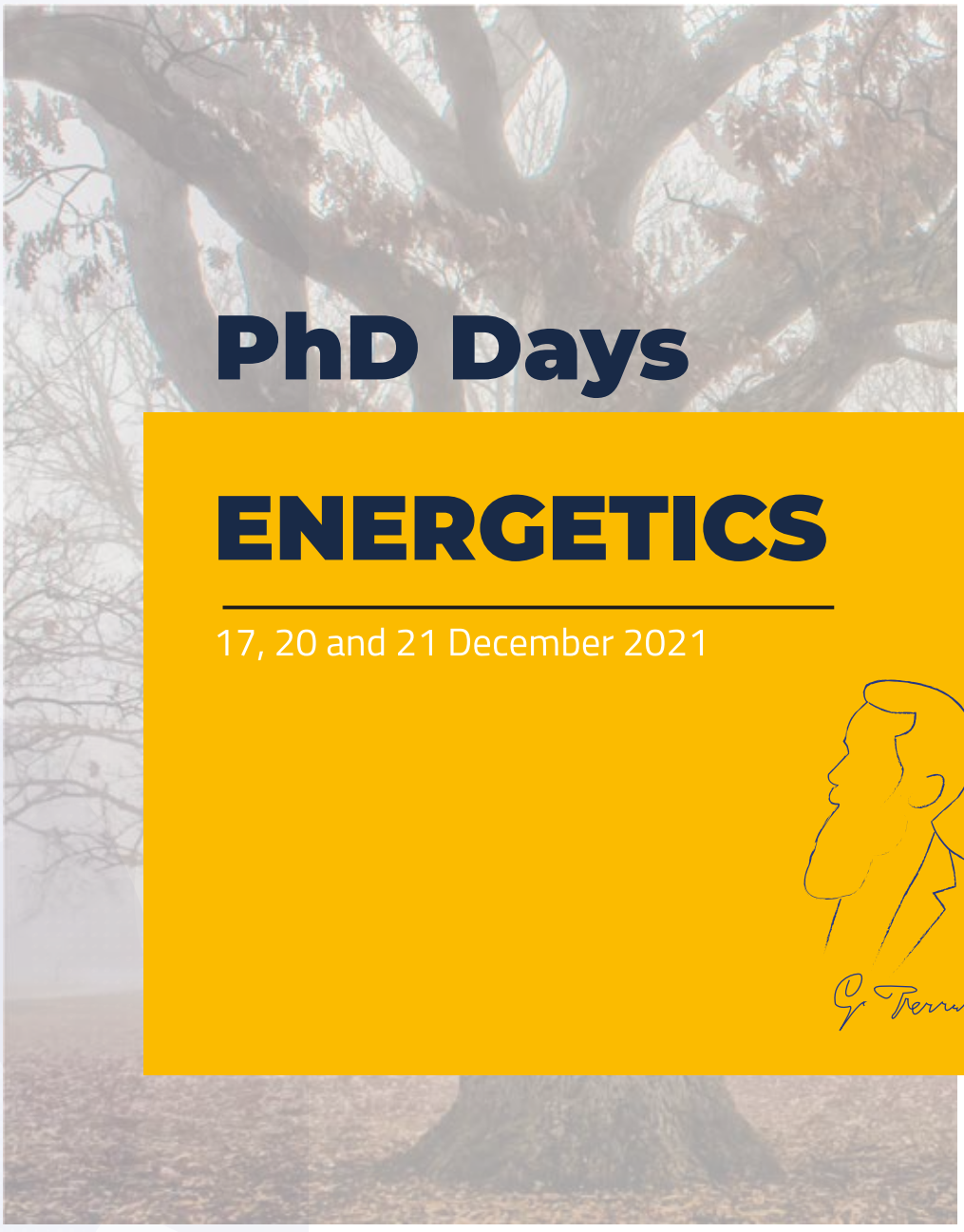
Politecnico di Torino

Department of Energy
"G.Ferraris"



PhD Days

ENERGETICS

17, 20 and 21 December 2021

ENERGETICS PHD ANNUAL REPORT

2021

DECEMBER 17, 2021

DIPARTIMENTO ENERGIA “GALILEO FERRRARIS“
POLITECNICO DI TORINO

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Acknowledgments

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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- ETAS (for ASCMO)
- Gamma Technologies (for GT-Suite)
- Siemens (for STAR CCM+, STAR-CD, ES-ICE)
- Simerics (for SimericsMP+)

CONTENT

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

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

Course year: 1st **Tutor(s)**: Stefano P. CORGNATI, Ettore F. BOMPARD, C. SANDRONI, A. LA BELLA

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] Krug, R., Mehrmann, V., & Schmidt, M. (2021). Nonlinear optimization of district heating networks. Optimization and Engineering, 22(2), 783-819.
[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.
- Information Technology for Humanitarian Assistance, Cooperation and Action - ITHACA S.r.l.
- RHOSS S.p.A.

