understanding the thermochemical mechanisms underlying these recycling processes and thus optimize their thermodynamic parameters, such as pressure and temperature. A detailed description of the degradation phenomena of composite materials would speed up the industrialization of these recycling methods, enabling a reduction in their energy consumption and environmental impact.
The research activity began by modeling materials crucial for supercritical water solvolysis, namely solvent and polymer composites, since analyzing their properties is essential to investigate the heat and mass transfer phenomena in which they are involved. First, different water models were used and compared to explore the properties of water under supercritical conditions. Different combinations of pressure and temperature were considered, and various properties (e.g., density and self-diffusion coefficient) were evaluated for each case.
Then, some representative polymer models (e.g., epoxy resin) were built through the development of specific algorithms, with the purpose of generating realistic polymer networks and accurately replicating their experimental properties. Next steps will include epoxy-based composite modeling and matrix-filler interaction analysis.



a) Molecular setup used to simulate water under supercritical conditions. b) Molecular model of a DGEBA-DETA epoxy resin network.

First name: MD Mizanur **LAST NAME**: RAHMAN

Topic: Sustainable materials, processes and systems for energy transition

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

Alessandro MONTEVERDE

Academic context

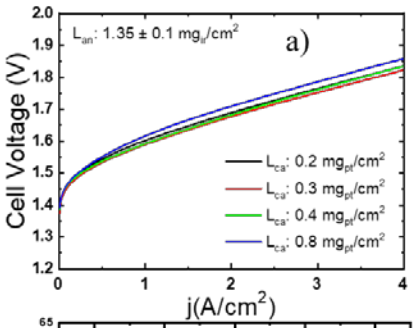
1. R. Fernández, P. Ferreira-Aparicio, and L. Daza, "PEMFC electrode preparation: Influence of the solvent composition and evaporation rate on the catalytic layer microstructure," in *Journal of Power Sources*, Oct. 2005, pp. 18–24. doi: 10.1016/j.jpowsour.2005.02.048.
2. M. Suermann, T. J. Schmidt, and F. N. Büchi, "Investigation of Mass Transport Losses in Polymer Electrolyte Electrolysis Cells," ECS Trans, vol. 69, no. 17, pp. 1141–1148, Sep. 2015, doi: 10.1149/06917.1141ecst.

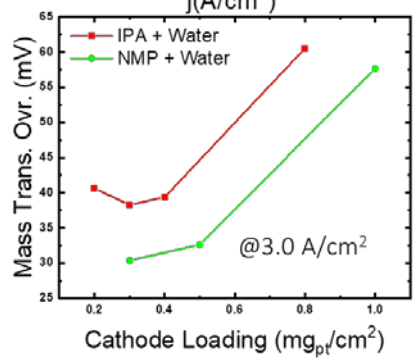
External collaborations

Highlights of the research activity

In 2023, I have been actively engaged in my academic pursuits, attending courses and delving deep into literature research on PEM water electrolyzer technology. My research focus revolves around the investigation of the effects of cathode thickness and ionomer particle size distribution on proton exchange membrane water electrolysis, with a specific emphasis on mass transport and hydrogen crossover analysis. Moreover, I presented at the "8th AIGE-IIETA International Conference and 18th AIGE Conference," organized by Politecnico.

Proton exchange membrane water electrolysis (PEMWE) stands at the forefront of efficient hydrogen production, particularly in the context of renewable or fluctuating power sources [1]. Its compact design, characterized by a solid and thin electrolyte, enables operation at high current densities of up to 10 A/cm2 and under substantial pressures of up to 700 bar. PEMWE's adaptability to load fluctuations further underscores its potential for sustainable hydrogen generation [2].





Within the PEM electrolysis cell, the Membrane Electrode Assembly plays a pivotal role, consisting of three critical layers: the anode, cathode, and solid electrolyte. The anode facilitates the oxygen evolution reaction, while the cathode promotes the hydrogen evolution reaction. The solid electrolyte ensures efficient proton transfer and gas separation. Achieving structural uniformity through solvent selection and fabrication processes is crucial for enhanced performance. Choi and colleagues' research highlighted the importance of electrode structure, demonstrating that uniform microcracks can significantly reduce hydrogen crossover.

The primary objective of this study is to investigate cathode mass transport resistance, focusing on cathode thickness and ionomer particle size distribution. By varying cathode loading and employing different solvent mixtures, we aim to achieve optimal cathode performance. Electrochemical techniques and gas analysis will be used to evaluate MEA effectiveness. This research will provide valuable insights into optimizing cathode mass transport in electrolyzers and advancing the field of electrolysis technology.

First name: Alessandro **LAST NAME**: RIBEZZO

Topic: Enhancing transport phenomena in phase-change composites for thermal energy storage

Course year: 3rd **Tutor(s)**: Eliodoro CHIAVAZZO, Matteo FASANO, Luca BERGAMASCO

Academic context

[1] A. Ribezzo *et al.*, An overview on the use of additives and preparation procedure in phase change materials for thermal energy storage with a focus on long term applications, Journal of Energy Storage, Vol. 53 (2022), 105140.
[2] A. Ribezzo *et al.*, Multi-scale numerical modelling for predicting thermo-physical properties of phase-change nanocomposites for cooling energy storage, TECNICA ITALIANA-Italian Journal of Engineering Science 65 (2021), 201-204.
[3] J. Gasia et al., Experimental evaluation of the use of fins and metal wool as heat transfer enhancement techniques in a latent heat thermal energy storage system, Energy Conversion and Management, Vol. 184 (2019)

External collaborations

- Research Center ENEA Portici
- Centro de Investigación en Energía Aplicada CREA - Universidad de Lleida

Highlights of the research activity

A literature review on enhancing thermo-physical properties of phase change materials (PCMs) through various inclusions led to a published paper. In the context of the collaboration with ENEA, a multi-scale model has been developed to i) estimate the thermal conductivity of phase change materials nanocomposites, and ii) perform an optimization analysis of a shell and tube heat storage tank containing the PCM nanocomposites. At the material scale, finite element simulations, mean field theory calculations, and experimental measurements have been exploited to estimate the thermal interface resistances within the nanocomposite and predict the effective thermal conductivity of the nanocomposite. At the plant scale, the optimization analysis has been carried out by exploiting a modified Stefan model, to develop a fast and reliable method for the thermal design of a thermal energy storage system. This approach has been also validated through CFD simulations. To overcome the phase segregation that occurs in PCM nanocomposites, a collaboration carried out with the GREiA group of the Universidad de Lleida, assessed the impact on the thermal properties of an organic PCM of continuous fibers (copper wool), which can represent an already available in the market, easily adaptable, and relatively cheap technology. This analysis has been performed through charging and discharging experiments of a heat exchanger containing the PCM and the wool, and by means of CFD simulations to develop an optimization framework to find an optimum between costs, power, and energy of the specific application under study.

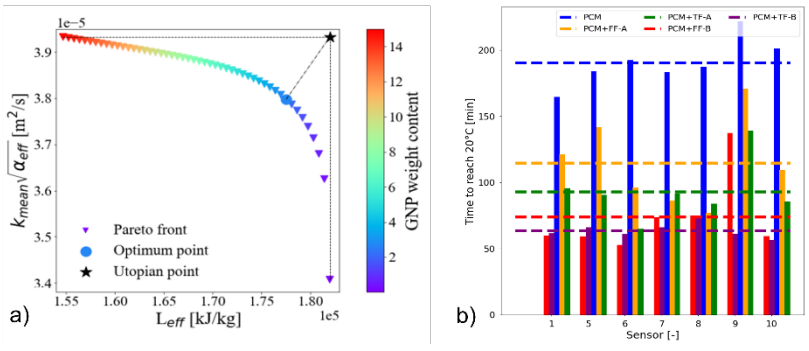


Fig. Optimum point among the Pareto front obtained for the nanocomposite PCM in the project in collaboration with ENEA a), and comparison between the discharging times of the PCM and four different configurations of copper wools within the heat exchanger b).

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

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

Course year: 2st **Tutor(s)**: Andrea LANZINI, Massimo SANTARELLI

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.

External collaborations

- Italgas S.p.A

Highlights of the research activity

Addressing the urgent need to mitigate methane emissions, a greenhouse gas with 80 times the global warming potential of CO2 over 20 years, is pivotal in our research. The scientific community emphasizes the urgency of transitioning from estimates to direct measurements when assessing methane emissions. Our collaboration with Italy's largest gas distribution grid operator is aligned with the ambitious goals of the European Green Deal, which targets the European Union's climate neutrality by 2050. Our research encompasses monitoring, reporting, and mitigating gas emissions across the gas infrastructure within the gas distribution network.

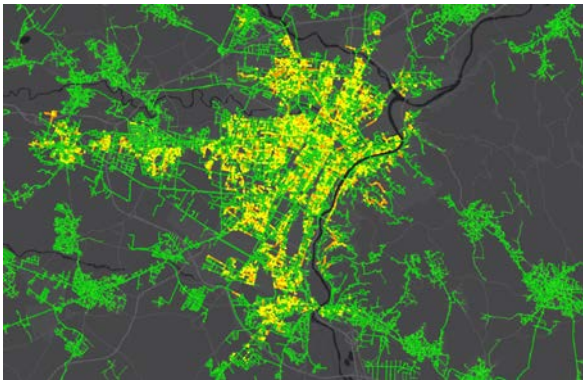


Fig. Map of the leak probability of the gas distribution grid.

The research activity includes a thorough analysis of Europe's regulatory framework on methane emissions, aligning with the Oil & Gas Methane Partnership 2.0 (OGMP 2.0) to enhance reporting accuracy. Additionally, the statistical analyses conducted using Python and QGIS, identify correlations between emission events and gas infrastructure characteristics, supporting prioritized monitoring and maintenance activities.
A cornerstone of our research involved the quantification of the Italy's national gas distribution network methane emissions using an advanced mobile method. This approach facilitated a comprehensive survey, ensuring a detailed analysis of the network's emission landscape. The obtained emission estimates not only contribute to reporting purpose, but also serve as a valuable dataset for developing targeted mitigation strategies. This quantification effort provides a robust foundation for understanding the scale and patterns of methane emissions within the gas distribution network.
We correlated leak events with specific pipeline characteristics, including age, material type, corrosion protection, pipeline geometry, nominal operating pressure, and joint type. Additionally, we examined exogenous predictors such as the distance from the sea, railways, and roads, as well as hydrogeological risk. To estimate leaks in underground pipelines, we employed a Bayesian Poisson regression model, while a linear regression model was used for above ground infrastructure estimations.
This modeling approach provides valuable insights for targeted maintenance activities and a detailed understanding of the complex interplay among various factors influencing methane emissions in both underground and above-ground gas distribution infrastructure.

First name: Umberto **LAST NAME**: TESIO

Topic: Modelling for the optimization of power plants and energy systems for combined production of energy vectors

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

Academic context

[1] Chicco, G., & Mancarella, P. (2009). Distributed multi-generation: A comprehensive view. Renewable and sustainable energy reviews, 13(3), 535-551.
[2] Xu, Y., Yan, C., Liu, H., Wang, J., Yang, Z., & Jiang, Y. (2020). Smart energy systems: A critical review on design and operation optimization. Sustainable Cities and Society, 102369.
[3] Theo, W. L., Lim, J. S., Ho, W. S., Hashim, H., & Lee, C. T. (2017). Review of distributed generation (DG) system planning and optimisation techniques: Comparison of numerical and mathematical modelling methods. Renewable and Sustainable Energy Reviews, 67, 531-573.

External collaborations

- Yanmar
- University of Seville

Highlights of the research activity

The aim of my research activity is to investigate the field of power generation and multi energy systems in order to develop mathematical models able to deal with some of the criticalities that characterize the implementation of these optimization problems. In order to realize what is the state of the art in the research, I have conducted, in collaboration with my researchteam, a detailed literature review. As a resulting outlook, very structured models have been developed, which are able to perform the optimization of synthesis, design and operation of energy systems. Most of the fundamental features of energy systems have been implemented, but some others are still missing. Among these there are: a detailed simulation of heating/cooling networks, and a reliable modelling of energy storages. A review paper was written in collaboration with the components of my research group, which was published on an international journal. The scope is to guide the implementation of the optimization problem by giving the mathematical formulation of the most effective methodologies available. In the meanwhile, I started the development of a model for the operation optimization of an energy system in the framework of a collaboration with the research center of an international company. The management of the heat storage, the mass flowrates and temperatures of the thermal network were included, and a decomposition approach was employed. The model demonstrated to be able to quickly find high-quality near-optimal solutions. This study was presented at the ECOS2022 conference and published on an international journal. Another model was successively developed to include the thermal inertia of a District Heating Network and demand side management, and was used on a case study of small size.

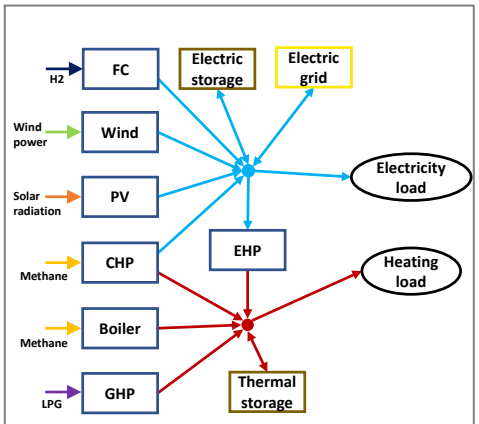


Fig. Conceptual layout of the Multi Energy System assumed as case study in the analysis exposed at ECOS2022

Concerning the study of the optimization of power plants, the topic is an innovative ThermoChemical Energy Storage for a central tower Concentrated Solar Power plant, which is under development in the European project SOCRATCES. The model developed during the research grant has been employed to perform comparisons in both energy end economic terms of the direct and indirect integration of some power cycles (Rankine, sCO2 Brayton and He Brayton). The results obtained have been presented at the ATI2020 conference, at the ICSREE2021 international conference and at the SOCRATCES webinar. The He Brayton integration has been analyzed and the study has been published on an international journal. This one resulted to be a promising integration, showing the highest performances among the alternatives investigated. Finally, the comparison between the He and sCO2 Brayton cycles integration has been published on an international journal.

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

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

Course year: 2nd **Tutor**: Massimo SANTARELLI

Academic context

[1] D. Trapani et al., "Optimal Design of Renewable Power-To-Hydrogen Systems for the Decarbonization of a Semiconductor Industry," in 36th ECOS Conference doi: 10.52202/069564-0227.
[2] P. Marocco et al., "Assessment of the role of hydrogen to produce high-temperature heat in the steel industry," J Clean Prod, vol. 388, Feb. 2023, doi: 10.1016/j.jclepro.2023.135969.
[3] A. Martinez Alonso et al., "Phasing out steam methane reformers with water electrolysis in producing renewable hydrogen and ammonia: A case study based on the Spanish energy markets," Int J Hydrogen Energy, 2023, doi: 10.1016/j.ijhydene.2023.07.347.

External collaborations

- Environment Park, Torino (Italy)
- SINTEF, Trondheim (Norway)
- Enel Green Power, Milano (Italy)

Highlights of the research activity

Green hydrogen is widely considered as a promising solution for reducing the CO_2 emissions of hard-to-abate industries, but some techno-economic barriers have still to be overcome. The PhD research activity thus focuses on the modelling and the design of power-to-hydrogen (P-t-H) systems with the aim of identifying the most suitable and cost-effective configuration for the different industrial processes. During the second year of my PhD, significant improvements have been introduced in the techno-economic optimization tool. New size-dependent cost functions and efficiency curves were included in the model for both PEM and alkaline electrolyzers. In addition, the lifetime of the components is estimated based on the real number of annual operating hours. These modifications allow for a more accurate cost estimation and enhance the overall accuracy of the sizing procedure. Moreover, a convergence study of the optimization algorithm was performed and the solver parameters were tuned to achieve reliable results while limiting the computational burden. Alternative optimization techniques were also investigated, and the Multi-Objective Genetic Algorithm (MOGA) scheme was implemented to simultaneously address the minimization of the levelized cost of hydrogen (LCOH) and the reduction of the CO_2 emissions. The optimization tool was adopted to carry out the design of a renewable P-t-H system for a semiconductor industry, which currently relies on grey hydrogen. Multiple decarbonization targets were explored and the cost-effectiveness of exploiting green hydrogen was assessed for different fossil-based hydrogen prices.

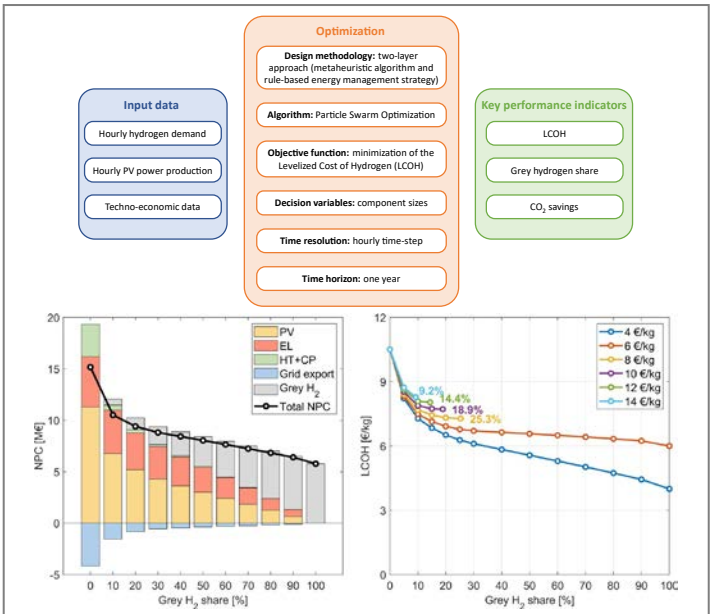


Fig. Optimization framework (top) and main techno-economic results (bottom).

First name: Giovanni **LAST NAME**: TREZZA

Topic: Artificial Intelligence based screening of materials for energy storage applications

Course year: 3rd **Tutors**: Eliodoro CHIAVAZZO, Matteo FASANO, Luca BERGAMASCO

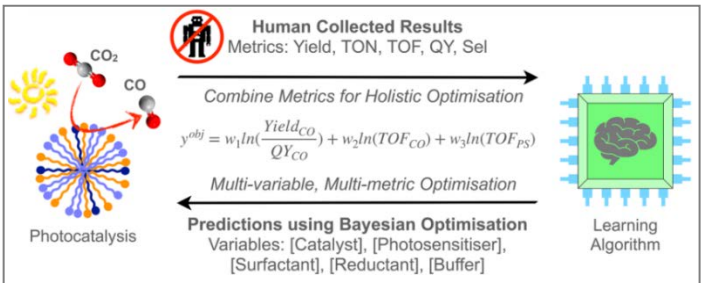
Academic context

[1] Trezza, Giovanni, and Eliodoro Chiavazzo. "Leveraging composition-based energy material descriptors for machine learning models." *Materials Today Communications* 36 (2023): 106579.
[2] Bonke, Shannon, et al. "Multi-Variable Multi-Metric Optimisation of Self-Assembled Photocatalytic CO2 Reduction Performance using Machine Learning Algorithms." *10.26434/chemrxiv-2023-g5hkm* (2023).
[3] Thomas, Nathaniel, et al. "Tensor field networks: Rotation-and translation-equivariant neural networks for 3d point clouds." *arXiv preprint arXiv:1802.08219* (2018).

External collaborations

- École Polytechnique Fédérale de Lausanne (EPFL)
- University of Cambridge, UK

Highlights of the research activity



Workflow overview of holistic BO optimization applied to micelles experiments for solar fuel production.