Highlights of the research activity

The current energy transition is having an impact on the whole energy chain and the progression of energy systems towards carbon neutrality involves supply, transmission, conversion and demand sides. In particular, the increasing deployment of distributed generation technologies allows exploiting local renewable energy sources, transforming consumers from passive to active actors (i.e., the so-called prosumers). This shifting in the way energy is produced and consumed clearly represents a challenge for transmission and distribution networks, and in this context, the concept of flexibility will play a crucial role. In this framework, the necessity of new and more flexibility sources to correctly guarantee the energy demand meeting puts the attention on the interaction between different energy vectors, converging towards the so-called Multi-Energy Systems (MESs). Specifically, if on one side the interaction between energy vectors can bring multiple benefits, among which the possible exploitation of different "types" of flexibility, on the other side, MESs ask for effective and optimal management. In this framework, my Ph.D. research, developed in collaboration with RSE S.p.A., aims: (i) to study the behavior of MESs and to model and simulate their operation dynamics; and (ii) to evaluate the types of flexibilities that MESs can provide to the supply network, by defining a methodology to easily quantify the amount of available flexibility. Going into detail, during this first year, attention was mainly devoted to the MES modelling and simulation. Starting from the definition of a base model, the Simscape simulation software was identified in order to dynamically simulate the system, and a preliminary case study was developed. The simulation was developed in the form of a reference benchmark model from literature constituted of a district heating network fueled by a CHP and a gas boiler and five final users. Moreover, to fine-tune the demand side inputs, a limited set of residential and office archetypes were modelled and simulated using the energy-dynamic simulation software EnergyPlus, to obtain typical buildings hourly demand profiles. Next steps will be devoted to the modelling of the electrical network, using a network developed by IEEE as a benchmark, and to explore how demand-response actions will affect flexibility in MESs.

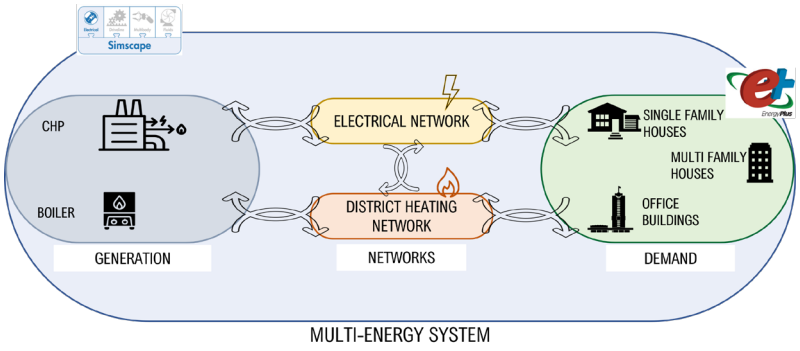


Figure 1 – MES model scheme and corresponding software used for simulation

First name: Nicolò **LAST NAME**: ABRATE

Topic: Methods for safety and stability analysis of nuclear systems

Course year: 3rd **Tutor(s)**: Sandra DULLA, Nicola PEDRONI

Academic context

[1] "A parametrized non-intrusive reduced order model and error analysis for general time-dependent nonlinear partial differential equations and its applications", D. Xiao, F. Fang, C.C. Pain, I.M. Navon, Comput. Methods Appl. Mech. Engrg., **317**, 868-889, 2017.
[2], "Assessment of numerical methods for the evaluation of higher-order harmonics in diffusion theory", Abrate, N.; Bruna, G.; Dulla, S.; Ravetto, P., Annals of Nuclear Energy, **128**, 455-470, 2019
[3] "The impact of heavy reflectors on power distribution perturbations in large PWR reactor cores", A. Sargeni, K.W. Burn, G.B. Bruna, Annals of Nuclear Energy, **94**, 566-575, 2016.

External collaborations

- INFN Genova

Highlights of the research activity

This PhD research focuses on the study and development of advanced computational methods for the safety and stability assessment of complex systems, focusing on advanced nuclear reactors, like GEN-III+ and GEN-IV designs. The main objective is to provide an innovative, safety-oriented simulation approach, combining legacy reactor physics methods with Reduced Order Modelling (ROM) techniques, with the aim of reducing the computational burden associated to the several simulations typically required for the quantitative risk analysis of nuclear reactors.

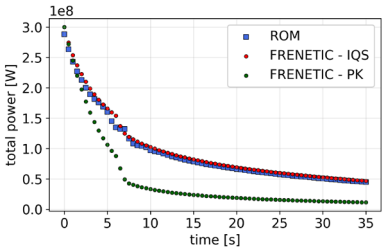


Figure 1 – Comparison between the fission power evolution computed by ROM, Improved Quasi-Static and Point Kinetics.

First, an analysis concerning the spectrum of the different neutron transport eigenvalue formulations was carried out, focusing on the impact of the numerical approximations commonly employed in neutron transport. This analysis allowed to remark the importance of the eigenvalue separation as a figure of merit for the stability of the system and to estimate the impact of the different formulations on the neutron energy spectrum. Moreover, this activity stimulated the introduction of innovative eigenvalue formulations, e.g., the capture eigenvalue, which allow to approach criticality by acting directly on the density of specific nuclides. These formulations could be extremely useful to support both the reactor design and operation, e.g., the reactivity control with the chemical shim. Then, the research activity was focused on the development of a non-intrusive ROM for the parametric study of accidental scenarios in complex systems. The first application involved the accidental insertion of one control rod inside the ALFRED reactor design. The ROM, trained using few reference solutions computed with the FRENETIC code, proved its effectiveness in reproducing the original model behaviour with a fair accuracy (see Figure) and a strong reduction in the computational burden. Another application of the ROM regarded the accidental gas releases in congested plants, e.g., oil&gas offshore plants. In this case, the ROM was applied to estimate the gas flow fields after the release phase, which were then employed as input for the gas dispersion simulations.
Finally, one of the most challenging steps in the licensing of a reactor is the propagation of the nuclear data uncertainty to the main operating parameters of the reactor: due to the huge size of the uncertain parameter space, appropriate reduction techniques are needed for an efficient study. First, the performances of an innovative ROM available in the Serpent 2 Monte Carlo code was compared to the legacy Generalised Perturbation Theory for the case of the ALFRED reactor, showing a very good consistency and a fair reduction in the computational time to propagate the uncertainties from the raw nuclear data to the macroscopic parameter. Then, alternative, non-intrusive techniques like fast Total Monte Carlo and GRS have been tested, providing sufficiently accurate results with a strong reduction in the computational effort.