I focused on the Machine Learning (ML)-based screening of superconductors, namely materials characterized by zero resistivity when cooled below a superconducting critical temperature T_c. Due to this property, such compounds have attracted attention in a wide range of different fields. Energetic applications include fusion reactors like tokamak, batteries, fast fault current limiters, low-loss power cables. Specifically, this activity – in collaboration with EPFL (Prof. Nicola Marzari's group) – aimed at providing ML-based predictions of T_cs computed via *ab initio* methodologies. Indeed, I have taken advantage of ~300 materials structures for which superconductivity properties have been computed by means of different methodologies. To this end, given the relatively few data available, I employed modern Equivariant Graph Neural Networks (EGNNs), which, by incorporating structure symmetries, enhance data efficiency if compared to traditional ML. Due to noise of this kind of simulations, errors are in line with other similar works in the literature. In a further project, I have also analyzed the role of data quality in AI-based discovery. As main case study, I utilized the updated version of the SuperCon database, containing chemical formulae of the materials, their experimental critical temperatures, the publication years and some partial information about the pressure needed to elicit superconductivity. Beyond the analysis of possible hidden variables and disparate data age, I proposed a methodology to quantify bias in such database by measuring the performance of a binary classifier which correctly recognizes materials in/out of the SuperCon; similar results come with employing this method on a database of thermoelectric materials, namely the Starrydata2. This bias arises because such materials have not been tested randomly over the years, but were rather selected based on the intuition from field scientists. As a result, predictions made with a model trained on a biased database can be misleading. Finally, during this year, I also collaborated remotely with the University of Cambridge, UK (Prof. Erwin Reisner's group) on Bayesian Optimization (BO) for orchestrating solar fuel generation experiments. Employing BO techniques, we aimed to minimize the number of costly experiments towards the maximization of a proper objective function considering CO production by means of photocatalytic micelles. I also proposed alternative parameter combinations, leveraging a recent method we introduced, to achieve comparable performance by employing a lower amount of the most expensive components, properly re-balancing the others.

Building physics and energy systems in future buildings and communities

First name: Ilaria **LAST NAME**: ABBA'

Topic: Multi-Vector Energy Integrated Networks for Local Energy Systems

Course year: 3rd **Tutor(s)**: Stefano Paolo CORGNATI, Ettore Francesco BOMPARD, Carlo SANDRONI, Edoardo CORSETTI

Academic context

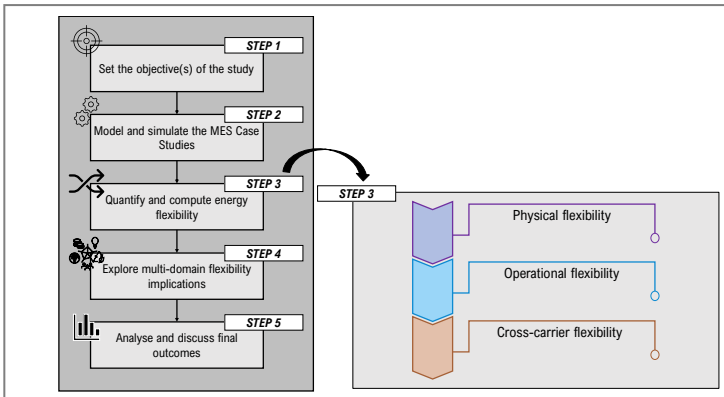
[1] Chicco, G., Riaz, S., Mazza, A., & Mancarella, P. (2020). Flexibility from distributed multi energy systems. Proceedings of the IEEE, 108(9), 1496-1517.
[2] Corsetti, E., Riaz, S., Riello, M., & Mancarella, P. (2021). Modelling and deploying multi-energy flexibility: The energy lattice framework. Advances in Applied Energy, *2*, 100030.
[3] Luc, K. M., Li, R., Xu, L., Nielsen, T. R., & Hensen, J. L. (2020). Energy flexibility potential of a small district connected to a district heating system. Energy and Buildings, 225, 110074.

External collaborations

- Ricerca sul Sistema Energetico – RSE S.p.A.
- LINKS Foundation
- REAM SGR S.p.A.

Highlights of the research activity

Addressing the inherent uncertainty and volatility arising from renewable sources necessitates a increased level of flexibility within the energy system. This adaptability is crucial for maintaining a consistent power balance between generation and demand. Against this backdrop, there is a growing interest in Multi-Energy Systems (MESs), where various energy vectors coexist and interact optimally. My Ph.D. research, conducted in collaboration with RSE S.p.A., is dedicated to modeling and simulating the operational dynamics of MESs. The primary objective is to assess the diverse flexibilities that MESs can offer to enhance the resilience and efficiency of the supply network. In detail, starting from the methodology developed in previous years, this year has been dedicated to its application on a case study involving a 5th generation district heating system, in line with future district heating trends. Building upon the simulator created in the first year for a 3rd generation district heating system, a novel simulator tailored for a low-temperature district heating setup has been developed. This system incorporates a groundwater source heat pump at the central thermal plant and a water-to-water heat pump system in the district substations. At the user level, six building districts have been considered, each composed of a diverse portfolio of buildings varying in construction period, use, and installed HVAC systems. The simulation of the district heating generation and distribution system utilized Simscape software, while EnergyPlus was employed for the dynamic simulation of buildings. Given that the all-electric heat pump system is inherently inflexible, as heat pumps are demand-oriented technologies, the assessment of system flexibility focused on exploring demand flexibility. Interventions involving the shifting of thermal consumption were thus modeled and simulated, always ensuring internal comfort within the buildings.



Overall methodology with a focus on the flexibility calculation step.

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

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

Course year: 2nd **Tutor(s)**: Stefano FANTUCCI, Valentina SERRA

Academic context

[1] H. Cuce, M.P. Cuce, J.C. Wood, B.S. Riffat, Toward aerogel based thermal superinsulation in buildings: A comprehensive review , Renewable and Sustainable Energy Reviews (2014), https://doi.org/10.1016/j.rser.2014.03.017
[2] M. Zinzi, S. Agnoli, G. Ulpiani, B. Mattoni, On the potential of switching cool roofs to optimize the thermal response of residential buildings in the Mediterranean region, Energy and Buildings,(2021), doi: https://doi.org/10.1016/j.enbuild.2020.110698.
[3] V. Gentile, M. Libralato, S. Fantucci, L. Shtrepi, G. Autretto, Enhancement of the hygroscopic and acoustic properties of indoor plasters with a Super Adsorbent Calcium Alginate BioPolymer, Journal of building engineering (2023), doi: https://dx.doi.org/10.1016/j.jobe.2023.107147

External collaborations

- Brunel University – London – United Kingdom
- ETH – Zurich –Switzerland
- University of Udine – Udine – Italy

Highlights of the research activity

The construction industry faces a growing interest in innovative solutions for building energy refurbishment to reduce the energy demand. Multifunctional climate control materials and coatings, such as Phase Change Materials (PCM), Super Insulating Materials (SIM), thermochromic layers, advanced coatings and cladding components for moisture buffering offer a consistent energy efficiency potential without increasing significantly the envelope thickness. Current methods for assessing the energy performance of these materials follow traditional and simplified procedures, leading to inaccurate representations of their behaviour. This discrepancy, coupled with the rising demand for building cooling, particularly in the Mediterranean area, highlights the importance of accurately estimating the buildings transient hygrothermal behaviour. The research activity is thus focused on the assessment, through numerical and experimental analyses of the performance of optimised advanced building envelope surface technologies characterised by their applications in thin layers and implementing different functionalities, including thermal and moisture buffering, high solar reflectance, and thermal insulation. The research aims to measure their properties, dynamic behaviour, and key performance indicators for reliable assessments of their impact on energy efficiency, environmental quality, and user well-being. During the first year, activities included the assessment of the impact of the moisture content on the thermal conductivity of loose aerogel particles (Super Insulating Materials) and the development of testing procedures for the characterisation of thermal and optical performance of thermochromic coatings. Moreover, an experimental analysis on the characterisation of hygroscopic and moisture buffering properties of indoor plaster additives with Super Adsorbent Calcium Alginate BioPolymers and 3D printed clay components has been carried out. Results indicate the potential of these technologies in significantly increasing the moisture buffering capacity of a building (Fig.). Ongoing investigations are now focusing on comprehensive hygrothermal properties characterization to retrieve essential input data for the building scale energy performance simulation, contextually developing and validating a simulation workflow.

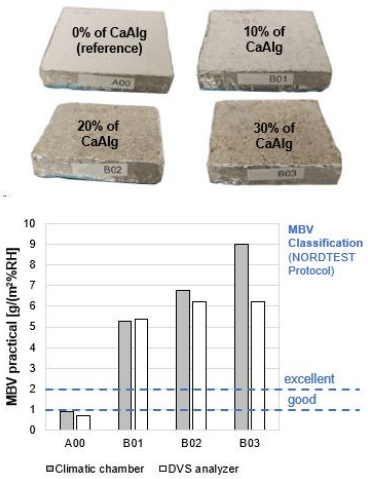


Fig. The MBV practical results measured on plaster additives with two different experimental setups.

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

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

Course year: 2nd **Tutor(s)**: Fabio FAVOINO, Valentina SERRA

Academic context

[1] R. C. G. M. Loonen, F. Favoino, J. L. M. Hensen, and M. Overend, "Review of current status, requirements and opportunities for building performance simulation of adaptive facades," J. Build. Perform. Simul., vol. 10, no. 2, pp. 205–223, Mar. 2017, doi: 10.1080/19401493.2016.1152303.
[2] 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.
[3] Giovannini L., Baracani M., Favoino F., Serra V. (2021). Occupant-centric control of transparent dynamic façades through an integrated co-simulation framework. 10.26868/25222708.2021.30754. BS2021 Conference, 1-3 September 2021. Bruges, Belgium.

External collaborations

- Horizon 2020 project Iclimabuilt
- PTR ENEA 2019/21, LA 18 "Controlli avanzati ed integrati di elementi di involucro trasparente dinamico per Smart Zero Energy Buildings"
- PRIN 2022 MIRABLE – Measurement Infrastructure for Research on heAlthy and zero energy Buildings in novel Living lab Ecosystems

Highlights of the research activity

My Phd research work investigates the multi-domain design, operation and integration of AFS in buildings with a dual objective: i) to investigate and develop models and an integrated co-simulation architecture to assess the multidomain behavior of AFS ii) to develop a methodology for the design and monitoring in field of AFs in buildings integrating the presence and actions of occupants. In this framework an investigation of fundamental variables and KPIs influenced by the technology in two case studies (water-flow glazing system, ventilated window with PCM heat exchanger) was carried out. Also, some preliminary simulations to design the components using simplified comfort proxies were performed: the cavity depth, the layers number and position, the coating location, together with the water-flow layer location in the first technology and the PCM melting temperature in the second one were selected. For what regards the design of the control of adaptive components in 2021 a co-simulation workflow including the thermal, visual and IAQ domains was applied in the PTR ENEA 2019/21 research activity, to investigate the performance of different rule-based and model-based strategies for the control of operable windows and venetian blinds. As a further step the development of a co-simulation workflow (including Energy Plus, Python, Contam) to simulate the behavior of the ventilated window investigating different operation logics and the IAQ, TC and energy performance depending on the given domain priorities, is in progress.

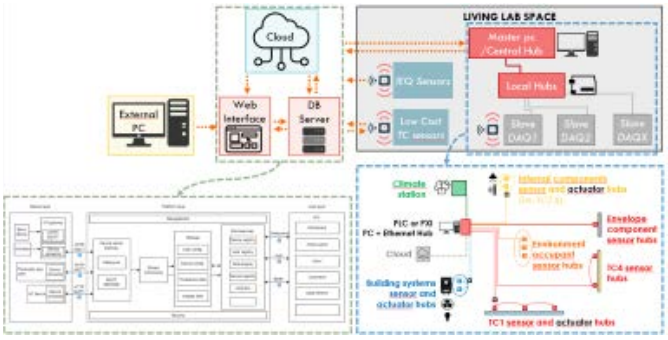


Fig. in-field acquisition system and IoT platform

The inclusion of the occupant in the design would be investigated at the experimental level by a campaign of objective and subjective measuring. To do this an office in Politecnico di Torino, named TEBE L2AB, was designed to test technologies in field with a Living Lab approach, including an occupant in a real life environment while collecting IEQ measurement. The first step in the design was the investigation and selection of sensor accuracy and design of the acquisition chain to record the variables with different DAQs in the long-term monitoring of the office. Also a preliminary study on the influence of the DAQs accuracy and resolution on the calculation of thermal comfort KPIs has been carried out in the office after the installation of high-cost, lab-grade and low-cost monitoring systems

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

Topic: Low enthalpy geothermal energy

Course year: 1st **Tutor(s)**: Glenda TADDIA, Vittorio VERDA

Academic context

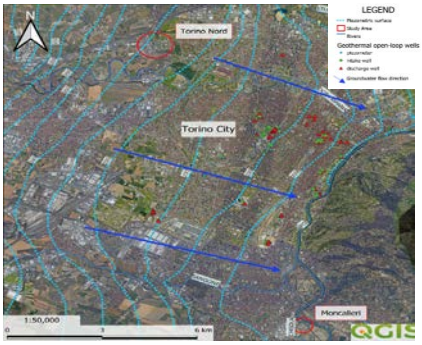
[1] Applied Geology
[2] Geothermal Energy
[3] Hydrogeology

External collaborations

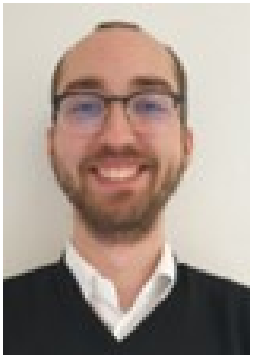
- IREN S.p.A.
- Norwegian University of Science and Technology (NTNU)

Highlights of the research activity

- Groundwater heat pumps are a promising solution for meeting the thermal demands of Buildings;
- The lack of a clear regulatory framework makes it challenging to develop GWHPs in Italian urban areas;
- Urban planning instruments should aim at a rapid diffusion of GWHPs and a protection of the exploted shallow aquifers;
- Numerical modelling is the most appropriate methodological tool for properly managing GWHPs distribution in densely urbanised contexts;
- Solely open-source software has been employed for simulating the surface aquifer, and the resulting model underwent calibration using uncertainty analysis codes;
- Investigative efforts are underway to study the geology and hydrogeology of the Turin plain, aiming to create precise geological and hydrogeological models;
- Various scenarios are conceptualized, encompassing all geothermal facilities in Turin, to enhance efficient management and contribute to territorial planning.



Hydrogeological context of Torino with location of open-loop geothermal plants for feasibility study at two IREN sites Torino Nord and Moncalieri



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: 2nd

Tutor(s): Vincenzo CORRADO, Ilaria BALLARINI

Academic context

[1] Judkoff, R., Wortman, D., O'Doherty, B., and Burch, J. (2008). A methodology for Validating Building Energy Analysis Simulations. Technical Report NREL/TP-550-42059, National Renewable Energy Laboratory (NREL).
[2] Ballarini, I., Costantino, A., Fabrizio, E., and Corrado, V. (2019). The dynamic model of EN ISO 52016-1 for the energy assessment of buildings compared to simplified and detailed simulation methods. Proceedings from BS2019: Building Simulation Conference. Rome (IT), 1-4 September 2019.
[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.

External collaborations

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

Highlights of the research activity

In the context of improving energy efficiency and reducing carbon emissions in buildings, one approach involves developing and enhancing design methodologies and tools. Simplified calculation procedures intended for building energy assessments face a significant challenge: balancing simplicity and accuracy. These methodologies must be user-friendly to minimize user errors while aiming to accurately represent the building's actual performance. Despite being user-friendly, existing simplified models lack precision. To bridge this gap, the focus of the Ph.D. research is on enhancing simplified calculation methodologies for assessing the performance of HVAC systems. After a literature review on simplified procedures, the focus was at first placed on the generation subsystem. Two comparative analyses were performed on different chiller performance methodologies assessing the deviation between procedures. A group of twelve case studies (indicated in Figure 1 as C1 - C12), with the same building geometries, but different in parameters such as the generator properties, the climatic data, and the building properties, was tested. The analysis, partially presented in Figure 1, confirmed previous results regarding the accuracy quality of these methods and provided useful insights regarding the influence of the analysed parameters. The focus was then moved to the emission subsystem to deepen the interaction between the building, the user, and the HVAC system. The available simplified calculation procedures for modelling emitters and control systems currently lack application flexibility and rely on tabular fixed values. The complex phenomena that occur inside a heated or cooled space, such as the spatial variation of the air temperature, the non-uniformity of the radiant temperature, or the imperfect control of the air temperature are often neglected or oversimplified by the current models. Therefore, there is a particular need for enhancement. The analysis of the existing calculation methods, already performed, was enriched with an analysis of the most relevant parameters, including the heat emitter properties. In the future steps, the next-generation control systems will be highlighted. These components are becoming increasingly relevant due to the demonstrated possibilities in energy efficiency, but the current simplified methodologies are not sufficient to evaluate their performances.

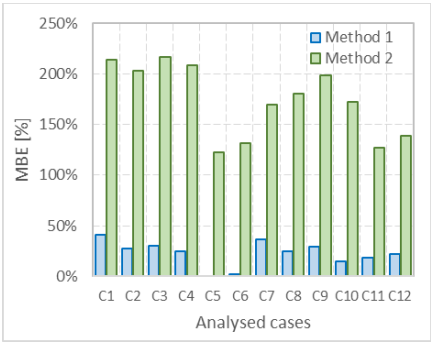


Fig. For a chiller, mean bias error (MBE) of the monthly energy consumption for a year of two simplified methods compared against a reference detailed method.

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

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

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

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] Pinto, G., Kathirgamanathan, A., Mangina, E., Finn, D., Capozzoli, A. ***Enhancing energy management in grid-interactive buildings: A comparison among cooperative and coordinated architectures***. Elsevier, Applied Energy. 2022. https://doi.org/10.1016/j.apenergy.2021.118497
[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

External collaborations

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

Highlights of the research activity

In the first PhD year, the research focused on the PRIN 2020 project: "Optimal refurbishment design and management of small energy micro-grids". A methodological process was developed for understanding demand dynamics, utilizing advanced techniques like pattern recognition and time series analytics to extract typical demand load profiles from buildings. This methodology found practical application in micro-grid energy demand scenarios, including case studies at Sannio University and Politecnico di Torino. A significant part of the research involved the creation of an advanced co-simulation environment, seamlessly integrating a non-residential building micro-grid model from TRNSYS with a Python-based control system. This innovative approach aimed to bridge the gap between proprietary software like TRNSYS and dynamic Python-based control systems.