First name: Francesco **LAST NAME**: ACCURSO

Topic: Large Bore Gas Combustion Technology Development by Predictive Combustion Model

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

Academic context

[1] Millo, F., Accurso, F., Piano, A., Caputo, G., Cafari, A., Hyvönen, J. "Experimental and numerical investigation of the ignition process in a large bore dual fuel engine". Fuel 2021, 290, 120073.
[2] Wenig M, Roggendorf K. Development of a Predictive Dual-Fuel Combustion and Prechamber Model for Large Two-Stroke Engines within a Fast 0D / 1D-Simulation Environment. 29th CIMAC World Congr. 2019.
[3] García Valladolid P, Tunestål P, Monsalve-Serrano J, García A, Hyvönen J. Impact of diesel pilot distribution on the ignition process of a dual fuel medium speed marine engine. Energy Convers Manag 2017;149:192–205.

External collaborations

- Wärtsilä
- Gamma Technologies LLC
- Powertech Engineering

Highlights of the research activity

The research activity, sponsored by Wärtsilä, concerns the development and validation of a predictive combustion model for dual fuel engines. The dual fuel combustion model recently introduced by Gamma Technologies in the commercially available software GT-SUITE was considered for this work. During my PhD the dual fuel model was optimized for large bore gas engines operating with lean mixtures, by developing accuarate submodels for both ignition proocess and flame propagation simulation.

In the third year of my PhD I focused on the assesemment of the predictive capabilities of the model for two Wärtsilä engines, namely a laboratory single-cylinder and a new 6-cylinder engine (cylinder bore equal to 310 and 460 mm respectively). The developed model demonstrated to be capable to capture the influence of the main calibration parameters (i.e., injection timing, duration and pressure, boost conditions) and engine modifications (i.e., compression ratio and valve timings) on combustion process, providing accurate predictions in terms of ignition timing, combustion phasing and peak cylinder pressure, as shown in Figure 1.

Additionally, with the aim to extend the validity of the model in terms of emission predictions and to consider a possible knocking tendency, a NOx emissions model and a knock model were considered. The developed NOx model, accounts for the mixture composition and temperature distribution of the burned gasses by dividing the overall cylinder in multiple zones and computing their temperature evolution and related NOx formation.
As far as the knock model is concerned, a kinetics-fit model for the natural gas was introduced and calibrated by achieving at a given knock-limited engine condition a good agreement in terms of knocking frequency between experiments and predicted results.

The proposed dual fuel model can be therefore used for preliminary optimization of the engine and for virtual calibration activities.

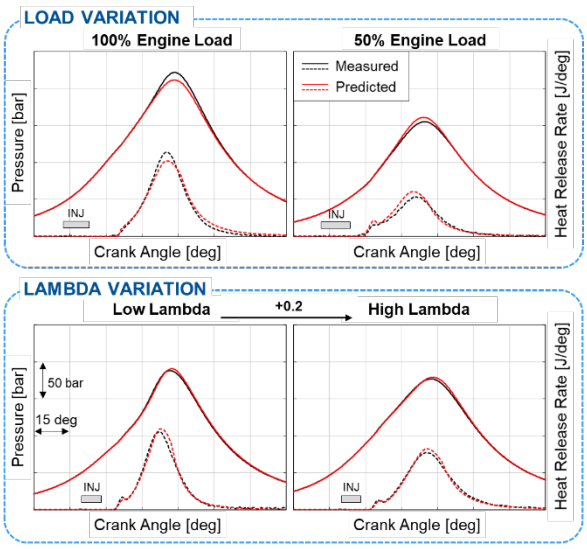


Figure 1 – Experimental and simulated Pressure and Heat Release Rate for a load variation (top figure) and lambda variation (bottom figure).

First name: Ciro **LAST NAME**: ALBERGHI

Topic: Analysis of MHD and tritium transport in liquid breeders for fusion applications

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

Academic context

[1] Alberghi, C., Candido, L., Testoni, R., Utili, M., Zucchetti, M., "*Verification and Validation of COMSOL Magnetohydrodynamic Models for Liquid Metal Breeding Blankets Technologies*", Energies, 14(2021), https://doi.org/10.3390/en14175413
[2] Mistrangelo, C., Bühler, L., Alberghi, C., Bassini, S., Candido, L., Courtessole, C., Tassone, A., Urgorri, F.R., Zikanov, O., "*MHD R&D Activities for Liquid Metal Blankets*", Energies, 14(2021), https://doi.org/10.3390/en14206640
[3] Alberghi, C., Candido, L., Testoni, R., Utili, M., Zucchetti, M., "Magneto-convective effect on tritium transport at breeder unit level for the WCLL breeding blanket of DEMO", Fusion Engineering and Design, 160(2020), https://doi.org/10.1016/j.fusengdes.2020.111996