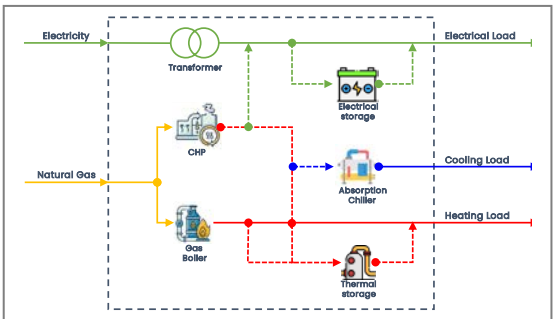


Fig. Multi carriers energy hub schema

Additionally, contributions were given to the CityLearn project, led by Prof. Zoltan Nagy of the University of Texas at Austin, to develop a robust co-simulation platform for advanced controller applications. The collaboration integrated data-driven modeling of building thermal dynamics through LSTM neural networks to comprehensively assess control effects on both energy balance and indoor air temperature evolution in each building. Furthermore, eXplainable Artificial Intelligence (XAI) algorithms were explored, focusing on algorithms to enhance output interpretations and deepen understanding of AI-based systems. The primary goal was to address the challenge of low interpretability in prediction models and AI-based controllers, significantly contributing to transparency and trustworthiness in the field. Eventually, the research activity has the objective to integrate Reinforcement Learning based control in the energy hub sector. The objective is to optimize energy flows within the hub, aiming to minimize the demand for input energy carriers and mitigate CO2 emissions. This work also aims to put in relation the optimization of Energy Hub operations with the optimal design of each constitutive component, providing comprehensive solutions for sustainable and environmentally friendly energy management.

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

Topic: Hydrogels for air/water separation

Course year: 1st **Tutors**: Marco SIMONETTI, Vincenzo Maria GENTILE

Academic context

[1] V. Gentile, M. Bozlar, F. Meggers, M. Simonetti, "Liter-scale atmospheric water harvesting for dry climates driven by low temperature solar heat", Energy (2022), https://doi.org/10.1016/j.energy.2022.124295.
[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. 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.

External collaborations

- AQUASEEK SRL SB
- Sorption Technologies Srl

Highlights of the research activity

This research project focuses on the study of sorbent hydrogels for air-water separation. Applications can range from humidity control in industrial and domestic environments to cooling, from atmospheric water harvesting to desalination. Given the high potentiality of such materials, the first year focused on the theoretical and experimental study of the hydrogels' properties.
A literature review was conducted, leading to the selection of diffusion models such as Fick diffusion and Linear Driving Force approximation. The models were tested over experimental data available on different hydrogel compositions, allowing to estimate samples diffusivity. It was found that increasing $CaCl_2$ content and decreasing Sodium Alginate amount in the composition have a positive influence on the overall equilibrium water uptake and on the kinetics during the adsorption and desorption transients. The results were collected in a conference paper and presented during the 2023 HPC conference in Edinburgh.
Afterwards, a new model was proposed: the dependence of concentration on diffusivity was included, and an analytical expression was derived. The resulting 2-parameters model "LDFDw" was tested over experimental data, proving able to well estimate adsorption and desorption kinetics of hydrogels at different temperatures and relative humidities. This showed that hydrogels' diffusivity is not constant, but instead strongly dependent on the amount of collected water, especially at high temperatures. Also, a positive influence of small concentrations of graphite in the hydrogel composition was found, as far as the amount of additive is not so high such to cause pore occlusion, thus leading to a decrease in the material performances. The results were collected in the published journal paper [3]: "Water Vapor Mass Transfer in Alginate-Graphite Bio-based Hydrogel for Atmospheric Water Harvesting".

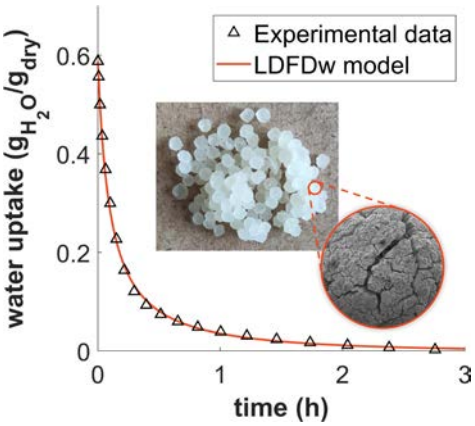


Fig. water uptake data and model in comparison during a desorption phase. The picture shows some beads of hydrogel and a SEM magnification.

In the final stages of the year, a numerical model was developed in order to include the influence of water concentration also in Fick-based models, where no analytical solution can be found for a generic functional dependence. The 1D time-dependent model was written in MATLAB and tested over experimental data available on a plane sheet of material: this allowed to estimate diffusivity and to perform simulations of the sorbent behavior over time, when the material is subject to cycling external conditions.

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

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

Course year: 2nd **Tutor(s)**: Alfonso CAPOZZOLI, Cheng FAN

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] Capozzoli, A., Piscitelli, M. S., Brandi, S., Grassi, D., & Chicco, G. (2018). Automated load pattern learning and anomaly detection for enhancing energy management in smart buildings. Energy, 157, 336-352
[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.

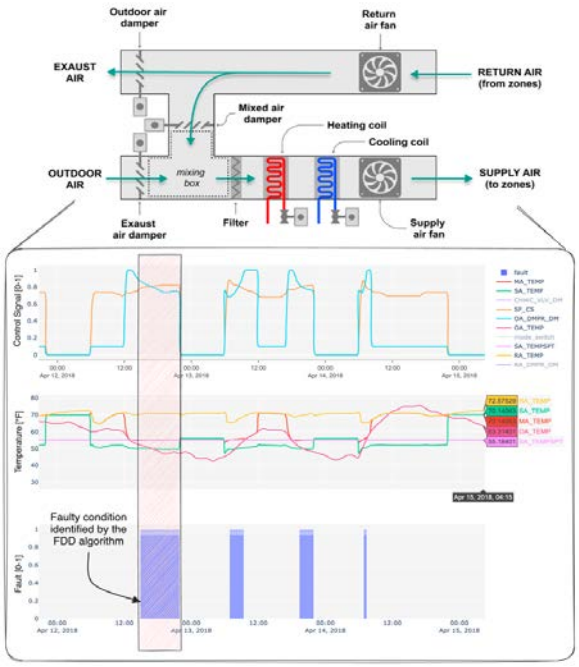
External collaborations

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

Highlights of the research activity

Within the second year of activities, I shifted the focus from meter level anomaly detection to system level fault detection and diagnosis. As an active member in IEA EBC - Annex 81 subtask C2 (Automated Fault Detection, Diagnostics, and Recommissioning Applications) I contributed to the publication of a review paper discussing data driven Fault Detection and Diagnosis (FDD) applications at the system level in Heating Ventilation and Conditioning (HVAC) systems [1].

Fig. Schematic of an AHU system with the representation of the outcome of an FDD tool



In my ongoing efforts to promote the practical adoption of Decision Support System (DSS) frameworks, I am currently involved in a project at Politecnico di Torino with the aim to modernize the electrical monitoring infrastructure by implementing cloud-based microservices for collecting, monitoring, and analysing energy metering data with the goal is to enhance energy management on the campus.

To address real-world challenges in EMIS adoption (e.g., data scarcity, interoperability constraints), I focused on transfer learning and semantic interoperability. Transfer learning involves applying knowledge from source domains to facilitate data-driven tasks in target domains and an application was investigated in the following publication [2]. On the other hand, semantic interoperability has the potential to provide a common ground for EIS application development though the standard definition of metadata in buildings. Those methods provided the basis for the development of a methodological process for scalable, portable, and interoperable Fault Detection and Diagnosis (FDD) developed during my visiting period at LBNL in Q2 2023. The introduction of standardized and flexible data and metadata organization (i.e., Brick schema) was capable to handle the complexity and heterogeneity of building data. The outcomes of these analyses are currently in progress and under investigation.

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

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

Course year: 2nd **Tutor(s)**: Alfonso CAPOZZOLI, Tianzhen HONG

Academic context

[1] Coraci, D.; Brandi, S.; Capozzoli, A. Effective pre-training of a deep reinforcement learning agent by means of long short-term memory models for thermal energy management in buildings. *Energy Conversion and Management* (2023), *291, 117303*. doi: https://doi.org/10.1016/j.enconman.2023.117303.
[2] Coraci, D.; Brandi, S.; Hong, T.; Capozzoli, A. Online transfer learning strategy for enhancing the scalability and deployment of deep reinforcement learning control in smart buildings. *Applied Energy* (2022), *333, 120598*. doi: https://doi.org/10.1016/j.apenergy.2022.120598.
[3] Pinto G., Wang Z., Roy A., Hong T., Capozzoli A. Transfer learning for smart buildings: A critical review of algorithms, applications, and future perspectives, *Advances in Applied Energy 5* (2022) *100084*. doi: https://doi.org/10.1016/j.adapen.2022.100084.

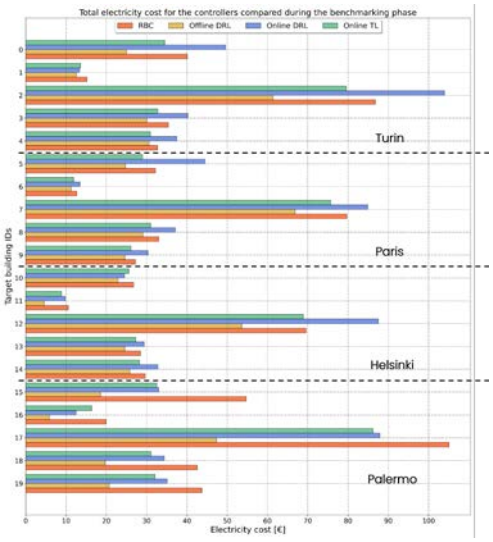
External collaborations

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

Highlights of the research activity

Deep Reinforcement Learning (DRL) has emerged recently as promising solution to change the way of managing energy systems in buildings. However, implementing DRL controllers directly in real buildings is not practical due to economic and safety constraints. In this framework, researchers developed surrogate models of buildings to pre-train DRL controllers. However, the definition of those models represents a time-consuming task requiring expert knowledge and detailed information. To address this gap, the first activity conducted in 2023 involves the development of a framework leveraging a LSTM neural network as building model to offline pre-train DRL agent managing heating power provided while improving indoor temperature conditions. This approach includes periodic re-training of LSTM and DRL agent, coupled with safety constraints. The results validate the potential of LSTM as powerful tool for increasing the DRL agents scalability, even facing with limited data availability. Moreover, Transfer Learning (TL) emerges as promising solution to avoid the development of any building surrogate model and enhance the scalability of DRL controllers. The second activity explored in 2023 involves the implementation of a heterogeneous Online TL (OTL) strategy to share a DRL controller pre-trained on a source building with target buildings characterised by different price/occupancy schedules, thermal properties, weather conditions, objective function and configuration of the energy systems. The developed DRL controller was capable to reduce electricity cost and enhance indoor temperature control by managing the cooling system operation mode and the energy cooling fraction to building. The figure indicates that OTL offers a practical and efficient approach for transferring DRL controllers in buildings implementing different energy systems, since its performances matches or is slightly worse than those of offline DRL while it performs better than baseline RBC and online DRL.

Fig. Performance comparison for OTL, offline/online DRL, RBC



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

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

Course year: 2nd

Tutor(s): Arianna ASTOLFI, Stefano Paolo CORGNATI, Anna PELLEGRINO

Academic context

[1] T. Parkinson, A. Parkinson, R. de Dear, Continuous IEQ monitoring system: Context and development, Build. Environ. 149 (2019) 15–25. https://doi.org/10.1016/j.buildenv.2018.12.010.

[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. https://doi.org/https://doi.org/10.1016/j.buildenv.2020.107535.

[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. https://doi.org/10.1016/j.buildenv.2020.106804.

External collaborations

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

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 PREP, 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 and comfort of the building. To this aim, it pursues the development of a low-cost and accurate monitoring system, which includes a multisensor able to monitor 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 multisensor hardware components are integrated in a single-case 3D printed device, with a cylindric shape (height 19 cm, diameter 13 cm), drilled through small holes and larger openings to provide air ventilation. Ten LEDs placed on each side of the case indicate the IEQ level of the environment. Calibration procedures of the sensors were defined to ensure the measurements traceability. In addition, the questionnaire to get users' feedback on comfort perception and information on personal and behavioural factors 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. Two pilot studies were conducted for both questionnaire and dashboard validation, whereas a study on the monitoring of IEQ and comfort perception started in April 2023 in the "Aule P" of Politecnico di Torino for the further validation of the algorithms for the comfort indexes calculation.

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

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

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

Course year: 1st **Tutor(s)**: Alfonso CAPOZZOLI; Co-Tutors: Stefano Paolo CORGNATI, Cristina BECCHIO

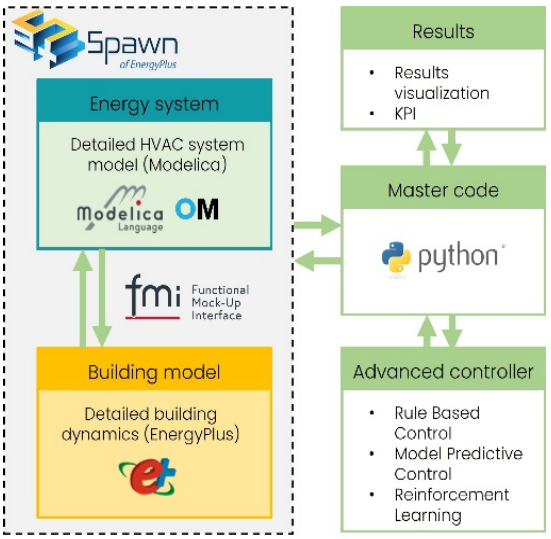
Academic context

[1] J. Drgoňa, J.Arroyo, I.Cupeiro Figueroa, D.Blum, K.Arendt, D. Kim, E.Perarnau Ollé, J. Oravec, M. Wetter, Draguna L. Vrabie, L. Helsen, All you need to know about model predictive control for buildings, Annual Reviews in Control, Volume 50, 2020, https://doi.org/10.1016/j.arcontrol.2020.09.001
[2] D. Blum, J. Arroyo, S. Huang, J. Drgoňa, F. Jorissen, H. Taxt Walnum, Y. Chen, K. Benne, D. Vrabie, M. Wetter & 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, DOI: 10.1080/19401493.2021.1986574
[3] D. Kim, Z. Wang, J. Brugger, D. Blum, M. Wetter, T. Hong, M. A. Piette,
Site demonstration and performance evaluation of MPC for a large chiller plant with TES for renewable energy integration and grid decarbonization, Applied Energy, Volume 321, 2022, 119343, ISSN 0306-2619, https://doi.org/10.1016/j.apenergy.2022.119343.

Highlights of the research activity

The research that was conducted during the first year of my PhD program focused on the topic of optimal control of building energy systems through the use of advanced control strategies, and their testing on high fidelity emulators. Firstly, an extensive literature review allowed to assess the state of the art in the field of control for building energy systems, enabling the identification of the current gaps that are limiting the widespread adoption of advanced control strategies on a larger scale. Potentials of tools for building performance simulation tools have also been explored, with particular attention to co-simulation platforms that allow to integrate accurate building thermal dynamics simulators (i.e. EnergyPlus) with the state of the art in dynamic systems modelling (i.e. Modelica language). These simulation tools were integrated with suitable coding languages (Python, MATLAB) for the definition of control strategies.

Fig. Conceptual representation of the Co-simulation framework



As far as advanced controllers, particular attention was devoted to model-based control paradigms such as Model Predictive Control, which integrates the knowledge of the controlled system dynamical behaviour with predictions of the disturbances acting upon the system so that, thanks to an optimizer, an optimal control action can be computed which minimizes the set objective function. The performance of such controllers can be conveniently assessed through the use of the forementioned simulation testbeds. Ongoing effort is being devoted to the testing of advanced, model-based controllers on the Building Optimization Performance TESTbed (BOPTEST) platform.
The model on which Model Predictive Control is based can be of different type; during the research so far, attention has been devoted to the performance of the grey box modelling paradigm, which is referred to as "hybrid" since it leverages both knowledge derived from physical first-principles and information extracted from monitoring data. The exploitation of physical knowledge has been proven to speed up the process of obtaining an accurate prediction model reducing the amount of data required for the training phase, with respect to a purely data-driven methodology.

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

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

Course year: 2nd **Tutor(s)**: Alfonso CAPOZZOLI

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

External collaborations

- IEA EBC Annex 82
- ABB s.p.a.
- Aarhus University

Highlights of the research activity

A district of buildings can offer energy flexibility to the electrical grid through the adoption of advanced energy management strategies. To analyse this aspect, the activities carried out during the 2023 were aimed at developing a decentralized control approach for a Renewable Energy Community (REC). The main goal was to understand the impact on grid-wide indicators with an emphasis on Shared Energy (SE) as a crucial metric for building energy flexibility in REC, prioritizing local consumption of renewable energy to minimize reliance on potentially costly energy storage solutions. Reinforcement Learning (RL) controllers operate the flexibility assets of the building within a REC of 100 members, while relying only on the observed state variables of the building where it operates. The buildings can be equipped with Photovoltaic (PV), and energy storage solutions. Three control strategies were developed, including a baseline strategy and two RL-based strategies (S1 and S2) with distinct reward functions.

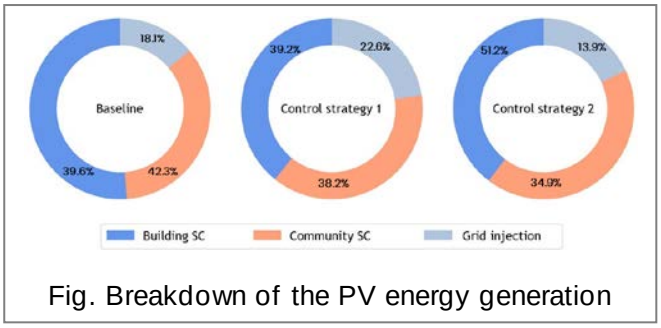


Fig. Breakdown of the PV energy generation

S2 aims at maximizing the share of prosumers self-consumption (SC) and shows an increase in total energy cost but reduces the peak of both positive and negative net load exchange, resulting in a flatter load profile. S2 achieves a higher share of Self-Sufficiency (SS) and SC, indicating a more effective utilization of locally generated energy. S1, with a cost minimization strategy, increases SS and reduces the overall cost compared to the baseline, but it does not achieve the same level of SE as S2. In Fig., it is shown where the PV generation is consumed. Building SC refers to the amount of energy that is produced by the PV-BESS system of a building and consumed by itself, community SC refers to the amount of energy that is produced by the REC and consumed in the perimeter of the REC itself, and grid injection refers to the amount of energy that is exported to the main grid. S2 can reduce the perimeter where energy is consumed by increasing only building SC since there is no coordination among members. The transition from S1 to S2 may not be justified solely by the incentive for SE, as the increase in SE primarily benefits consumers. Eventually, cost-efficient strategies like S1 reduce total energy cost but can compromise SE. Conversely, S2 increases demand during PV generation, improving grid compliance with a flatter consumption profile, reduced negative peak loads.

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

Topic: Scalable and interoperable Artificial Intelligence based Decision Support Systems (DSSs) for enhancing energy management in buildings.

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

Academic context

[1] M. S. Piscitelli, S. Brandi, A. Capozzoli, Recognition and classification of typical load profiles in buildings with non-intrusive learning approach, Applied Energy 255 (2019).
[2] Z. Tian, X. Shi, Proposing energy performance indicators to identify energy-wasting operations on big time series data, Energy and Buildings 269 (2022).
[3] M. Hu, B. Stephen, J. Browell, S. Haben, D. C. Wallom, Impacts of building load dispersion level on its load forecasting accuracy: Data or algorithms? importance of reliability and interpretability in machine learning, Energy and Buildings (2023).