External collaborations

- ENEA
- EUROfusion
- ITER organization

Highlights of the research activity

The MHD and tritium transport code for WCLL breeding blanket developed in 2020 has been upgraded. Lithium-lead flow in a 3D portion of the WCLL 2018 was simulated, considering a magnetic field of 4 T and buoyancy forces. The velocity field was used as input for the tritium transport calculations. The temperature field and velocity profile of lithium-lead (shown in Fig. 1) and tritium inventories and losses were obtained. A model that includes the pulsed operation of DEMO reactor is under development. The tritium transport code has been verificated and validated against the commercial code TMAP7. A new mathematical tool to describe the different permeation regimes in the hydrogen isotope permeators, sensors, PAV and Liquid Vacuum Contactor (LVC) systems has been developed. Regarding the experimental activities, the first campaign of Hyper-Quarch (Hydrogen Permeation Quartz Chamber) facility at ENEA C. R. Brasimone has been carried out. A first value of the Sievert constant of solubility of hydrogen in lithium-lead has been obtained. In 2022 the campaign will proceed in order to determine a relation for the Sievert constant as a function of temperature. Two experimental campaigns on TRIEX-II facility at ENEA C.R. Brasimone have been followed. a) Characterization of Hydrogen extraction efficiency of the Gas Liquid Contactor under ITER operative conditions. b) Characterization of Alumina based PLD (pulsed laser deposition) hydrogen permeation barrier on EUROFER samples. The design of a new experimental facility that characterizes the hydrogen permeation performance of a 2-meter-long pipe with anti-permeation coating and having an uncoated welding area has been performed. The facility construction has been completed in november at RINA Consulting CSM (Roma)

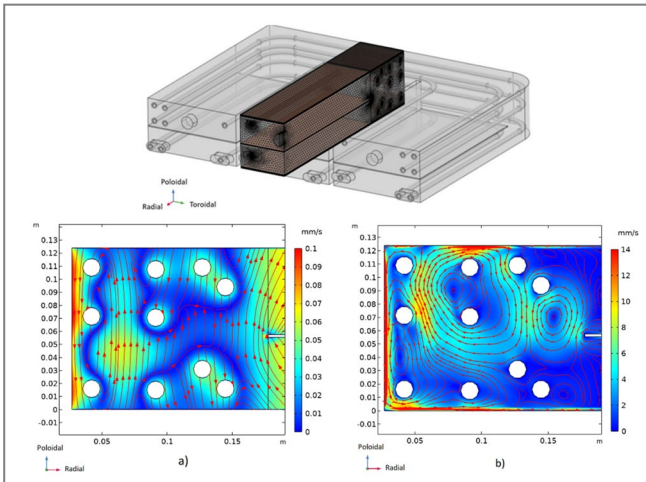


Figure 2 – Pure hydrodynamic B_0=0 T (left) and magnetoconvective B_0=4 T (right) velocity profile of the LiPb in a portion of the WCLL BB module.

First name: Matteo **LAST NAME**: ALBERGHINI

Topic: Heat and mass transfer in porous and structured materials for energy-conversion devices: towards the water-energy nexus

Course year: 3rd **Tutors**: Pietro ASINARI, Eliodoro CHIAVAZZO, Alberto TIRAFERRI

Academic context

[1] Alberghini, M., Morciano, M., Fasano, M., Bertiglia, F., Fernicola, V., Asinari, P., & Chiavazzo, E. (2020). Multistage and passive cooling process driven by salinity difference. *Science advances*, 6(11), eaax5015
[2] Alberghini, M., Hong, S., Lozano, L. M., Korolovych, V., Huang, Y., Signorato, F., ... & Boriskina, S. V. (2021). Sustainable polyethylene fabrics with engineered moisture transport for passive cooling. *Nature Sustainability*, 1-10.
[3] Vaartstra, G., Zhang, L., Lu, Z., Díaz-Marín, C. D., Grossman, J. C., & Wang, E. N. (2020). Capillary-fed, thin film evaporation devices. *Journal of Applied Physics*, 128(13), 130901.

External collaborations

- Massachusetts Institute of Technology (MIT)
- Istituto Nazionale di Ricerca Metrologica (INRiM)

Highlights of the research activity

Porous materials with engineered multi-functionalities are particularly desirable for passive energy conversion devices. These devices typically require low maintenance, are cost-effective and offer a robust and cost-effective alternative in a wide variety of applications. They typically use non-structured capillary materials, such as paper or commercial textiles, as passive component to move working fluids. These materials, however, offer limited degrees of optimization given their non-ordered structure.

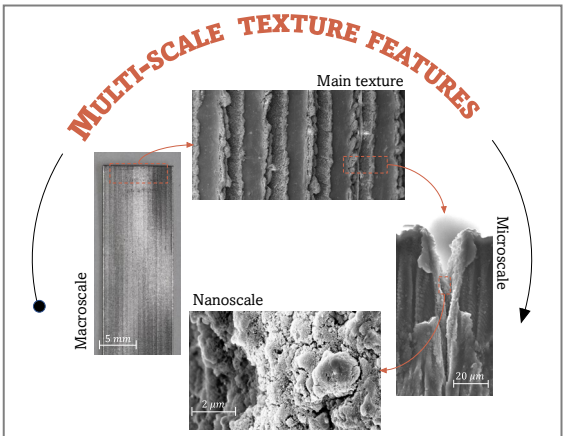


Figure 1 – The optimized micro- and nano-features and the provided surface functionalization provide the material with high performance and long-term durability.