External collaborations

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

Highlights of the research activity

The research activities, conducted in the first year, focused on improving the generalization and scalability of AI-based Decision Support Systems (DSS) in the building sector, including Anomaly/Fault Detection and Diagnosis (A/FDD) and energy benchmarking. Firstly, an extensive literature review was conducted to identify the current state of the art of DSSs in buildings, deepening the study on different levels: multiple-buildings level, single building level, and system level (such as Air Handling Units/HVAC systems). Concerning the generalization of DSS tools at the multiple-buildings level, the Ph.D. activity primarily focused on the development of a holistic data-driven energy benchmarking system. The aim was to overcome existing limitations by developing a methodology to define a clear pipeline for benchmarking electrical energy consumption of a building against a consistent set of peers. The evaluation of the energy performance of the building relies on defining a set of meaningful Key Performance Indicators (KPIs) based on time-series feature extraction processes. This new approach significantly enhances the accuracy of the benchmarking process when it is compared with a conventional approach leading to an average variation of the calculated KPIs of about 14%. Additionally, the research activitiy also focused on the scalability of data-driven solutions for energy management, investigating the exploitation of metadata schemas and ontologies for the in-field deployment of DSSs. In this context, the conceptualization and implementation of an anomaly detection and diagnosis tool for energy consumption and photovoltaic production across a group of buildings has been developed, employing ontologies to achieve scalability targets. Finally, the research focuses on enhancing the generalization and scalability of DSS tools at the system level, particularly regarding Fault Detection and Diagnosis (FDD) on Air Handling Units (AHUs). A systematic literature review has been carried out to understand the current limitations of data-driven FDD tools and how to incorporate domain knowledge and robust physical rules to improve the reliability of all FDD steps.

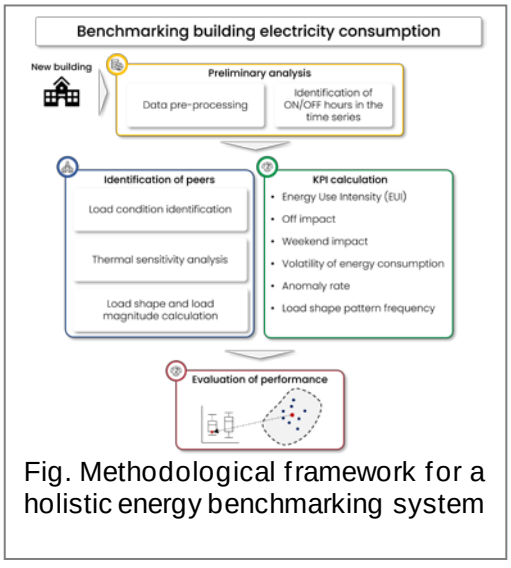
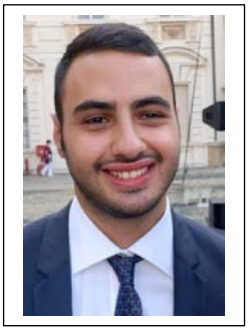


Fig. Methodological framework for a holistic energy benchmarking system



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

Topic: Advanced energy performance assessment of building stocks

Course year: 1st **Tutor(s)**: Ilaria BALLARINI, Vincenzo CORRADO

Academic context

[1] Swan, L. G., & Ugursal, V. I. (2009). Modeling of end-use energy consumption in the residential sector: A review of modeling techniques. *Renewable and Sustainable Energy Reviews, 13*(8), 1819-1835.
[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.
[3] Reinhart, C. F., & Cerezo Davila, C. (2016). Urban building energy modeling – A review of a nascent field. *Building and Environment, 97*, 196-202.

External collaborations

- La Salle – Ramon Llull University (Spain)
- Jožef Stefan Institute (Slovenia)
- Politecnico di Milano

Highlights of the research activity

The enhancement of building stock energy efficiency relies on the spread and advancement of the Urban Building Energy Model (UBEM). UBEM employs a bottom-up approach based on an engineering model, aimed at assessing the energy and environmental performance of a set of buildings and evaluating their mutual interactions. The creation of an energy model on a city scale, to analyse the energy *status* of a city's environment and to guide the deep renovation of the building stock, is a crucial activity for urban planners, public administrations, energy agencies, and validation bodies.
In this context, the Ph.D. research is aimed at discovering the potentialities, capabilities, and future perspectives of the UBEMs, thereby supporting key actors in mapping the energy performance of the building stock.
A recent paradigm shift is taking place, moving from the Building Energy Model (BEM) at the scale of a single building to the Urban Building Energy Model (UBEM) at a city-level scale. The modelling differences in terms of geometry, building envelope, zoning, internal heat gains, technical building systems, and calculation modules between BEM and UBEM have been deepened. Next, a case study application investigating the interactions between the building and the surrounding environment has been assessed. Specifically, the short-wave (as shown in Figure) and long-wave energy exchange within the urban environment have been explored and discussed both in BEM and UBEM scenarios.

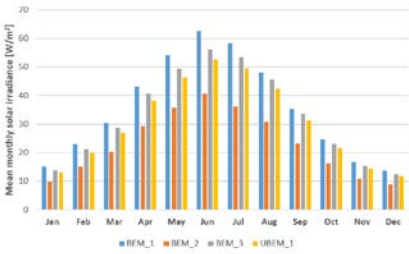
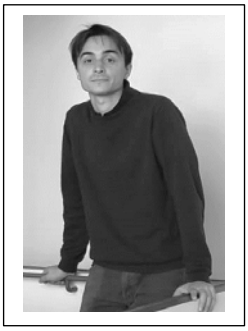


Fig. Short-wave energy mutual interactions between BEMs and UBEM scenarios (Piro et al., 2023).

UBEMs require a huge amount of information from different informative sources to bridge the uncertainty gap in the model creation. The collected data flow into the generation of the reference buildings (RBs). The RB approach is a trade-off to reduce complexity and enhance the model's accuracy. From this perspective, the work has been oriented to review, list, and organise the available public and private local, regional, and national databases to catalogue the information requested to run a large-scale energy model. In this perspective, the Energy Performance Certificate (EPC) repositories represent indispensable and central sources of information. However, the low quality of EPCs has imposed the development of a procedure to verify the reliability of the energy certificates. The EPC data quality checking process is based on the attribution of tailored rules and scores to crucial EPC parameters. Then, the overall EPC score is compared to an acceptability threshold value beyond which the EPC is considered *unreliable*. Instead, *reliable* EPCs have been used to generate residential and non-residential building archetypes, i.e., virtual buildings (subset of RBs). The future steps will be focused on the development and validation of RBs, to be used in UBEMs, by combining multiple databases.



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

Topic: Towards digital twins enhanced services for high performance facades

Course year: 1st **Tutor(s)**: Fabio FAVOINO, Valentina SERRA

Academic context

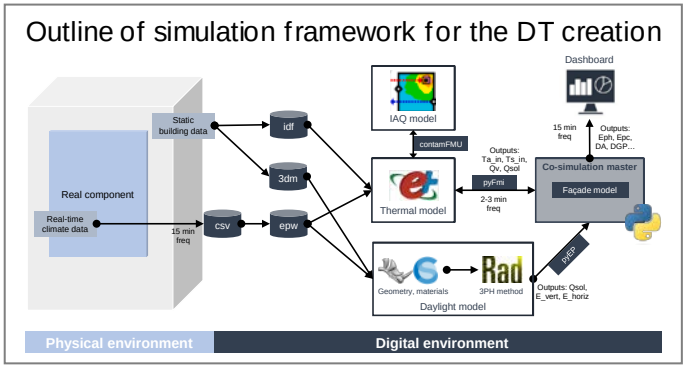
[1] Van Berkel, P., Kruit, K., Van de Poll, F., Rooijers, F., & Vendrik, J. (2020). Zero carbon buildings 2050 - background report
[2] Favoino, F., Loonen, R. C., Michael, M., De Michele, G., & Avesani, S. (2022). Advanced fenestration—technologies, performance and building integration. In Rethinking Building Skins (pp. 117-154). Woodhead Publishing
[3] P. de Wilde, Building performance simulation in the brave new world of Artificial Intelligence and Digital Twins: a systematic review, Energy and Buildings. (2023) 113171.

External collaborations

- Norwegian University of Science and Technology (NTNU) – Norway
- Eurecat Centre Tecnològic – Spain

Highlights of the research activity

The focus of the PhD project is the development of **digital twin (DT)** services for transparent building envelope technologies to enhance energy efficiency while maintaining indoor environmental quality conditions. The initial phase of the research involved a literature review of the subject matter to explore the main **aims and features** of a DT creation in building facades and laid the foundation for the first case study.



In the construction sector, a DT refers to the interaction between the real-world building's indoor environment and a virtual representation of the built environment. The concept of DT can exhibit varying development levels when it comes to its maturity in terms of achievable capabilities. The simplest maturity level is the "**Descriptive DT**", where the digital model is only enhanced with a sensor network for real-time data monitoring. Then, an "**Informative DT**" gives insights by means of simple post processing of the acquired dataset. A further analysis can be done by a "**Predictive DT**", where the integration of complex simulation models gives dataset enhancement in spatial and time dimensions. As a completion of the co-simulation outcomes, a "**Prescriptive DT**" gives informed feedbacks to the system through a decision-making process. Finally, the most comprehensive "**Transformative DT**" automatically actuates in field the optimal control configuration.

Among the various services that each level of DT can provide, the following ones were specifically selected for the case of building facades: **technical and raw data visualization**; **dataset enhancement**; **fault detection** (to detect malfunctioning sensors or damages to physical components); **renewable resources availability** (to calculate the potential on-site energy generation through renewable sources in real time); **data granularity enhancement** (to simulate variables not directly measured in the physical asset); **what-if scenarios** (to simulate and analyze various façade and control configurations as alternatives to the in-field benchmark); **predictive maintenance** (to enhance the operational efficiency of the building façade by planning maintenance interventions based on simulated predictions); **automation of optimal/improved controls** (to implement in field through actuators the effective optimization of specific parameters).

For the development of a DT infrastructure for building facades, a **co-simulation framework** is helpful to provide a comprehensive understanding of a building's performance. Various domains, including thermal, daylight, acoustic, indoor air quality, energy loads, and energy production, are captured by different BPS tools. The first selected case study for the proposed framework to create a DT of a façade is the "Test Case 1" (TC1) of iClimabuilt H2020 EU project. The TC1 is a full-scale façade mock-up installed on the south facade of an outdoor test facility at DENERG and comprises a ventilated window with an air-PCM heat exchanger on top.

First name: Hamed **LAST NAME**: RASAM

Topic: Spreading of biologically active aerosol in the indoor environment: analysis of local airflow control systems

Course year: 3rd **Tutor(s)**: Marco SIMONETTI, Paolo TRONVILLE, Vincenzo GENTILE

Academic context

[1] L. Bourouiba, "Turbulent gas clouds and respiratory pathogen emissions: Potential implications for reducing transmission of COVID-19," Jama, vol. 323, no. 18, pp. 1837–1838, 2020.
[2] G. Cortellessa et al., "Close proximity risk assessment for SARS-CoV-2 infection," Sci. Total Environ., vol. 794, p. 148749, 2021.
[3] L. Liu, Y. Li, P. V. Nielsen, J. Wei, and R. L. Jensen, "Short-range airborne transmission of expiratory droplets between two people," Indoor Air, vol. 27, no. 2, pp. 452–462, 2017.

External collaborations

Highlights of the research activity

In the pursuit of advancing our understanding of respiratory pathogen transmission, my research during the past academic year focused on two key activities: Computational Fluid Dynamics (CFD) simulations and experimental investigations.
The primary emphasis of the research year was on CFD modeling, where the goal was to elucidate the dynamics of respiratory particle transmission from infected individuals to susceptible subjects in close proximity. The research aimed to assess the effectiveness of a portable desktop fan as a barrier against the diffusion of airborne pathogens.
The CFD simulations involved Star-CCM+ software, utilizing a finite volume approach and Eulerian-Lagrangian model to comprehensively analyze airflow dynamics and droplet interactions. The simulations considered specific conditions, such as spherical droplets with a log-normal size distribution and incorporated a two-way coupling method for particle-air interaction.
Mesh generation played a crucial role, with polyhedral-based unstructured grids and a mesh sensitivity analysis leading to an optimal configuration of 2,529,932 cells. Experimental measurements were carried out utilizing Hotwire anemometers in order to supply vital inputs for the desktop fan simulation.
The research included a detailed analysis of particle dispersion, revealing the desktop fan's ability to create a protective zone and redirect particles, effectively mitigating exposure risks. Furthermore, to evaluate the range of effectiveness of the device, a parametric analysis investigated the key parameters such as fan position, height, and outlet velocity that affect desktop fan effectiveness.

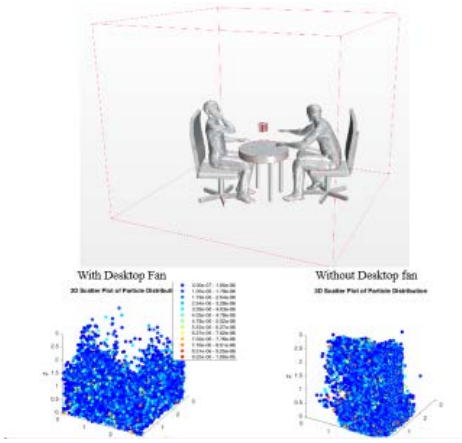


Fig. Problem geometry and assessment of desktop fan effectiveness against the diffusion of airborne particles

Validation efforts showed a satisfactory agreement between experimental and CFD results, instilling confidence in the utility of the CFD model. Following the initial modeling phase, current research integrates mechanical ventilation systems to thoroughly evaluate particle dispersion in confined areas.
In addition to CFD simulations, a portion of the research was dedicated to the experimental exploration of desiccant-coated heat exchangers. The study assessed an intermittent dehumidification system's efficiency and performance, providing insights into dehumidification effectiveness, thermal performance, and energy efficiency.

First name: Silvia **LAST NAME**: SANTANTONIO

Topic: Urban energy atlas for a sustainable development

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

Academic context

[1] *Urban-Scale energy models: the relationship between cooling energy demand and urban form*, G. Mutani, V. Todeschi, S. Santantonio, 2022, Journal of Physics: Conference Series, doi:10.1088/1742-6596/2177/1/012016.
[2] *QGIS-based tools to evaluate air flow rate by natural ventilation in buildings at urban scale*, S. Santantonio, G. Mutani, Building Simulation Applications 2022, doi: 10.13124/9788860461919.
[3] *Wind-driven and buoyancy effects for modeling natural ventilation in buildings at urban scale*, S. Santantonio, C. Moscoloni, O. Dell'Edera, C. Bertani, G. Bracco, G. Mutani, Energy Efficiency collection "Energy Conversion, Management, Recovery, Saving, Storage and Renewable Systems", 2023, in press.

External collaborations

- ACEA SpA, Environment Park SpA, CIDIU Servizi SpA, GAL Meridaunia Scarl, La Salle Municipality

Highlights of the research activity

Sustainable and resilient cities should rely on territorial strategic energy planning that requires supporting models and tools in exploring the spatial distribution of energy consumption of buildings, local RES, GHG emissions and liveability of urban environment, integrating different levels of analysis at proper scales and comparing different scenarios. Urban energy atlas can facilitate the identification of critical areas and real local potentiality, defining flexible measures for each context. My research activity starts with the application of a GIS place-based process-driven UBEM to evaluate how the urban morphology and local climate influence cooling energy demand of buildings, after re-scaling the input parameters to apply the model at the block of building scale [1]. Then, it focuses on modelling the urban local wind environment, as the wind profile affects buildings' energy consumption for space heating and cooling. QGIS tools are applied to calculate aerodynamic parameters at neighborhood scale, correcting wind speed in presence of roughness elements and assessing the spatial variation of wind pressure across windward and leeward buildings' façades. Compared to existing parametric models, this flexible methodology considers real obstructions and spatial relationships between buildings, providing short-term simulations even at larger scale [2]. To assess wind paths and momentum inside urban canyons where turbulent flows occur, 2D-CFD simulations are processed to investigate urban airflows patterns in non-isothermal conditions and for classes of aspect ratio. A three-zone air flow lumped parameters model is implemented to assess the hourly variation of the air changes per hour (ach), considering the combined effect of wind-driven and buoyancy, generating pressure variations and air flow motion through leakages on building envelope [3]. Results are used to calibrate and optimize the GIS-based engineering energy model, evaluating the ventilation loads of thermal energy balance and the overall building energy performance, with applications on case study at urban scale in the city of Turin.

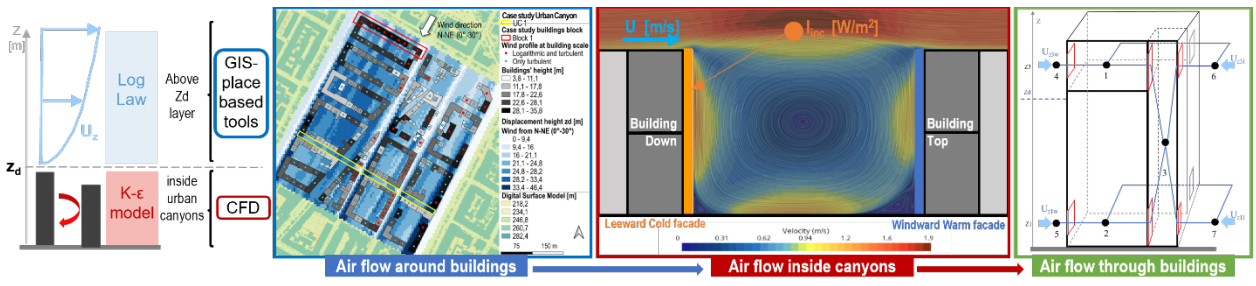


Fig. Spatial distribution of wind profile at urban scale (left) and inside urban canyons on building façades (center) which impacts on ach parameters and ventilation loads in building thermal energy balance, assessed with a three-zone air flow lumped parameters model (right).

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

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

Course year: 2nd **Tutor(s)**: Guglielmina MUTANI, Cristina BERTANI

Academic context

[1] Statistical Building Energy Model from Data Collection, Place-Based Assessment to Sustainable Scenarios for the City of Milan. Mutani, G.; Alehasin, M.; Usta, Y.; Fiermonte, F.; Mariano, A. *Sustainability*. 2023, 15, 14921. https://doi.org/10.3390/su152014921
[2] Impact of the COVID-19 pandemic on the energy performance of residential neighborhoods and their occupancy behavior. Todeschi, V., Javanroodi, K., Castello, R., Mohajeri, N., Mutani, G., Scartezzini, J. L. *Sustainable Cities and Society*. 2022, Volume 82, 103896. https://doi.org/10.1016/j.scs.2022.103896.
[3] Design and Modeling Renewable Energy Communities: A Case Study in Cagliari (Italy). Mutani, G., Usta, Y. *International Journal of Sustainable Development and Planning*. 2022, 17, 4, pp. 1041-1051. https://doi.org/10.18280/ijsdp.170401

External collaborations

- Gruppo Iren,Torino, IT
- IDIAP Research Institute, Martigny, CH
- Joint Research Center, Ispra, IT

Highlights of the research activity

In urban areas dominated by existing building stock, the importance of building energy modeling is vital to enable the assessment of energy use and the identification of strategies for consumption reduction. This extensive research involves a process-driven Urban Building Energy Modeling (UBEM) with a place-based approach considering both buildings and urban parameters (i.e., buildings' density, built shape, wind field, solar exposure, ect.) [1]. The broad aim of this research is to consider the complex urban dynamics in improving the energy efficiency of buildings and integrating smart and renewable technologies to reduce dependence on fossil fuels and achieve a higher energy independence. A more distinctive aim of this research is to implement robust UBEM with a decision-making tool for all stakeholders: citizens, companies, policymakers, and urban planners.

The current goal is modeling and analyzing the existing building stock, considering all site-specific technical, historical, economical, and environmental constraints. The research work is implemented by integrating optimization tools (such as QGIS, Python and MATLAB tools) in data-driven, process-driven, and hybrid models [2]. Further scenarios will be applied to test the contribution of various interventions to reach energy and climate targets: retrofit measures, renewable energy technologies, and smart networks to optimize the demand response for all energy services and the storage and sharing of energy between consumers and prosumers [3]. The outcome of the ongoing research is believed to have an effective role in achieving the targets for clean energy transition, especially in critical urban environments. In this regard, UBEMs can play an important role in analyzing the spatial distribution of energy-uses and relative variables (for a better comprehension of results) and finding more effective solutions for each specific city or territory.

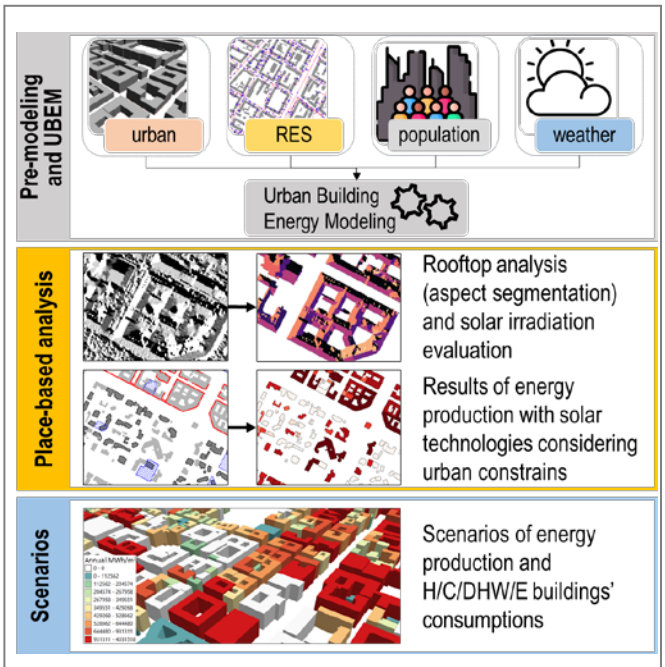


Fig. UBEM and RES production

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

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

Course year: 2nd **Tutor(s)**: Fabio FAVOINO

Academic context

[1] Y. Zhou, G. Gennaro, S. Fantucci, M. Ibrahim, E. Franquet& F. Favoino, "Building performance simulation of Advanced Building Envelope (ABE): towards a python-based open-source library to support co-simulation for design and operations", IBPSA, Shanghai, China, 2023
[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

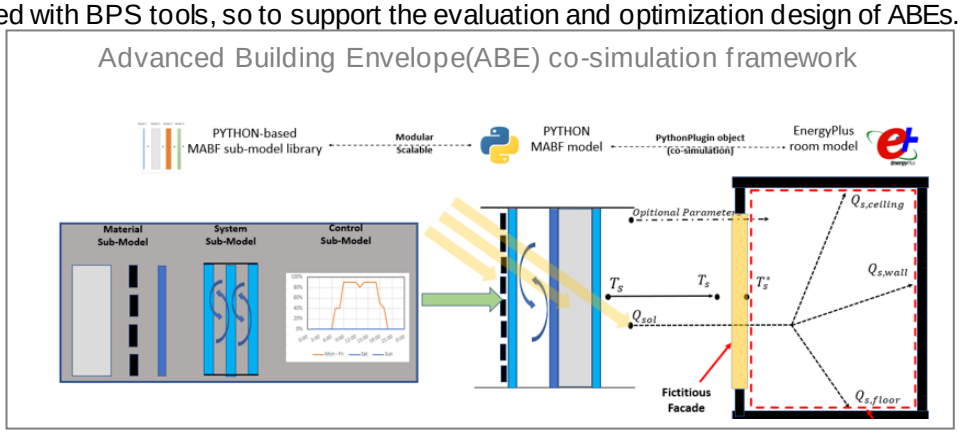
External collaborations

- Polytech'Lab, UPR UCA 7498, Université Cote d'Azur Sophia Antipolis, France

Highlights of the research activity

-Numerical Modeling of Micro-Fluidic Glazing(MFG):
MicroFluidic Glazing (MFG), features fluid flow within laminated micro-channels, enabling the harvesting of solar radiation, transmission of visible light, and adjustment of indoor thermal environments. In this part, a Thermal Capacitance-Resistance (RC) numerical model for a triple-glazing type MFG is developed and validated by the experimental data obtained at a flow rate of 9.6 l/h (0.00062m/s) with a component size of 0.68m*0.58m. Furthermore, the performance of this model is evaluated under different control strategies at the building level, utilizing generic co-simulation framework. The annual solar radiation harvesting ratio under different constant and dynamic control show a relatively low idea heating and cooling need, with constant control strategy ratios of 23.08% and dynamic control strategy ratios of 24.26%. These figures demonstrate the substantial potential advantages in energy saving and harvesting of MFG.

-Generic Co-simulation Frame Work for Advanced Building Envelope systems:
Assessing performance of Advanced Building Envelope (ABEs) using state-of-the-art Building Performance Simulation (BPS) tools poses significant challenges due to the absence of specific models, difficulties in integrating advanced controls, and simulating performance across multiple physical domains. EnergyPlus has introduced the Energy Management System (EMS) and integrated Python capabilities, enabling the co-simulation of Python-based models and control strategies developed by users. The purpose of this part work is to showcase a scalable co-simulation approach, aimed at defining an opensource python-based library of ABEs, that can be interfaced with BPS tools, so to support the evaluation and optimization design of ABEs. The approach is done by co-simulating with EnergyPlus, evaluating the performance of two highly complex ABEs (1) Micro-Fluidic Triple Glazing (MFTG) and (2) flexible Double Skin Façade (DSF).



Sustainable nuclear energy

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

Topic: Multiphysics modelling of fusion machines liquid-breeder blankets

Course year: 2nd **Tutors**: Sandra DULLA, Antonio FROIO

Academic context

[1] A. Aimetta; N. Abrate; S. Dulla; A. Froio; (2022); Neutronic Analysis of the Fusion Reactor ARC: Monte Carlo Simulations with the Serpent Code. In: FUSION SCIENCE AND TECHNOLOGY, vol. 78, pp. 275-290;
[2] A. Aimetta, M. Caravello, N. Abrate, A. Froio, S. Dulla, 'Non-intrusive uncertainty propagation in the ARC fusion reactor through the nemoFOAM multi-physics tool', M&C 2023 International Conference, Niagara Falls, Canada., August 13-17, 2023.
[3] 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, vol. 100, pp. 378-405.

External collaborations

- Tokamak Energy
- ENEA-Argonne National Laboratory

Highlights of the research activity

The research activity concerns the multiphysics modelling of liquid-breeder blankets for fusion machines, like the Affordable Robust Compact (ARC) reactor [3]. During the 2nd year of PhD, the Serpent model of the ARC reactor developed in [1] has been employed to generate nuclear properties to be used as input in the multiphysics code *nemoFOAM*, developed at Politecnico di Torino. *nemoFOAM* is a multiphysics tool written in the OpenFOAM environment for the solution of the multigroup neutron diffusion and the mono-kinetic photon diffusion equations. Then, the nuclear power deposited by neutrons (see Fig.) and photons is passed as an input to the thermal-hydraulic module of *nemoFOAM*, written using the standard solvers available in OpenFOAM. Particular attention has been devoted to the implementation of the photonic module and to the evaluation of the required photonic properties evaluated with the Serpent Monte Carlo code, since the contribution of the photons to the total power deposition in ARC is non-negligible, as reported in [1]. Serpent is not specifically developed for the generation of multigroup photonic properties, for this reason *nemoFOAM* is currently forced to solve the one-group photon diffusion equation. An important term in the photonic equation is the one related to the generation of secondary photons emitted by Bremsstrahlung, fluorescence, and annihilation, which significantly contribute to the total number of photons in ARC. Neglecting this contribution means to neglect ≈30% the power deposited by photons in ARC. Currently, the contribution of secondary photons is approximately implemented in *nemoFOAM* by means of an external source term, but in the future a more realistic and multi-group photonic model will be implemented.

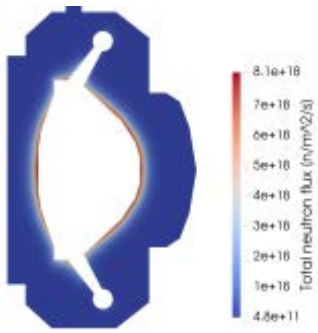


Fig. Map of the neutron flux in the blanket of ARC, computed with *nemoFOAM*

In the context of multiphysics modelling, a non-negligible period of the 2nd year of PhD has been dedicated to the evaluation of the impact of nuclear data and thermo-physical properties uncertainties on thermal-hydraulic responses of interest in ARC computed with *nemoFOAM*. Employing uncertainty propagation techniques already exploited during the 1st year of PhD (e.g., Total Monte Carlo, Unscented Transform and Polynomial Chaos Expansion), it has been found out that the effect of nuclear data uncertainties appears limited, while thermo-physical uncertainties have signifcant impact on representative results [2]. The acquired knowledge acquired in the field of uncertainty propagation is also going to be exploited to assess the impact of the nuclear data uncertainty in the computation of various integral parameters of interest for fission reactor physics, with a specific focus on their application in noise analysis in the TAPIRO (TAratura PIla Rapida a potenza zerO) research reactor, in collaboration with ENEA-Casaccia and Argonne National Laboratory.

First name: Simone **LAST NAME**: BLEYNAT

Topic: Monte Carlo modelling and variance reduction technique applications for heavily shielded geometries

Course year: 3rd **Tutors**: Roberto ZANINO, Sandra DULLA

Academic context

[1] J. Leppänen. 2019. "Response Matrix Method–Based Importance Solver and Variance Reduction Scheme in the Serpent 2 Monte Carlo Code." *Nuclear Technology* 205 (11): 1416–32.
[2] M. Pantelias Garcés. 2013. "Activation Neutronics for the Swiss Nuclear Power Plants" Diss. ETH No. 21623
[3] S. Bleynat, S. Dulla, F. Pancotti, L. Ricci, C. Vicini, R. Zanino. 2023. "Hybrid Monte Carlo/deterministic activation calculation to support the decommissioning of PWRs: Validation against data from the thermal shield of the Enrico Fermi NPP." *Annals of Nuclear Energy*, Volume 181, 109527, ISSN 0306-4549, https://doi.org/10.1016/j.anucene.2022.109527.

External collaborations

- Sogin

Highlights of the research activity

The research carried out during the third year of the PhD program focused on refining and expanding a hybrid calculation methodology for examining residual activation in pressurized water reactors (PWRs). Initially centered on the thermal shield of the Enrico Fermi nuclear power plant in Trino, the study methodology evolved through multiple phases employing Monte Carlo and deterministic tools like Serpent-2 and FISPACT-II. The first two phases developed a detailed model of the Trino reactor and optimized neutron propagation through variance reduction techniques, enabling precise assessments of neutron fluxes and spectra across the shield. The subsequent phases involved using FISPACT-II to simulate irradiation effects on specific points of the shield, considering the reactor operational history. Expanding from the thermal shield analysis, the study targeted then the reactor pressure vessel, a component to be carefully characterized for an efficient decommissioning. Addressing the vessel's stainless-steel liner's activation due to neutron exposure, the research accounted for nine operational cycles and significant design modifications along the plan lifetime. Multiple core configurations were developed to encompass these changes, impacting neutron fluence and subsequently, residual activation levels.

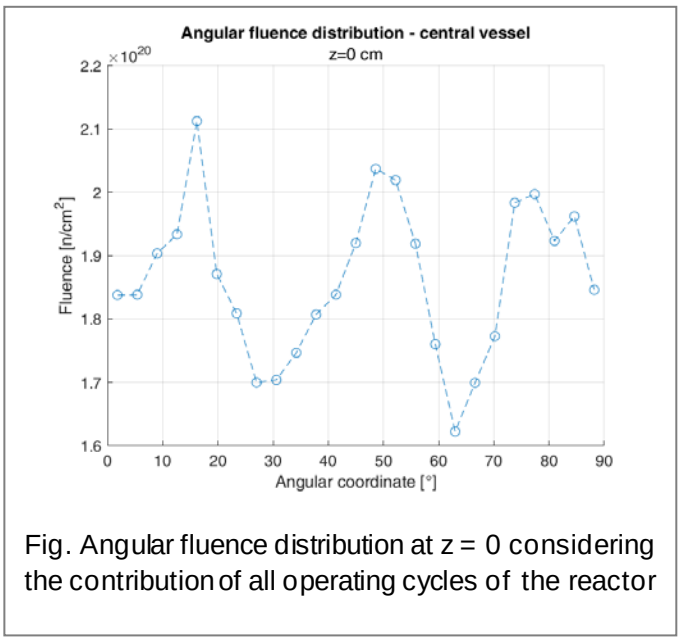
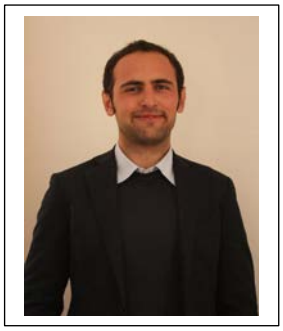


Fig. Angular fluence distribution at z = 0 considering the contribution of all operating cycles of the reactor

The analysis of neutron flux angular profiles, such as the one shown in Fig., highlighted significant variations near the core and upper sections, due to design alterations and control rod placements. These variations influenced activation levels, impacting subsequent dismantling operations. Comparisons between modeling choices indicated potential differences in activation values, especially when considering maximum activation points versus uniform irradiation assumptions. The study also assessed the Representative Operating Cycle (ROC) hypothesis, concluding that while it slightly overestimates residual activities and dose rates, it nevertheless serves as an effective approximation for Trino's complex operational history.



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

Topic: Multi-physics modelling of Molten Salt Blanket
Course year: 1st **Tutor(s)**: Antonio FROIO, Roberto ZANINO

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] Aimetta, A.; Caravello, M.; Abrate, N.; Dulla, S.; Froio, A. (2023); Non-intrusive Uncertainty Propagation in the ARC Fusion Reactor through the nemoFOAM Multi-physics Tool.. In: M&C 2023 - The International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, Niagara Falls (Canada), August 13 – 17, 2023
[3] Meng, Zi & Zhang, Shichao & Jia, Jiangtao & Chen, Zhibin & Ni, Muyi. (2017). A K-Epsilon RANS turbulence model for incompressible MHD flow at high Hartmann number in fusion liquid metal blankets. International Journal of Energy Research. 42. 10.1002/er.3891.

External collaborations

- ENI

Highlights of the research activity

The PhD research topic is focused on multi-physics modeling of molten salt blankets for nuclear fusion reactors. The primary focus of our research is the ARC reactor [1]. The concept behind the ARC reactor involves a fully liquid immersion blanket filled with FLiBe molten salt, serving multiple purposes, including coolant for the blanket, heat carrier to the secondary loop, neutron multiplier (due to Beryllium), tritium breeder (due to Lithium), and neutron shield. In tokamak devices, and particularly within the ARC reactor, strong magnetic fields are generated to control the D-T plasma shape. Since molten salts are electrical conductors, they experience additional forces, known as the Lorentz force, when moving within a magnetic field. This specific branch of thermal-hydraulics is referred to as Magnetohydrodynamics (MHD) and requires special attention. The required modeling approach is inherently multi-physics, focusing on the coupling of MHD (power management) and neutronics (power production and deposition). A multi-physics tool is under development within the OpenFOAM environment, that currently couples neutronics (implementing the multi-group diffusion equation for neutrons and the monokinetic equation for photons) with standard thermal-hydraulics equations, including continuity, Navier-Stokes, and energy equations (neutronics power production is an additional source term). The module also models photons directly generated by neutrons (due to radiative capture) and secondary photons (bremsstrahlung, fluorescence, and annihilation). The definition of this last term representing secondary photons is still a work in progress. A comparison of results generated by the nemoFoam tool and Monte Carlo simulations conducted with the Serpent code, by another PhD student at our institution (Alex Aimetta), has shown good agreement and was presented at the SOFE 2023 conference. The nemoFoam tool has also been used for non-intrusive uncertainty propagation analysis for the ARC reactor, and the results have been presented at the M&C 2023 conference [2]. In terms of MHD modeling, an OpenFOAM solver incorporating the electromagnetic equations for electric potential is under development. The implementations proceeds incrementally, starting from laminar cases with single-unit Reynolds and Hartmann numbers up to slightly turbulent regimes with Hartmann values in the order of hundreds. Currently, dedicated turbulence models for MHD regimes, introducing additional source/sink terms in the standard RANS k-epsilon model [3], are being implemented.

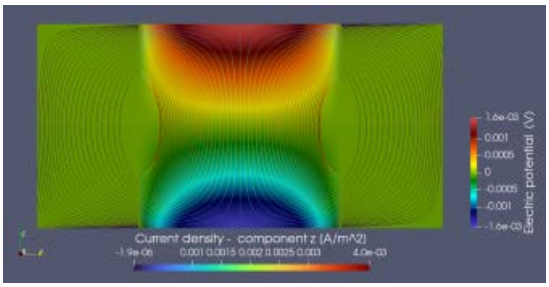


Fig. Map of electric potential and streamlines of the induced current density, computed by the MHD code under development. The case study is defined by a square section pipe, with Hartmann walls in contact with the surrounding walls and side walls (top and bottom walls).

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

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

Course year: 2nd **Tutor**: Roberto ZANINO

Academic context

[1] V. Moreau, M. Profir, A. Alemberti, M. Frignani, F. Merli, M. Belka, O. Frybort, T. Melichar, M. Tarantino, S. Franke, S. Eckert, A. Class, J. Yanez, D. Grishchenko, M. Jeltsov, P. Kudinov, F. Roelofs, K. Zwijsen, D.C. Visser, A. Badillo, B. Niceno, D. Martelli, Pool CFD modelling: Lessons from the SESAME project, *Nucl. Eng. Des*., 355, 110343, 2019.
[2] L. Mengali, M. Lanfredini, F. Moretti, F. D'Auria, Stato dell'arte dell'accoppiamento fra codici di sistema e di fluidodinamica computazionale. Applicazione generale su sistemi a metallo liquido pesante. Report Ricerca di Sistema Elettrico, 2012.
[3] P. Cioli Puviani, R. Zanino, T. Del Moro, F. Giannetti, B. Gonfiotti, I. Di Piazza, D. Martelli, M. Tarantino, 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.

External collaborations

- ENEA
- EUROFusion
- Westinghosue

Highlights of the research activity

My research topic is focused on GEN-IV Lead-cooled Fast Reactor technology, with specific reference to the Advanced Lead-cooled Fast Reactor European Demonstrator (ALFRED). This research is carried out in collaboration with ENEA Brasimone. During the second year of my PhD program, the focus of my work has been the further development and application of a thermal-hydraulic simulation tool, that exploits the advantages of the CFD ANSYS CFX code and the system code RELAP5, through a coupled approach. The coupling strategy, established in the first year and based on in-house developed FORTRAN 77 routines and Python executables, demonstrated good performance in simplified cases. Throughout the second year, the structure has been refined, incorporating a new numerical scheme and enhanced control over memory consumption. The tool underwent validation in a test case within the IAEA Coordinated Research Project titled "Benchmark of Transition from Forced to Natural Circulation Experiment with Heavy Liquid Metal Loop" on the NACIE-UP experimental campaign. Results from standalone simulations using ANSYS CFX and RELAP5, as well as coupled simulations, demonstrated good agreement with experimental results (Fig.). The coupled tool replicated system-level behavior similar to the standalone code, allowing for the representation of time-varying temperature inside the fuel pin bundle simulator. This application served as a proof of concept of the coupled tool, which will be further tested in cases where the addition of a 3D component representation could enhance system-level prediction capabilities, such as for the TALL3D and ATHENA facilities.