In the framework of passive solar desalination, the research activity envisions to replace traditional non-structured porous materials with rigid capillary layers engraved with optimized V-shaped grooves. The concept has been tested using aluminum sheets, which were machined by femtolaser (see Figure 1). The etching procedure provided the treated metal layer with efficient capillary properties, which, however, were depleted by prolonged exposure to water. Therefore, the material was coated by SiO_2 or functionalized by oxygen plasma. Notably, the wettability and capillary performance remained exceptionally stable for the whole duration of the aging tests, both in distilled and salt water at 35 g L^{-1} (approximately 250 hours). Then, the experimental capillary properties were used to calibrate a novel theoretical model relating the geometry and surface chemistry of the grooves to their wicking performance.
Finally, the rigid capillary material was envisaged for use in a passive desalination device: a comprehensive heat and mass transfer theoretical framework was used to investigate the optimal size and total productivity of the engineered assembly in a real-scale application. Interestingly, the proposed rigid capillary material allows to replace commercial hydrophobic membranes, essential in a typical multistage device layout, with air gaps, thus removing the most expensive component of the assembly. According to modeling estimates, this configuration achieves a specific throughput 58% higher than the best performing reference in literature. Concluding, a combination of the adopted design approach and the proposed structured and rigid capillary material paves the way for the transition of passive applications from lab-scale prototypes to real-scale devices.

First name: Andrea **LAST NAME**: ALLIO

Topic: Advancing the numerical modeling of 2-phase heat transfer

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

Academic context

[1] M. Shiea, et al., “Evaluation of Hydrodynamic Closures for Bubbly Regime CFD Simulations in Developing Pipe Flow,” Chemical Engineering \& Technology, vol. 42(8), pp. 1618–1626, 2019.
[2] Y. Liao and D. Lucas, “Poly-disperse simulation of condensing steam-water flow inside a large verti-cal pipe,” International Journal of Thermal Sciences, vol. 104, pp. 194–207, 2016.
[3] M. Colombo and M. Fairweather, “Multi-Fluid Computational Fluid Dynamic Predictions of Turbulent Bubbly Flows Using an Elliptic-Blending Reynolds Stress Turbulence Closure,” Frontiers in Energy Research, vol. 8, p. 44, 2020.

External collaborations

- THALES Electron Devices S.a.S., Vélizy-Villacoublay Cedex, France

Highlights of the research activity

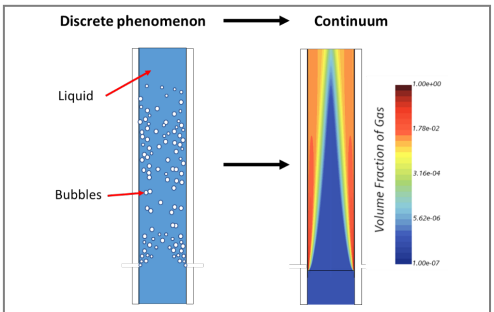


Figure 1 – Schematic of the Eulerian-Eulerian two-fluid modelling approach for bubbly flows in vertical pipes

During 2021 I investigated the CFD modelling of boiling phase change phenomena, which include fluid dynamics phenomena of two flow phases and their interaction. First, a large number of experimental data from experiments datasets available in the literature was collected. Then, a CFD model was developed, suitable to simulate multiphase bubbly flows using the commercial software STAR-CCM+ using an Eulerian-Eulerian two-fluid computational approach. The model was applied to simple geometries, in particular vertical cylindrical pipes with different diameters, in which a mixture of water and gas bubbles moves upward. Water was considered as continuous phase and air or steam as dispersed phase. A set of conservation equations was solved for each phase. In the momentum equations a term considering the interfacial momentum transfer between the phases per unit volume source is included. It is defined by the closure relations that model the interfacial forces: drag, lift, turbulence dispersion, and wall lubrication. It was not possible to derive a single CFD model able to well reproduce the complex physics beyond all the different experimental cases analyzed. So, three models were developed: A, B, and C. Model A was used to simulate vertical pipes with large (200 mm) diameter, and it uses Tomiyama drag coefficient, Sugrue lift coefficient, Burns turbulent dispersion force and Antal’s wall lubrication coefficient as closure relations. In this model the turbulence of the continuous phase, is solved using a standard $k-\varepsilon$ model with a high-Reynolds wall treatment. Model A was also utilized to simulate some cases with steam bubbles injected inside a slightly subcooled water flow, instead of air. To account for the phenomenon of condensation of the steam bubbles, an interphase mass transfer model was needed, and a semi-empirical correlation proposed by Tomiyama was used. Model B and C were developed to treat the bubbly flow phenomenon in small pipes, with diameter < 40 mm. They use a Reynolds stress equation model with a low-Reynolds wall treatment. In all analyzed air-water cases, a good agreement between computed and experimental volume fraction and velocity profiles along the radius of the pipes was reached. Some discrepancies, especially near the wall, are affected not only by the accuracy of the modelling but also by the large uncertainties of the experimental data. In the steam-water cases, however, the discrepancies are significant, and the modeling still needs improvement.

First name: Elena **LAST NAME**: BADINO

Topic: Optimization of building façade features to enhance environmental quality at the urban microscale

Course year: 2nd **Tutor(s)**: Arianna ASTOLFI, Valentina SERRA, Louena SHTREPI

Academic context

[1] W. Yang, J.Y. Jeon, Design strategies and elements of building envelope for urban acoustic environment, Build. Environ. 182 (2020)
[2] E. Badino, R. Manca, L. Shtrepi, C. Calleri, A. Astolfi, Effect of façade shape and acoustic cladding on reduction of leisure noise levels in a street canyon, Build. Environ. 157 (2019)
[3] C.V. Gál, N. Kántor, Modeling mean radiant temperature in outdoor spaces, A comparative numerical simulation and validation study, Urban Clim. 32 (2020)

External collaborations

- University of Naples Federico II, Naples, Italy
- CEMEX Research Group AG, Brügg, Switzerland
- ENEA, Roma, Italy

Highlights of the research activity

The research endorses the conception of buildings façades as interfaces between indoor and outdoor environments, capable to benefit both conditions. In particular, it focuses on the potential contribution of façade design to **outdoor thermal and acoustic comfort** for dwellers and pedestrians. In cities, such conditions are influenced by the geometric and material features of surrounding buildings, and a performance-wise design approach can provide a long-lasting contribution to public health. During the past year, the research activities have mainly focused on **façade design solutions** for improving outdoor conditions over the façade itself and at the street level, by means of simulation and experimental work. A parametric simulation study assessing how the design of the façade facing a courtyard can influence outdoor and indoor noise levels in presence of chatting noise within the courtyard has been carried out, using a calibrated model of the courtyard of the Department of Energy as case-study. In the attempt to identify **performance simulation tools** able to provide reliable information during design phases to optimize outdoor thermal comfort, the mean radiant temperature models implemented in common simulation tools (ENVI-met, TRNSYS, CitySim, Ladybug and Honeybee, SOLENE-microclimat) were compared, evidencing the radiative components included and the simplification applied in the calculation. Since the mean radiant temperature is the main parameter influencing outdoor thermal comfort in hot conditions, it is crucial to obtain reliable predictions. Moreover, a study on the use of **thermochromic materials** as cladding solution for building facades and roofs has been carried out in an outdoor test facility and in the laboratory to characterize their behavior in both free-running and controlled conditions. These materials can dynamically modulate the rate of solar radiation absorbed/reflected based on their surface temperature. The working mechanism influences both indoor and outdoor conditions and therefore, the application of these materials needs to be carefully defined to promote comfort in both settings.

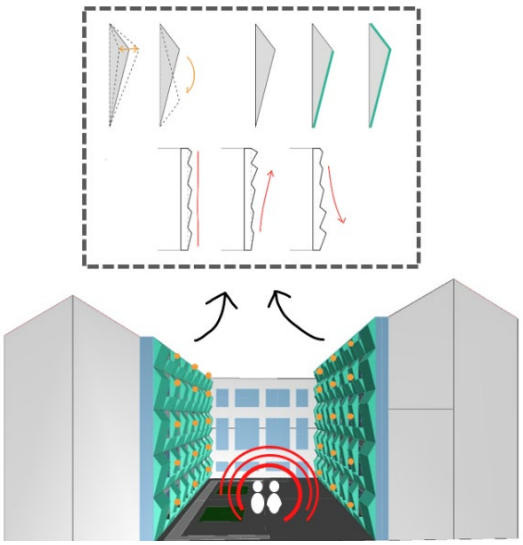
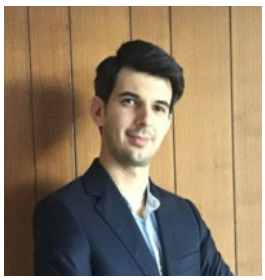


Figure 1 – Example of the set of facade design alternatives applied to the side buildings of the courtyard to investigate the resulting outdoor noise level variations



First name: Stefano **LAST NAME**: BAZZOLO

Topic: Cable driven innovative systems for urban transport: engineering, design and energy consumption (Ph.D. in apprenticeship)

Course year: 2nd **Tutor(s)**: Bruno DALLA CHIARA, Sergio BLENGINI

Academic context

[1]. Navone M., Dalla Chiara B., Blengini S., Vair E., Cable driven Automated People Movers for urban applications: modelling the roller for investigating energy consumption, Ingegneria Ferroviaria, vol. LXX, N 9, pp 631-663, Sept.2017
[2]. Affatato M., Blengini S., Dalla Chiara B., Vair E., Automated People Mover with rope traction: engineering and modelling an innovative hybrid solution to optimise energy use, Ingegneria Ferroviaria, vol. LXX, ISSN: N. 11, pp. 901-923, Nov. 2015
[3]. UNI, "Linee guida per la progettazione dei sistemi di trasporto persone ad automazione integrale (APM) con trazione a fune", 2018

External collaborations

- Dimensione Ingenierie S.r.l.

Highlights of the research activity

Main goal of the research activities during the three-years PhD program is to analyse the urban transport systems derived by cable car technologies, with particular reference to hybrid systems, where propulsion can be given to the vehicle through two different ways: 1) the clamping or gripping to a cable, similarly to a traditional cable car; or 2) through motorized wheels mounted on the vehicle, similarly to a monorail or to a small light rail.

A comparative analysis on energy consumption between the hybrid cable car-motorized wheels and other public transport systems has been carried on. This analysis shows that the above-mentioned hybrid system has better performances in terms of energetic impact [kWh/(pass*km)] and emissions [gCO_2/(pass*km)]. The analysis has been made about the line segment on motorized wheels, as scientific literature already contained studies made about cable car sectors. Energy simulation has been carried on by considering different traffic scenarios and different cities (London, Dubai City, Torino and New Delhi), and it was shown that the request of energy to the net can be further reduced until 50% in Torino and until 70% in cities with particularly advantageous conditions weather by installing photovoltaic plant and an energy storage system through batteries. The above descripted analysis was published in the paper “Energy load analysis of a fully automated hybrid cable-driven public transport system: simulation with a photovoltaic system and storage” (Bazzolo S., Dalla Chiara B., Blengini S.) published in December 2019 issue of “Ingegneria Ferroviaria” (Scopus).