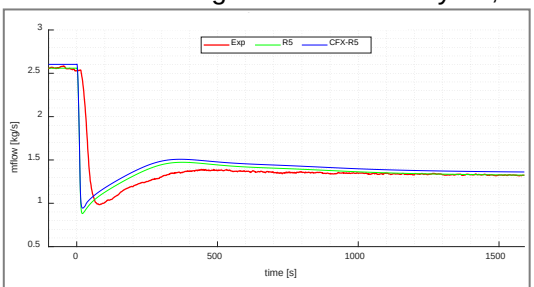


Fig. Code to experiment comparison of the mass flow rate

Additional activities have been carried out in the framework of HLM applications: support to the design of the ATHENA facility, contribution to the development of a simplified multiscale model of the Westinghouse LFR heat exchanger; testing of a new thermal mass flow meter for applications in fusion technologies (EUROFusion), designed in the first year, and its accuracy estimation; assessment of potential heavy liquid metal applications as targets or dumpers in particle accelerators, in collaboration with the CERN research center.

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

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

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

Academic context

[1] J. Zhao, X. Li, A review of polymer electrolyte membrane fuel cell durability for vehicular applications: Degradation modes and experimental techniques, Energy Convers. Manag. 199 (2019) 112022. https://doi.org/10.1016/j.enconman.2019.112022

[2] M. Gong, X. Zhang, M. Chen, Y. Ren, Proton Exchange Membrane Fuel Cell as an Alternative to the Internal Combustion Engine for Emission Reduction: A Review on the Effect of Gas Flow Channel Structures, Atmosphere. 14 (2023) 439. https://doi.org/10.3390/atmos14030439

[3] O. Brakni, Y. Kerkoub, F. Amrouche, A. Mohammedi, Y.K. Ziari, CFD investigation of the effect of flow field channel design based on constriction and enlargement configurations on PEMFC performance, Fuel. 357 (2024) 129920. https://doi.org/10.1016/j.fuel.2023.129920

External collaborations

- Politecnico di Milano, Energy Department

Highlights of the research activity

Proton Exchange membrane Fuel Cells, PEMFCs, are at the forefront of green energy solutions, playing a crucial role in the development of clean and efficient power systems. A fuel cell generates electricity through an electrochemical reaction between hydrogen and oxygen. Hydrogen is fed into the anode, where it undergoes a catalyst-mediated process to produce electrons and protons. Electrons flow through an external circuit, generating electric power, while protons migrate through the electrolyte to the cathode. At the cathode, oxygen combines with electrons and protons to produce water as the only byproduct, making fuel cells a clean and efficient energy conversion technology. However, their performance is influenced by complex interactions between different physical processes and phases, such as heat transfer, electrochemical reactions, and mass transport. My research activity addresses this complexity by employing a multi-physics approach, which involves integrating and simulating these diverse phenomena simultaneously by means of CFD softwares such as the STAR-CCM+ and openFOAM. One of the figures of a PEMFC performance is given by its polarization curve that relates the fuel cell voltage to the current density. A standard fuel cell polarization curve exhibits three well-defined regions, each highlighting the primary factor limiting performance. At low current densities, up to 1 A/cm2, the activation overpotential required to drive electrochemical reactions becomes the dominant factor. Intermediate current densities are characterized by the presence of ohmic resistance, while at high current densities, over 4 A/cm2, mass transport resistance takes precedence in influencing the overall performance. The open-source library openFuelCell has been validate against experimental results carried out by the MRT lab at Politecnico di Milano. The geometry consists in two circuits of parallel straight channels. The component presents an active surface area of 10 cm2. The Membrane Electrode Assembly (MEA) between the two sides of the FC is made of two gas diffusive layer (GDL), two Micro Porous Layer (MPL), two thin Catalyst Layer (CL) and eventually the Proton Exchange Membrane (PEM) permeable only to the transport of hydrogen ions, from anode to cathode, and water molecules. The polarization curve replicated with openFOAM, under the same operating condition, exhibits a good agreement with the experimental results as can be appreciated in Figure.

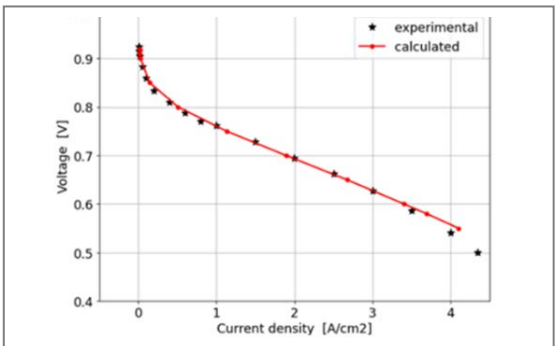


Fig. Experimental polarization curve results, in black, against OpenFOAM CFD results, in red, of the MRT-Lab fuel cell.

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

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

Course year: 2nd **Tutor(s)**: Laura SAVOLDI, Valeria DI COSMO

Academic context

[1] M. Nicoli, F. Gracceva, D. Lerede, L. Savoldi, "Can We Rely on Open-Source Energy System Optimization Models? The TEMOA-Italy Case Study", Energies, vol. 15(18), 6505, 2022.
[2] IEA (2023), Global Hydrogen Review 2023, IEA, Paris https://www.iea.org/reports/global-hydrogen-review-2023, License: CC BY 4.0
[3] S. Carrara et al., "Supply chain analysis and material demand forecast in strategic technologies and sectors in the EU – A foresight study", Publications Office of the European Union, Luxembourg, 2023.

External collaborations

- Università di Torino
- Ruhr University Bochum
- EUROfusion

Highlights of the research activity

My PhD project aims to expand the current paradigm of the bottom-up energy system optimization models (ESOMs) behind the traditional macro-economic schemes, integrating the social, environmental, and economic dimensions of the sustainable development issue. In this regard, the development and maintenance of several ESOMs (i.e., TIMES-Italy, ETM, and TEMOA-Italy), the core of my PhD first year, continued also for this year. In particular, the techno-economic modules for the hydrogen and synfuel value chains developed during last year research activity were applied to the TEMOA-Italy model, in collaboration with the PhD student Matteo Nicoli and the former MSc student Alessandro Balbo, and were adopted in several cases studies. The modeling of such value chains implied a review of the traditional emission computation scheme. Indeed, in ESOMs the emissions are usually computed through commodity-emission factors (CEFs) based on a given static fuel composition: hence, this static accounting method (see Figure (a)) is not capable to track the avoided emissions from the possible blending between fossil fuels and low-carbon fuels (LCFs), such as hydrogen, biofuels, and synfuels. Instead, the new proposed methodology is dynamic (see Figure (b)) in the sense that it accounts for such avoided emissions by using negative process-emission factors (PEFs) proportional to the LCF fractions in the blends with fossil fuels. The TEMOA-Italy model extension also included the review of the technology-specific discount rates, that are among the techno-economic parameters used to characterize technologies in ESOMs. Then, the maintenance activity concerned the ETM model, in the framework of the EUROfusion socio-economic EUROfusion Socio-Economic Studies Workpackage (WPSES), in collaboration with the postdoctoral researcher Daniele Lerede. The second part of the year was completely devoted to the off-site activities carried out at the Chair of Energy Systems and Energy Economics at the Ruhr-Universität Bochum, from April to September 2023, co-supervised by Prof. Valentin Bertsch. The ongoing collaboration aims to assess the energy and critical raw material import dependency through the application of multi-objective optimization in a TEMOA model.

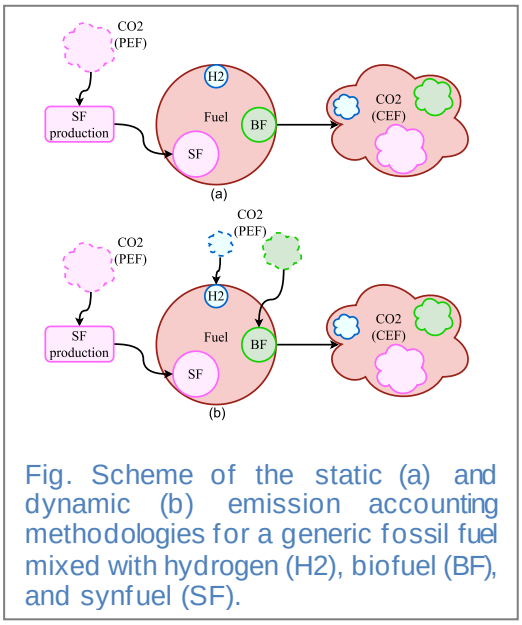


Fig. Scheme of the static (a) and dynamic (b) emission accounting methodologies for a generic fossil fuel mixed with hydrogen (H2), biofuel (BF), and synfuel (SF).

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

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

Course year: 1st **Tutor(s)**: Laura SAVOLDI, Nicola FACCIN

Academic context

[1] Hafeez MA, Singh BK, Yang SH, Kim J, Kim B, Shin Y, et al. Recent advances in Fenton-like treatment of radioactive ion exchange resins. Chemical Engineering Journal Advances 2023;14:100461. https://doi.org/https://doi.org/10.1016/j.ceja.2023.100461.
[2] Li J, Wang J. Advances in cement solidification technology for waste radioactive ion exchange resins: A review. J Hazard Mater 2006;135:443–8. https://doi.org/https://doi.org/10.1016/j.jhazmat.2005.11.053.
[3] Hill J, Prazska M, Jagatia M. Geo-polymer solidification technology approved by Czech / Slovak nuclear authority to immobilise NPP resins and sludge waste - 15555. WM2015: Annual Waste Management Symposium, United States: 2015.

External collaborations

- SOGIN

Highlights of the research activity

My PhD research activity, in collaboration with green-land, aims to develop of a new geopolymeric matrix (HYPEX®) able to safely conditionate the spent radioactive ion exchange resins (IEXs), which is one of the most problematic Medium Level waste (MLW) of Nucleare facilities (Fig. 1). Furthermore, the PhD is focused only on the design of a mock-up to demostrate the validity of the HYPEX® process on insustrial scale.

In this first year, a major revision of all the existing method on the conditioning of IEXs has been made, focusing on the major engineering and safety problems. A wide study of geopolymer matrix as a structural material has been made to validate its feasibility for nuclear waste conditioning. Chemical reactions occurring the formation of the geopolymer has been analysed, many geopolymers typologies have been manufactured and final macroscopic proprieties of the geopolymer matrix has been tested to prove its mechanical stability. The mechanical proprieties aimed to be achieved are the one of the Technical Guide N33 of Ispettorato Nucleare per la Sicurezza Nucleare (ISIN) for Medium Level Waste (MLW). Until now results suggests the new developed geopolymer can incorporated up to 30% of IEXs, maintaining good strength. Promising results have been achieved also by grinding the IEXs from a millimetre to a micrometre scale.

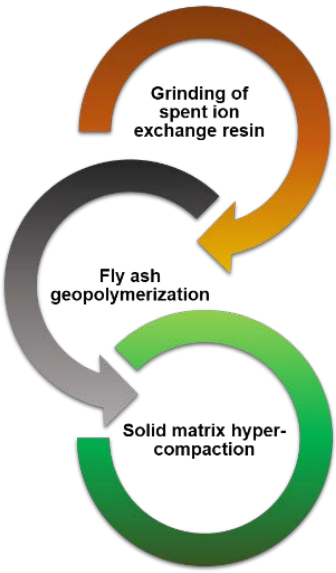
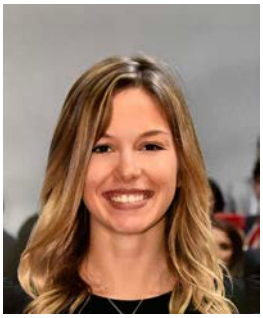


Fig. "The three main step in the HYPEX process"

Furthermore, a first draw of the mockup has been designed. The process of "incorporating IEXs in geopolymer matrix" will be carried out by a mobile plant formed by 2 units. The first unit addresses the problem of taking remotely the IEXs (the waste) out of the containers where they have been stocked. In the second unit the IEXs in mixed with the reagents of the geopolymer to form the final matrix. The design of the plant has been carried out in collaboration with "Sinergia Spa". A general sizing of all the equipment of the plant has been made to produce a Basic Pipe & Instrumentation Diagram (P&ID). High safety standards according to ASME VIII have been followed during the design of the plant.



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

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

Course year: 1st **Tutor(s)**: Laura SAVOLDI, Giancarlo VENTURA

Academic context

[1] Hafeez MA, Singh BK, Yang SH, Kim J, Kim B, Shin Y, et al. Recent advances in Fenton-like treatment of radioactive ion exchange resins. Chemical Engineering Journal Advances 2023;14:100461. https://doi.org/https://doi.org/10.1016/j.ceja.2023.100461.
[2] Li J, Wang J. Advances in cement solidification technology for waste radioactive ion exchange resins: A review. J Hazard Mater 2006;135:443–8. https://doi.org/https://doi.org/10.1016/j.jhazmat.2005.11.053.
[3] Hill J, Prazska M, Jagatia M. Geo-polymer solidification technology approved by Czech / Slovak nuclear authority to immobilise NPP resins and sludge waste - 15555. WM2015: Annual Waste Management Symposium, United States: 2015.

External collaborations

- SOGIN

Highlights of the research activity

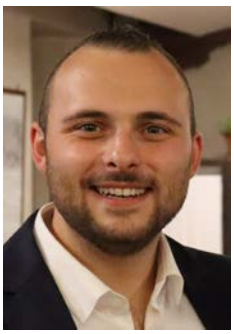
My PhD research activity, conducted in collaboration with green-land s.r.l., focuses on innovating the treatment and conditioning of ion-exchange resins (IEXs). The primary objective is to minimize the final waste volume and operational time and costs. To achieve this, I've contributed to formulate a novel conditioning matrix utilizing geopolymer, as opposed to the conventional use of cement for immobilizing radioactive waste. Geopolymer was selected for its superior mechanical properties compared to cement and its unique ability to incorporate boron within its chemical structure, a feature that adversely affects the chemical integrity of cement. Throughout this year, various types and families of geopolymers have undergone testing to identify the most suitable candidate capable of immobilizing the maximum quantity of resin while adhering to the International Safety Standards for radioactive waste management.
Also an in-depth investigation into the behavior of the resin was conducted to mitigate its swelling property, a characteristic that tends to compromise the matrix when exposed to water. Consequently, the treatment procedure will involve grinding and full resin hydration before conditioning, significantly reducing the resin's swelling pressure by a factor of 1000.

Fig. Fundamentals steps of the new process for the conditioning of IEXs

Resistance to radiation, compression, immersion, thermal cycles, leachability, fire and permeability to gas have been carried out in agreement with the standards established in Italy in the Technical Guide #33 (GT33) by the National Inspectorate for Nuclear Safety and Radiation Protection (ISIN). The selected geopolymer matrix with, at lest, 30%wt of resin has successfully met all these criteria.

This new process for the treatment and conditioning of ion-exchange resins has been developed at room temperature, to minimize the hazard in a radioactive environment.

The conventional Portland cement-based matrices are able to embed about the 10%wt of resins. The new geopolymer matrix formulated conditions 3 times the usual quantity of resin.



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: 2nd **Tutor(s)**: Roberto ZANINO

Academic context

[1] 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**", *accepted by IEEE Access*, 2022
[2] 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
[3] M. De Bastiani, R. Bonifetto, G. Messina, L. Morici, R. Zanino and A. Zappatore, "**Electro dynamic model of eddy currents in EU DEMO TF coil casing during major plasma disruption**", *Fusion Engineering and Design, vol 196, 2023*

External collaborations

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

Highlights of the research activity

This year my research has been mainly devoted to the development of two new models to be added to the multiphysics platform for superconducting magnet modelling which will be the final outcome of my PhD. The first one is the 4C/DC model, for the electrical (EL) simulation of superconducting magnet systems, directly connected to the 4C code (thermal-hydraulic - TH - model) by means of FMI standard. Accurate EL and TH coupled modelling is fundamental to obtain reliable numerical results, especially for accidental transients in which the coupling between the two physics is important.
The second model developed is dedicated to thermo-mechanics and is based on the commercial software ANSYS: it uses in input the temperature distribution computed by the 4C code to assess the thermal stresses induced during specific transients.
The 4C/DC has been developed in the object oriented Modelica language and thanks to its modularity can be used to simulate the magnet system with different levels of details, from the system level model of the magnet power supply, to the detailed EL connections within a non-insulated winding pack.
The first application of the 4C/DC has been the analysis of a EU DEMO TF coil short circuit during a fast discharge (FD) of the current, while the second has been the EL+TH simulation of the charge of the non-insulated version of the EU DEMO TF coil.

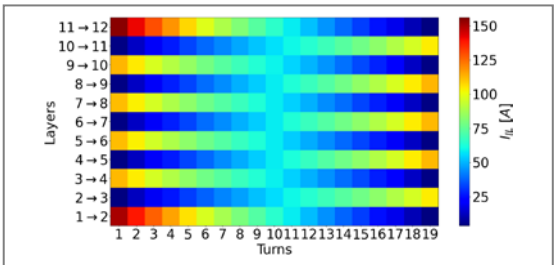


Fig. Inter-layer current distribution in the non-insulated version of the EU DEMO TF coil after 10 h (over 100 h) of charging.

The developed thermo-mechanical model is currently being used to evaluate the thermal stresses induced in the DTT TF magnets during their cooldown from ambient to cryogenic temperature; the aim is to assess which temperature *gradients* allow keeping the secondary stress below the threshold, possibly relaxing the simplistic constraint on the maximum temperature *difference* to optimize the cooldown speed and maximize the machine availability.
Additional analyses have been carried out to support the design of DTT and EU DEMO magnet systems:

- Quench + FD simulation of both EU DEMO and DTT TF coils, using the power deposition in the casing during FD evaluated with the 3D-FOX, the electromagnetic (EM) tool developed during the 1st year
- EL+EM+TH analysis of the DTT TF FD using varistors.

Moreover, I have supported the DTT thermal shield design team by means of TH simulations aiming at identifying the better shield configuration to reduce the radiative heat load to the magnets.

First name: Rosa **LAST NAME**: DIFONZO

Topic: Analysis, design and optimization of the cooling system of Gyrotron resonant cavities

Course year: 3rd **Tutor(s)**: Laura SAVOLDI, Antonio CAMMI

Academic context

[1] Savoldi, L. et al. Assessment and optimization of the cavity thermal performance for the Europena wave gyrotron. In Proceedings of the 27th IAEA fusion energy Conference (FEC 2018), Gāndhināgar, Indien, October 22 – 27 2018.
[2] Alexandersen J., and Andreasen C.S., A review of topology optimization for fluid-based problems, *Fluids*, Vol. 5, No.1, 2020, pp. 29.
[3] Kontoleontos E.A., Papoutsis-Kiachagias E.M., Zymaris A.S., Papadimitriou D.I., and Giannakoglou K.C., Adjoint-based constrained topology optimization for viscous flows, includin heat transfer, *Engineering Optimization*, Vol. 45, 2013, pp. 941-961.