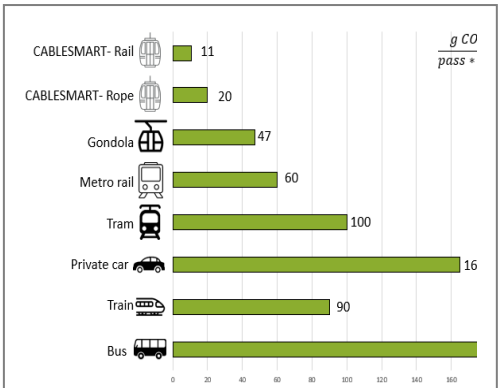


Figure 1 – Comparation among hybrid cable car- motorized wheels system and other transport system in terms of emissions [gCO_2(/pass·km)]

Moreover, the research activity has been focused in the pre-design of several installations of cable car-motorised wheel transport systems, with particular reference to the integration with the system in the urban context (strength of motorised wheel segments) and to the easy passing of natural and anthropic obstacles (strength of cable car segments). Pre-designs and designs were carried for Genova, Sorrento, Maiori and Courmayeur contexts. All the above-mentioned projects show that the hybrid system is able to answer to the needs of public urban transportation better than the conventional cable car in terms of energy impact, matching with the demand and integration in the urban context.

First name: Francesco M. **LAST NAME**: BELLUSSI

Topic: Heat and mass transfer phenomena at the soft matter interface for energy devices

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

Academic context

[1] Cardellini et al. “Integrated molecular dynamics and experimental approach to characterize low-free-energy perfluoro-decyl-acrylate (PFDA) coated silicon”. *Material & Design* 208 (2021) 109902.
[2] Bellussi et al. “Anisotropic Electrostatic Interactions in Coarse-Grained Water Models to Enhance Accuracy and Speed-up of Mesoscopic Simulations”. *J. Phys. Chem. B* 2021, 125, 43, 12020–12027
[3] Wang et al. "Design of robust superhydrophobic surfaces." *Nature* 582.7810 (2020): 55-59.

External collaborations

- Roma Tre University
- MaterialX
- Nanoforce / Queen Mary University

Highlights of the research activity

During the second year of the PhD, I focused the attention of my research activity on the development of a multiscale model for predicting the wettability properties of soft and hard surfaces. Such model ranges from the atomistic (AA) to the coarse grained (CG) and then to the continuum level. Specifically, I adopted classical molecular dynamics simulations to predict the contact angle of several polar and non-polar solvents, namely water, formamide, toluene and hexane, on polymer surfaces, namely perfluoro decanoic acid (PFDA) and polylactic-co-glycolic acid (PLGA). In the case of PFDA, we used a thermodynamic route to progressively tune the cross interaction between the solvent and surface, and thus compute the work of adhesion which is correlated to the contact angle via the Young-Dupré equation. In the case of PLGA, we reproduced the sessile droplet experiment, by allowing a drop of solvent to relax on the polymer surface. In this case, the contact angle was evaluated graphically from the simulated trajectory once the system reached its equilibrium in energy (see Figure 1 a). The obtained results were validated with experiments, showing good agreement, and highlighting the chemical and morphological contribution to the wettability properties.

With the aim of enhancing the accuracy and the speed-up factor of mesoscopic simulations, we developed a coarse grained (CG) model of water and polymers feasible for the prediction of the structural, thermodynamics and interface properties (see Figure 1 b). In such a model, the short-range interactions are accounted through the Gay-Berne potential, while electrostatic interactions are described by placing virtual charges within the CG ellipsoidal bead which describes grouped atoms. We initially validate the CG water model by evaluating some structural and thermodynamics properties under bulk and interfacial conditions. The results obtained were compared and validate with the reference AA models and with experimental evidence, showing excellent agreement and making the model as a good candidate for describing heat and mass transfer phenomena at the interface. As regards the polymer CG model, the work is still ongoing, as it requires an extension of the bonding interaction for ellipsoid and several modifications in the algorithms used in MD code (LAMMPS). Once the model will have been fully validated against AA models and experimental results, it will be employed to create nanopatterned surfaces to assess possible effects of the nano roughness.

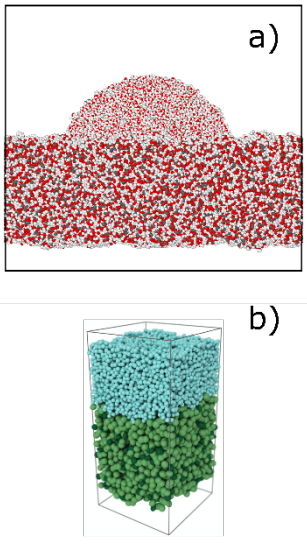


Figure 3 – a) Pictorial view of the droplet evolution onto the PLGA surface at the atomistic level. b) Pictorial view of the PLGA/water coupling at the CG level.

First name: Matteo **LAST NAME**: BILARDO

Topic: From Zero Energy to Zero Power Buildings

Course year: 2nd **Tutor(s)**: Enrico FABRIZIO

Academic context

[1] Bilardo, M.; Sandrone, F.; Zanzottera, G.; Fabrizio, E. Modelling a fifth-generation bidirectional low temperature district heating and cooling (5GDHC) network for nearly Zero Energy District (nZED). Energy Reports 2021, doi:10.1016/j.egyr.2021.04.054.
[2] Amato, A.; Bilardo, M.; Fabrizio, E.; Serra, V.; Spertino, F. Energy evaluation of a PV-based test facility for assessing future self-sufficient buildings. Energies 2021, 14, 329, doi:10.3390/en14020329.
[3] Ferrara, M.; Della Santa, F.; Bilardo, M.; De Gregorio, A.; Mastropietro, A.; Fugacci, U.; Vaccarino, F.; Fabrizio, E. Design optimization of renewable energy systems for NZEBs based on deep residual learning. Renew. Energy 2021, 176, 590–605, doi:10.1016/j.renene.2021.05.044.