External collaborations

- Karlsruhe Institute of technology
- Thales AVS France
- National Technical Institute of Athens

Highlights of the research activity

My research activity is mainly focused on the study and application of existing optimization methods to the design of the cooling system of the Gyrotron resonant cavity, for nuclear fusion applications. During the gyrotron normal operations, in fact, a high amount of heat is released on the cavity inner wall, causing displacements and consequently affecting the tube efficiency. Thus, the need of minimize the displacement on the inner wall, while keeping the pressure drop under a fixed value and keep the thermal stresses under the yield strength of the material. The most recent work has been focusing on the use of adjoint-based topology optimization method, in OpenFOAM, including fluid-dynamics and heat transfer. The s/w developed byt the Parallel CFD & Optimization Unit has been used during my research activity at NTUA. A sector of the whole circular cavity has been chosen as computational domain. The optimization problem included a weighted cost function with a contribution of the mean temperature on the heated wall, to reduce indirectly displacements, and its standard deviation, in order to reduce thermal gradients, to control stresses. Moreover, a constraint on the pressure drop was included. In Figure 1 the results of the thermal-hydraulic analysis of the body-fitted mesh of the optimized solution are represented. We can notice that similar "wedge" shape is obtained in opposite directions for inlet and outlet manifolds, forcing the flow in the azimuthal direction mainly in the central area where the peak of the heat load is experienced. This goes in the direction of a flatter temperature profile to reduce thermal stresses.

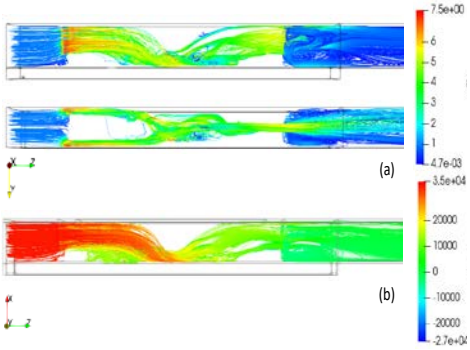


Fig. streamlines of the velocity field form lateral and bottom point of view (a) and pressure map (b) in the optimized configuration.

Another front of investigation has been the stability analysis of a previously optimized annular duct cooling configuration. During the normal operations of the Gyrotron, in fact, variation in the power can be experienced, leading variation in the deformations and hence in the cooling. The stability analysis had the aim to verify that, in the considered range of values, the response in time of the system to small perturbation, reaches a steady state. A 0D model was according to the Lyapunov's criterion. Moreover, the step responses of the system with linear and non-linear model showed very similar behaviors.

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

Topic: Characterization and mitigation of Runaway Electrons in the next generation of fusion reactors

Course year: 1st **Tutor(s)**: Fabio SUBBA, Giuseppe RAMOGIDA

Academic context

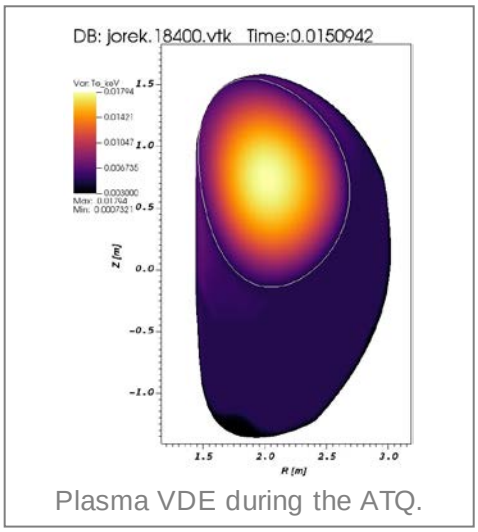
[1] Hoelzl M., Huijsmans G.T.A. et al. Nuclear Fusion 61, 065001 (2021)
[2] Bandaru V., Hoelzl M., Reux C. et al. Plasma Physics and Controlled Fusion, 63, 035024 (2021)
[3] Schwarz N., Artola F.J., Vannini F. et al. Nuclear Fusion 63, 126016 (2023)

External collaborations

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

Highlights of the research activity

The main objective of my activity is the study of 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. REs are relativistic electrons that can form beams of energies up to several 10s of MeV. Thus, they pose a considerable threat to the operation of future generations of fusion reactors, and proper avoidance and mitigation strategies have to be designed. In my PhD research activity, I am exploiting the non-linear magneto-hydrodynamic (MHD) code JOREK, which is able to resolve realistic toroidal tokamak X-point geometries and which implements a RE fluid model able to describe self-consistently the nonlinear coupled evolution of REs and plasma instabilities during disruptions. Similar work has already been carried out for other tokamaks (both in operation and in construction), such as JET, ASDEX Upgrade, ITER and EU-DEMO.



Plasma VDE during the ATQ.

In the initial part of my work, my main focus has been on importing the data from DTT inside JOREK in order to calculate the equilibrium of the chosen plasma scenario. This has been carried out both in simplified fixed boundary conditions and in free boundary conditions, thanks to the coupling of JOREK with another tool called STARWALL.
After working on some preliminary steps that were mainly useful to gain confidence with the software and the ATQ procedure, I worked on performing a so-called Artificial Thermal Quench (ATQ) in free boundary conditions, which is linked with a Vertical Displacement Event (VDE) of the plasma (Figure on the right). The ATQ mimics what really occurs during a disruption by artificially tuning some physical parameters (e.g. thermal diffusivities and electrical resistivity). In this way, it is possible to arrive in a relatively simple way to a post-disruption phase, without having to run ad-hoc simulations that are very complex and time-consuming. This is allowed since the main focus of my research activity is the current quench phase, which is then connected with the generation of REs.
Currently, I am working on the final steps of the ATQ. When this will be done, it will be possible to simulate the current quench phase (exploiting the RE module of JOREK to initialize the RE) and, switching to 3D simulations, to study the RE beams termination in DTT. This will follow with scans of the main parameters of interest (e.g. number of impurities after the mitigation) and evaluation of mitigation strategies such as the presence and the characteristics of sacrificial limiters.

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

Topic: Fusione termonucleare innovativa

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

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

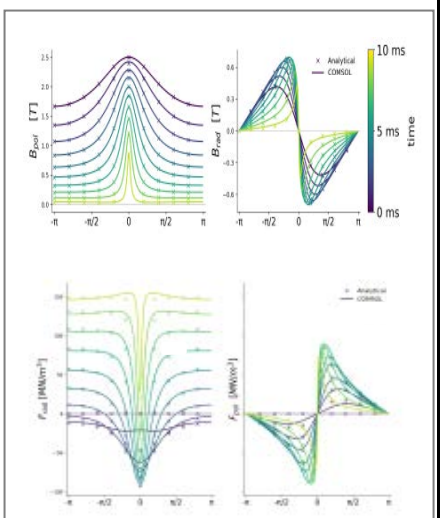
External collaborations

- ENI
- MIT – Plasma Science and Fusion Center

Highlights of the research activity

The activities in the second year contributed to:

- The analysis of the phenomena with Multiphysics connections which are relevant in an ARC-class reactor molten salt Liquid immersion blanket. Heat transfer mechanisms in molten salts, radiative heat transfer, and tritium transport analysis have been carried out, together with the electromagnetic responsive force of the vacuum vessel in response to a plasma disruption due to the induced currents.
- The evaluation of relevant heat transfer mechanisms in ARC-class reactors, temperature distribution, heat transfer coefficients, velocity field, and effective heat transfer enhancements methods to respect the material limits with decreased pressure drops. The determination of ARC blanket minimum operative conditions, outlet temperature, mass flow rate, pressure drops, and required pumping power through 3D CFD models [Ferrero, Gabriele, et al. "Exploration of ARC-class reactor vessel and divertor cooling system." *Fusion Engineering and Design* 192 (2023): 113818.]. An analysis of the impact of radiative heat transfer in ARC-class liquid immersion blankets has been published. [Ferrero, Gabriele, Raffaella Testoni, and Massimo Zucchetti. "Impact Assessment of Radiative Heat Transport in ARC-Class Reactor FLiBe Liquid Immersion Blanket." *Nuclear Science and Engineering* (2023): 1-16.]



Verification of the FEM model for disruption forces in VV with anisotropic conductivity

- 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 blanket design. Activities with the open-source Tritium transport code *festim* team have been conducted during the period spent at MIT PSFC.
- The analytical model to evaluate disruption forces in a VV with anisotropic conductivity has been verified through comparison with the FEM model as the main scope for the period spent at MIT PSFC.A poster on this activity has been presented at the APS DPP conference in Denver (30th October- 3rd November 2023) and the MITEI (13th-14th September 2023) conference in Boston.

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: 1st **Tutor(s)**: Laura SAVOLDI, Gianluca BOCCARDO, Antonio BUFFO

Academic context

[1] Rathore, Surendra Singh, et al. "Flow Characterization in Triply Periodic Minimal Surface (TPMS)-Based Porous Geometries: Part 1—Hydrodynamics". *Transport in Porous Media*, 2023

[2] Yeranee, K.; Rao, Y. A, *Review of Recent Investigations on Flow and Heat Transfer Enhancement in Cooling Channels Embedded with Triply Periodic Minimal Surfaces (TPMS),* Energies 2022, 15, 8994.

[3] Rathore, S.S., Mehta, B., Kumar, P. *et al.* Flow Characterization in Triply Periodic Minimal Surface (TPMS)-Based Porous Geometries: Part 1—Hydrodynamics. *Transp Porous Med* **146**, 669–701 (2023).

External collaborations

- Politecnico di Milano, Energy Department

Highlights of the research activity

The research activity focuses on the development of an equivalent macro-scale model to describe the Triply Periodic Minimal Surfaces (TPMS) from the hydraulic and thermal points of view. TPMS are non-intersecting, 3D periodic structures generated by combinations of trigonometric functions. They can be produced with Additive Manufacturing, and they form a structured porous medium utilizable as heat sinks or heat exchanger, increasing the heat transfer while simultaneously maintaining low pressure drop because of the smooth surfaces. During this first year of the PhD, a hydraulic model has been developed for some TPMS, in parallel with the design of the cooling systems of some fusion components, equipped with TPMS. An innovative TPMS-based cooling system has been considered for the mirrors in the Transmission Lines of the DTT Electron Cyclotron Heating (ECH) system. DTT (Divertor Tokamak Test). A wide range of parameters have been explored in the TPMS generation, varying the porosity, the cell dimension and the topology, thus characterizing the operational windows of such cooling system (see Fig., where the different colors and numbers refers to the cell size of a single TPMS unit cell). The mirror cooling system equipped with TPMS appears more effective than the traditional cooling for those mirrors (usually spiral-cooling): a TPMS cooling system can reach $P_o/\Delta T_{max} = 340\ MW\ m^2\ K^{-1}$, while the spiral cooling arrives at $P_o/\Delta T_{max} = 9\ MW\ m^2\ K^{-1}$. This figure of merit, the ratio between the peak heat flux and the maximum temperature increase, describes how efficiently the power can be removed, and larger values are beneficial.

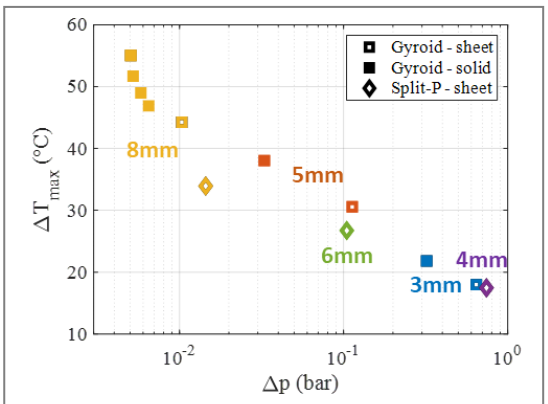


Fig. Thermal-hydraulic investigation of TPMS as cooling system for the mirrors in the transmission line of DTT ECH. Sheet or solid refers to the two or one channel topology of the TPMS.

A new design of the cooling system of the divertor tile of the stellarator W7-X has also been investigated using TPMS and this study has been presented at the 17th International heat Transfer Conference and submitted to its proceedings. This analysis compares the two (sheet-TPMS) or single (solid-TPMS) channel of TPMS as heat sink and the different orientation of the principal direction of the structure with respect to the heated side.

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

Topic: Macro-scale modeling of DTT cryogenic plant

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

Academic context

[1] R. Ambrosino, "DTT-Divertor Tokamak Test facility: A testbed for DEMO," Fusion Engineering and Design, vol. 167, p. 112330, 2021..
[2] R. Bonifetto, F. Casella, L. Savoldi Richard and R. Zanino, "Dynamic modeling of a supercritical helium closed loop with the 4C code," AIP Conference Proceedings, vol. 1434, no. 1, pp. 1743-1750, 2012.
[3] Lisanti, F., et al. "Design of the cryogenic loop for the superconducting toroidal-field magnets of the Divertor Tokamak Test." Cryogenics 136 (2023): 103757.

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

Highlights of the research activity

The research activity carried out during the first year of PhD focused on the development of system-level dynamic models of the cryogenic circuits of the Divertor Tokamak Test (DTT) superconducting tokamak [1].
To support the DTT cryogenic plant design, system-level models of the cryogenic circuits for the cooling of the DTT toroidal-field (TF) and pulsed (namely, poloidal field - PF - and central solenoid - CS) magnets were developed; the cryogenic circuit module of the 4C code has been used [2], a state-of-the-art numerical tool developed at Politecnico di Torino, based on the Modelica language. A preliminary 1D thermal-hydraulic analysis has been carried out for the dimensioning of the main distribution lines supplying He to the TF magnets, based on the trade-off between pressure drop and radiative heat loads; the resulting dimensions and radiative heat loads have been adopted as inputs for the entire TF cooling circuit model. At first, a reference layout for the TF cryogenic circuit has been implemented and simulated; then, alternative layouts (i.e. separate circuits and series cooling for TF coils and casings) and mitigation strategies (e.g. the reduction of the cold circulator – CC – speed during the plasma pulse) have been investigated to reduce the heat load transferred from the cryogenic circuit(s) to the He refrigerator of the DTT cryoplant. The results of this work have been presented at the CHATS on Applied Superconductivity conference, held in Turin in May, and included in a paper published in the Cryogenics journal [3], while some preliminary estimates of the overall heat load that will be suffered by the DTT He refrigerator (see e.g. Fig. 1) have been presented at the SOFE conference held in Oxford (UK) in July. In addition, a model of the PF and CS coils cooling circuit has been implemented and simulated, providing the evolution of the heat load transferred to the He bath by such circuit. Moreover, in parallel to the main stream, the system-level GETTHEM modelica model of the PbLi circuit of the water-cooled lithium-lead (WCLL) concept for the breeding-blanket (BB) of the EU DEMO reactor was supported. A model for the assessment of the generation and transport of Activated Corrosion Products (ACPs) was developed and presented in a paper published in the IEEE Access journal. Furthermore, the modelica implementation of the PAV (Permeator Against Vacuum, one of the candidates technologies for the tritium extraction unit of the WCLL BB) model and the related uncertainty quantification have been performed and presented in a paper published in the Nuclear Materials and Energy journal. First comparisons of the model with experimental data from tests performed on a PAV mock-up at ENEA Brasimone have also been presented at the ISFNT conference in September.

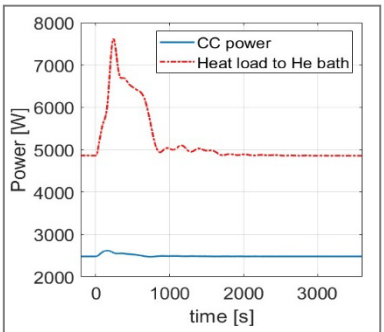


Fig. Thermal power delivered to the DTT He refrigerator and CC power consumption for the DTT TF cooling loop during one plasma pulse.

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

Topic: Modeling of the Climate Land Energy Water nexus

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

Academic context

[1] J. Krzywanski *et al.*, "Advanced Spatial and Technological Aggregation Scheme for Energy System Models," *Energies 2022, Vol. 15, Page 9517*, vol. 15, no. 24, p. 9517, Dec. 2022, doi: 10.3390/EN15249517.

[2] J. Liu *et al.*, "Nexus approaches to global sustainable development," *Nature Sustainability 2018 1:9*, vol. 1, no. 9, pp. 466–476, Sep. 2018, doi: 10.1038/s41893-018-0135-8.

[3] N. Wang, R. A. Verzijlbergh, P. W. Heijnen, and P. M. Herder, "A spatially explicit planning approach for power systems with a high share of renewable energy sources," *Appl Energy*, vol. 260, Accessed: Apr. 04, 2023. [Online]. Available: https://doi.org/10.1016/j.apenergy.2019.114233

External collaborations

- ENI S.P.A.

Highlights of the research activity

The rapid growth of renewable energy sources, the need for increased afforestation to sequester carbon, and soil degradation from climatic factors collectively constrain the availability of land for diverse purposes. Recent research, both scientific and non-scientific, has illuminated potential conflicts between soil resources and the energy transition, particularly highlighting challenges arising from the decarbonization of all sectors within regions facing primary resource limitations.

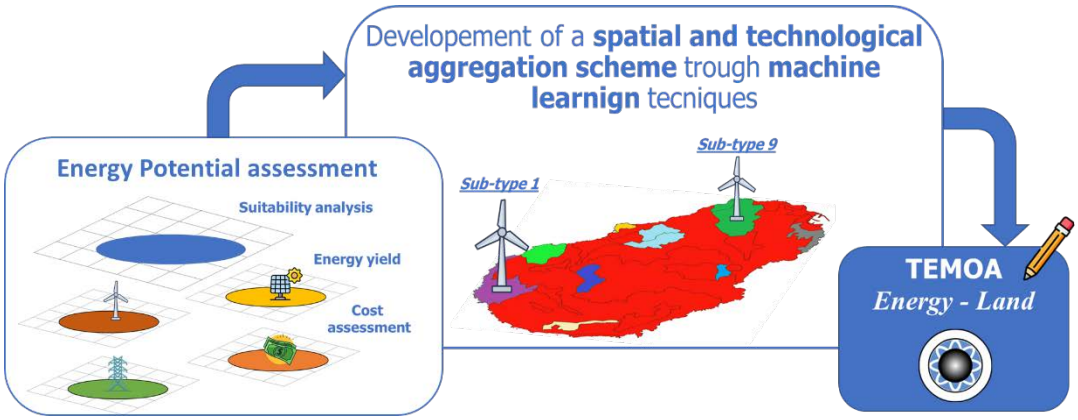


Fig. Workflow of the integration of land-use aspects in ESOMs

This underscores the pressing need to integrate land availability, both for energy and non-energy purposes, into energy models. However, such integration remains an underexplored area in the existing scientific literature, necessitating the development of novel methodologies. My ongoing research efforts comprise three primary components: characterizing a selected case study (Pantelleria Island) in terms of land availability and energy potential using geospatial analysis, translating resource assessment data into a model-interpretable format, and modifying the TEMOA model to incorporate this crucial new element.

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

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

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

Academic context

1. M. Nicoli, F. Gracceva, D. Lerede, and L. Savoldi, "Can We Rely on Open-Source Energy System Optimization Models? The TEMOA-Italy Case Study," Energies 2022, Vol. 15, Page 6505, vol. 15, no. 18, p. 6505, Sep. 2022, doi: 10.3390/EN15186505.
2. D. Lerede, M. Nicoli, L. Savoldi, and A. Trotta, "Analysis of the possible contribution of different nuclear fusion technologies to the global energy transition," Energy Strategy Reviews, vol. 49, no. 101144, Sep. 2023, doi: 10.1016/j.esr.2023.101144.
3. G. Colucci, D. Lerede, M. Nicoli, and L. Savoldi, "A dynamic accounting method for CO2 emissions to assess the penetration of low-carbon fuels: application to the TEMOA-Italy energy system optimization model," Appl Energy, vol. 352, no. 121951, Dec. 2023, doi: 10.1016/j.apenergy.2023.121951.

External collaborations

- North Carolina State University
- Eni S.p.A.
- ENEA

Highlights of the research activity

The research activity focuses to the development of open-source energy system modeling frameworks and models including innovative energy paradigms and aims at the assessment of the possibile future role of nuclear fusion in the energy system. Concerning open-source frameworks, an extended version of the already existing Tools for Energy Modeling Optimization and Analysis (TEMOA), developed by North Carolina State University, was produced [1]. Within the TEMOA modeling framework, a first preliminary study of the possible role of nuclear fusion in the future energy mix was carried out [2]. The paper presents a competitive study between alternative typologies of nuclear fusion power plants, which techno-economic parameters (e.g., the specific cost, the expected lifetime, and the efficiency) have been estimated, based on the last studies in the field. Three technological alternatives are presents in the paper (based on ARC, EU-DEMO and Asian-DEMO reactor concepts) and their contribution to the global energy transition is assessed for several socio-economic scenarios and regions of the world. The second year of my research activity was conducted at the North Carolina State University, under the co-supervision of Prof. Anderson Rodrigo De Queiroz. The joint research activity is aimed at analyzing the possible role of energy storage technologies in the future energy system through energy system optimization models. The activity includes the techno-economic characterization of a set of electricity and hydrogen technology options, implemented in the TEMOA-Italy model (as shown in Figure), and the development of a proper modeling strategy (focused on the refinement of the model time scale) to assess the possible role of storage in balancing the infra-day dynamics associated with the renewable energy sources intermittence. Summary results are available in a poster presented at the NCSU 2023 Climate Leaders Fall Symposyum.

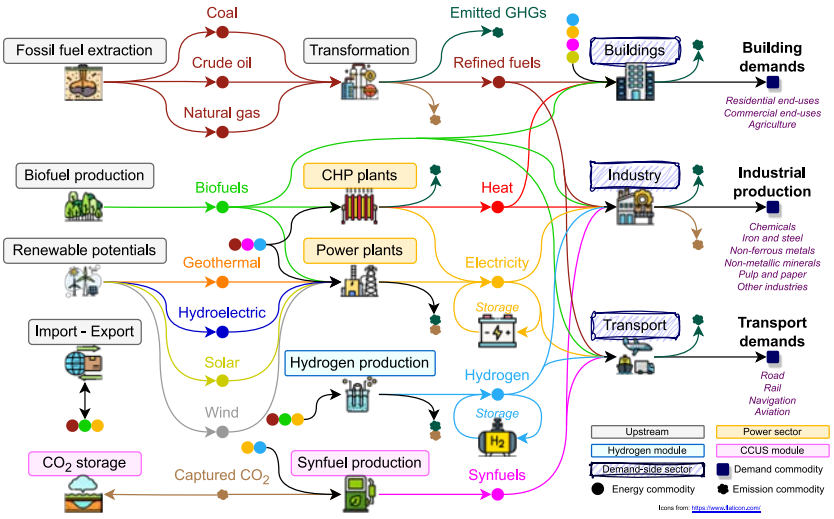


Fig. The TEMOA-Italy energy system, including electricity and hydrogen storage technologies.

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

Topic: ARC safety and siting studies

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

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.

External collaborations

- ENI
- Massachusetts Institute of Technology: MIT

Highlights of the research activity

The activities in the first year contributed to:

- Create a CAD model for an ARC-class reactor Fig., defining materials and a tokamak source to perform a neutron and activation analysis. These are very important to determine the machine's operation, the materials' lifetime over time, and disposal methods. The model creation and simulations of tokamak operations were conducted using OpenMC to evaluate: neutron economy, absorption rate on the materials, transmutation products, power density, neutron flux, neutron spectra and neutronic damage. The results obtained from the neutronic analysis were used as inputs for FISPACT-II to calculate: specific activity, dose rate, decay heat, displacements per atoms. Results of this work have been presented at the 30th Symposium on Fusion Engineering (Oxford 09/07-13/07 2023).
- Comparison between OpenMC and FISPACT-II for activation, transmutation, depletion, shutdown dose rate, and neutron damage.
- A literature review has specifically focused on materials currently proposed for use as structural components in nuclear fusion reactors, examining the required properties, corrosion phenomena, and the thermal stresses they undergo. Additionally, an analysis of regulatory constraints in the USA and Italy was conducted to identify the limits necessary for establishing such facilities in these countries.
- The comparison between the PHITS and OpenMC transport codes allowed for the assessment of their impact on key results such as the tritium production ratio and spatially resolved neutron spectra, considering various nuclear libraries, models, and codes. This analysis was carried out using a three-dimensional geometry imported from CAD, simulating a fusion machine similar to ARC. Additionally, the influence of different neutron source shapes was explored, ranging from a simple ring-like source to a realistic toroidal plasma distribution. A paper on this topic is under review.
- Comprehensive analysis of damages and energy deposition, including data on secondary particles, on a three-dimensional model of a VIPER cable (based on REBCO), starting from a 3D model of an ARC-class reactor. Results of this work have been presented at the European Conference on Applied Superconductivity (Bologna 03/09-07/09 2023)

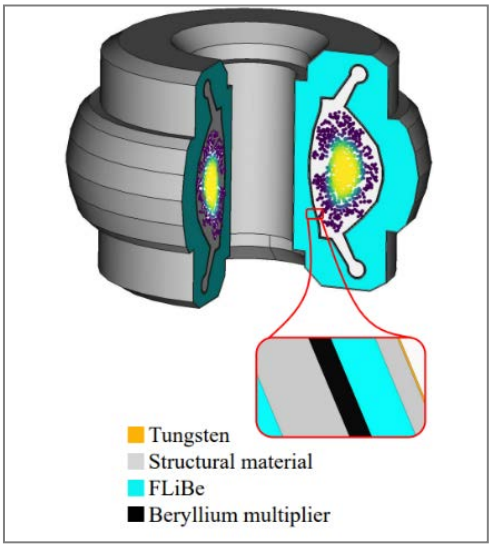


Fig. ARC-class reactor components and their material specifications

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

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

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

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 et all, https://doi.org/10.1016/j.cryogenics.2009.07.008.

External collaborations

- Plasma Science and Fusion Center (PSFC) at Massachusetts Institute of Technology (MIT)
- EPFL
- Università di Bologna

Highlights of the research activity

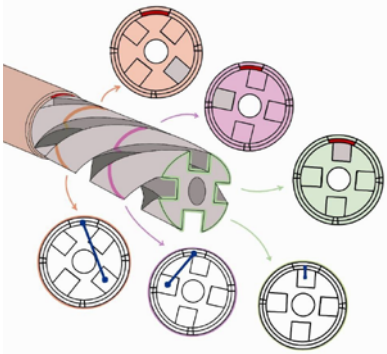


Fig. variable contact perimeters and heat transfer coefficients are required to suitably model the twist pitch of the stacks of tapes in the VIPER cable.

Whithin the framework of the design of superconducting (SC) cables used in nuclear fusion and power transport, most of the available tools for their modeling are proprietary sofware, not always provided with a well integrated multiphysic module. A new open source open access sofware (OPENSC^2) is being develop at Politecnico di Torino that deals with the thermal-hydraulic and electromagnetic modeling of SC cables. The main activity of the second year of the PhD focused on several tasks, namely code refactoring, models verification and validation as well as introduction of new features. Refactoring became necessary when we realized that the monolitic approach followed so far was not suitable in the long run for easy software development and management. To that purpose, an Application Programming Interface (API) needs to be developed. The main advantages are improved maitainability and readability, a simpler introduction of new features and the possibility to leverage them to develop a GUI. Much of the year has been devoted to validating the thermal-hydraulic model and verifying of the electric model. For the latter, a benchmark against the H4C software is underway for the ENEA HTS slotted core cable configuration with the help of a M.Sc. student. The thermal-hydraulic model was questioned in two different ways: on the one hand we validate it against the experimental measurements taken at the SULTAN test facility for the VIPER cable configuration, on the other hand we performed a code to code benchmark against THEA. The former activity, with the collaboration of prof. Hartwig and Dr. Riva of PFSC, MIT (Boston, MA, US) was discussed at the MT28 conference. During the Short Term Student Mission co-founded by COST Action undertook by the candidate in July, both a preliminary analysis of the experimental data and model set-up were conducted. This experience highlighted some criticalities in both the experimental data and the model; the latter, related to variable contact perimeters and heat transfer coefficients, were subsequently addressed and solved. The second activity involved Dr. Guarino from EPFL. The outcomes concerinig two scenarios for the BEST PATHS-like cable configuration for power transport were presented in a poster session of EUCAS conference.
Moreover, the introduction of new tecniques for discretizing the spatial and time derivatives that characterizes the thermal-hydraulic model of OPENSC^2 was inevstigated. The verification phase, carried out outside OPENSC^2, has been successfully completed while the implementation of the new discretizations in the sofware is still in progress.

First name: Mehdi **LAST NAME**: SHOKRNIA

Topic: Modeling of concentrated solar power systems

Course year: 3rd **Tutor(s)**: Roberto ZANINO, Mattia CAGNOLI

Academic context

[1] Ordóñez, F., Flores, E., Soria, R., 2021. Comprehensive analysis of the variables influencing the techno-economic optimization of medium temperature linear Fresnel collectors. Energy Rep. 7, 5747-5761.
[2] Cagnoli, M., Mazzei, D., Procopio, M., Russo, V., Savoldi, L., Zanino, R., 2018. Analysis of the performance of linear Fresnel collectors: Encapsulated vs. evacuated tubes. Sol. Energy 164, 119-138.
[3] Suresh, C., Saini, R.P., 2020. Experimental study on combined sensible-latent heat storage system for different volume fractions of PCM. Sol. Energy 212, 282-296.

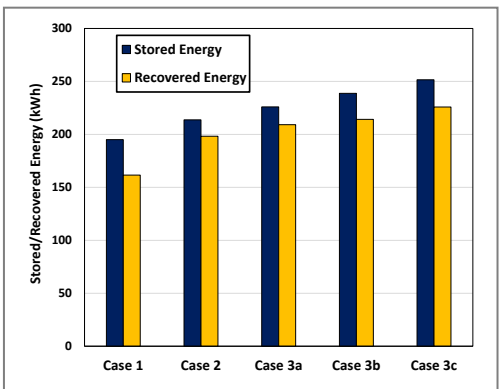
External collaborations

- ENEA, Casaccia, Italy

Highlights of the research activity

Three activities have been followed during my PhD program: (1) optimization of photothermal efficiency for a parabolic trough plant, (2) comparative techno-economic analysis of parabolic trough and Fresnel plants with encapsulated and evacuated tubes, and (3) optimization of a thermal energy storage (TES) system.

1) For the parabolic trough system, a system-level Modelica model was developed and validated against experimental data provided by ENEA. Then, the photo-thermal performance of the system was optimized by using 3 different coatings along the absorber tube. Such a strategy increased the photo-thermal efficiency nearly 1% on average, compared to the single-coating tubes, reducing the capital cost because the (expensive) coating suitable for high temperatures is adopted only for a small portion of the tube.
2) The techno-economic analysis of linear CSP systems was performed in terms of levelized cost of electricity (LCOE). The LCOE depends on economic parameters and on the net annual energy yield. The latter was computed by a 1D model that solves the energy balance along the receiver axis. The 1D model requires accurate boundary conditions, including a thermal driver and heat losses. The thermal driver, consisting of the incident solar power, was calculated by using an optical ray-tracing model, whereas a lumped-parameter model computed the heat losses. It was found that the PTC with an evacuated receiver tube allows obtaining the highest net annual energy yield, leading to the lowest LCOE. This is because the higher cost with respect to both the LFC system and the non-evacuated PTC are compensated by the higher net energy yield. Finally, a sensitivity analysis was carried out to evaluate the impact on the LCOE of the optical efficiency and of the economic parameters.
3) An optimized TES system was introduced by implementing two optimization measures on a case study in terms of geometrical optimization and phase change material (PCM) integration. In this respect, first, tank geometry was modified to involve the entire tank in thermal stratification, and then, toroidal PCM tubes were inserted at different heights inside the tank with three scenarios. A transient 2D CFD model was developed to determine heat losses and salt temperature distributions, coupled with a PCM lumped-parameter model which computes PCM temperature and corresponding heat transfer coefficient. Geometrical optimization of the TES system led to an improvement in the thermal performance in terms of all performance parameters. Moreover, PCM integration could increase the potential thermal storage capacity of the system by a maximum of ~23%. The TES system with PCM at both top/bottom locations indicated the most enhanced performance among all configurations.



Stored/recovered energy during charge/discharge process for different thermal energy storage systems

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

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

Course year: 2nd **Tutor(s)**: Fabio SUBBA, Daniela GRASSO

Academic context

[1] P. Helander et al., (2007). Resistive stability of a plasma with runaway electrons. Physics of Plasmas, 14(12), 122102, https://doi.org/10.1063/1.2817016
[2] Liu et al., (2021). Self-consistent simulation of resistive kink instabilities with runaway electrons. Plasma Physics and Controlled Fusion, 63(12), 125031
[3] Bandaru et al., Magnetohydrodynamic simulations of runaway electron beam termination in JET. Plasma Physics and Controlled Fusion 63, 035024 (2021)

External collaborations

- Max Planck institute for Plasma Physics, Garching bei Munchen, Germany
- CEA, Cadarache, France
- Consorzio RFX, Padova, Italy

Highlights of the research activity

The goal of the PhD activity is to develop a workflow that allows a thorough understanding of the RE dynamics in a post disruptive plasma starting from their interaction with the plasma core activity to their impact on the First Wall of a Tokamak.
In the underlined framework, the PhD activity has started focusing on:

1. Understanding the mutual influence of Runaway Electron current and a specific plasma instability often detected in tokamaks, the so called magnetic reconnection. This first part of the activity is called MARE (MAgnetic reconnection and Runway Electrons) in the following;
2. Modelling the impact of RE on the first wall materials of existing Tokamak. This second part of the activity is called DiRHaS (Disruption and Runaway electrons Handling Strategies) in the following.

MARE

We verified the results given by our code SCOPE3D against the theory presented in Liu et al, PoP, 27 (2020). Afterwards, we carried out the non linear analysis which represents the novelty of our work. In particular, we found out that while the resistive layer controls the transition of the island from the linear to the nonlinear stage, the microlayer width causes the runaways to become nonlinear once the island size becomes larger than the microlayer width. This transition of the runaways to the nonlinear phase is accompanied by the generation of a spiral-like structure inside the island changing drastically the distribution of runaways with respect to the symmetric case as shown in Fig.
The next step consists in benchmarking the SCOPE3D results, verified against theory, with the JOREK (a nonlinear MHD code) results considering a similar physical scenario. This would enable us to verify JOREK results in case of a magnetic reconnection event driven by a RE current.

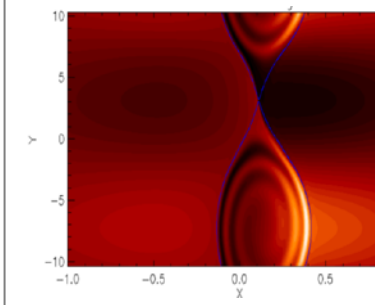


Fig. Distribution of the perturbed runaway electrons current with the corresponding magnetic island (blue line) during the nonlinear phase of the island evolution.

DiRHaS

The focus for this part of the activity has been the implementation and use of thermal models to compute the temperature evolution and melting caused by the RE impact on a First Wall (FW) tile using the FREEFEM code. These models have used as input the energy deposition profiles given as output by the Monte Carlo code FLUKA. The results obtained so far using FLUKA and FREEFEM are being written in a paper yet to be submitted. The models implemented, so far, in FLUKA and FREEFEM will be used in the next year of the PhD for the validation of RE induced damage on the JET First Wall tile.

First name: Sofia **LAST NAME**: VIARENGO

Topic: Development of numerical multi-physics models for the analysis of normal and off-normal operating conditions for HTS components

Course year: 3rd **Tutor(s)**: Laura SAVOLDI, Fabio FRESCHI

Academic context

[1] D. I. Meyer and R. Flasck, "A new configuration for a dipole magnet for use in high energy physics applications," Nucl. Instrum. Methods, vol. 80, no. 2, pp. 339–341, Apr. 1970.
[2] X. Wang et al., "A viable dipole magnet concept with REBCO CORC ® wires and further development needs for high-field magnet applications," Supercond. Sci. Technol., vol. 31, no. 4, p. 045007, Apr. 2018.
[3] D. C. van der Laan, J. D. Weiss, and D. M. McRae, "Status of CORC ® cables and wires for use in high-field magnets and power systems a decade after their introduction," Supercond. Sci. Technol., vol. 32, no. 3, p. 033001, Mar. 2019.

External collaborations

- Lawrence Berkeley National Laboratory (LBNL)
- Ricerca sul Sistema Energetico (RSE)
- ENEA

Highlights of the research activity

My activity is focused on the development of numerical multiphysics model for prediction of the critical current and the performance of the Conductor-on-Round-Core (CORC®) cable, specifically the voltage-current (V-I) curve. In CORC® cables, the high-temperature superconducting ReBCO tapes (Figure b) are helically wound around a copper core in opposite winding directions each layer. Since ReBCO tapes are strain-sensitive, these cables can degrade as a result of the winding process and operating conditions. The 3D multi-physics numerical model is based on a T – A formulation for straight cable (verified and validated) has been extended to a bended cable, see Figure a. The model is implemented in COMSOL Multiphysics® coupled with a thermal model. The tape is a composite multilayered material, treated as a single material through a homogenization. All properties are temperature dependent and weighted on thickness or on mass. The electrical resistivities are computed as an equivalent electrical resistivity. The ReBCO resistivity depends on the critical current density J_c and the current density which flows in the conductor through a power law. Moreover, the J_c scaling accounts for temperature, magnetic field, and local strain: a pure geometrical consideration allows to account for the punctual degradation of J_c, as an input for the multiphysics model. A map of strain has been extrapolated both from literature and from some simplified geometrical assumptions based on the definition of strain, considering: the intrinsic strain due to the tape winding on the copper core; compression\tension state and shrinkage due to the bending evaluated through pure analytical computations. The simulation results, considering a LN_2 bath at $77\ K$ and self-field conditions, have been compared to experimental data of a bended 6-tapes CORC® cable tested at the LBNL, showing a good agreement for the critical current prediction.

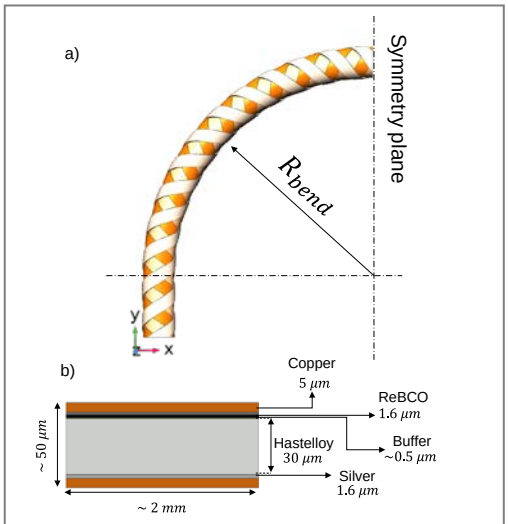


Fig. a) CORC® cable and b) tape layouts (not in scale).

Politecnico di Torino

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PhD. ENERGETICS

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