External collaborations

- SmartData@Polito, Department of Mathematical Sciences (DISMA), Politecnico di Torino
- COESA srl, Corso Francia 30, Torino, Italy
- Department of Agricultural, Forest and Food Sciences (DISAFA), Università degli Studi di Torino

Highlights of the research activity

The aim of the research activity is to study energy utilization and generation within the built environment by focusing on short time intervals. In this research scenario, the final objective is to explore the future transition from the most well-known and globally recognized nearly Zero Energy Building (nZEB) to a so-called nearly Zero Power Building (nZPB). The detailed analysis on short time intervals, ideally tending to zero, is therefore necessary to address this research. To better engage this topic, the research activity carried out so far has concentrated on different levels of detail.
The first result of this research was focused on the scale of the single device, analyzing the performance of an Integral Collector Storage (ICS) prototype for the production of domestic hot water (DHW) of a single family building. Moving on a larger scale, a further research task focused on the energy performance analysis of a solar cooling system designed to meet the cooling demand of a multi-family builing. This research activity initially made it possible to develop a dynamic model of the HVAC system to optimize its design. Afterwards, this work found a collaboration with the SmartData @ Polito research group with the aim of exploring how neural network might support the optimization process of such renewable systems.
To continue the analysis path on an even larger level of detail, a new line of research focused on entire districts, exploring the benefit of new generation district heating and cooling networks. The development of this new study aims to extend the concept of nearly zero energy/power buildings no longer in the perspective of the single building, but rather within a larger scenario where the energy exchange and interaction between more facilities becomes essential. The results of this work led to the generation of a dynamic network model of buildings whose heating and cooling needs are met by decentralized heat pumps, using a shared water loop as heat source. After analyzing different levels of detail in terms of energy use and energy efficiency, the new advances in this research topic are shifting the focus to the concept of primary energy. In this regard, the latest work under development aims to determine primary energy factors adaptable to the dynamic simulations performed. This step is in fact necessary to reach a Zero Power building target, freed form from the current use of constant primary energy factors.

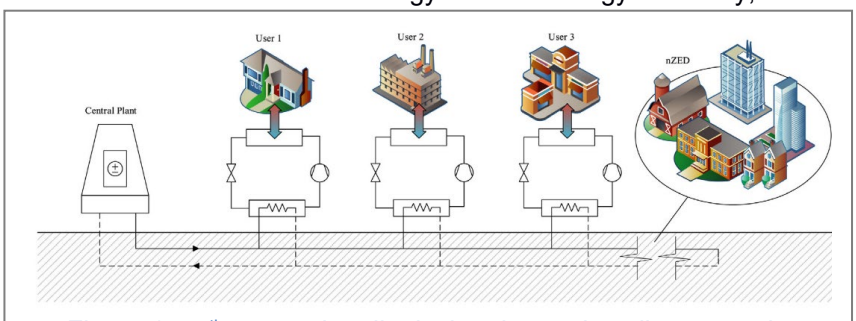


Figure 1 – 5th generation district heating and cooling network.

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

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

Course year: 1st **Tutor(s)**: Roberto ZANINO, Sandra DULLA

Academic context

[1] Leppänen, J. 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] Pantelias Garcés, M. 2013. "Activation Neutronics for the Swiss Nuclear Power Plants" Diss. ETH No. 21623
[3] Phlippen, P. W. et al. 2018. Numeric determination and validation of neutron-induced radioactive nuclideinventories for decommissioning and dismantling of light water reactors. *Nuclear Technology*, *201*(1), 66–79.

External collaborations

- Sogin

Highlights of the research activity

In the first part of the year the research activity has been focused on completing the work assigned by Sogin in the frame of a previous research project, therefore I mainly worked on the topic of cutting techniques applied to nuclear decommissioning activities. Afterwards, I focused on the development of a Serpent 2-based Monte Carlo model of the reactor of the Enrico Fermi nuclear power plant, located in Trino (VC). Sogin provided the data used for this activity, including drawings of the reactor geometry and details on the fuel composition of each operating cycle. The main goal of this activity is to evaluate the neutron flux in the structural components of the reactor and to use these data to calculate the residual activation in the material due to neutron irradiation by the means of a separate, dedicated activation model based on FISPACT II. Variance reduction techniques have been used in order to reach a reasonably good statistics in some areas far away from the neutron source due to the presence of thick layers of shielding materials, mainly water and steel. Two sets of experimental activation data were provided by Sogin and are currently being used to validate the model results. These two sets come from two separate sampling campaigns carried out in 1969 and in 1992 on the thermal shield, a component that was removed from the reactor at the end of the first operating cycle. Eventually, the long-term aim of the project is to expand current knowledge on the radiological status of the reactor and to support Sogin in the definition of a segmentation plan of the reactor vessel and internals, which will have to be dismantled as part of the ongoing efforts to decommission all the remaining nuclear related facilities in Italy. A more detailed map of the residual activity would be useful to determine which regions of the system are not activated and can therefore be cut and disposed as regular industrial waste, and which regions have to be treated as radioactive material. A precise characterization of the reactor vessel and internals would help in the selection of the right amount of waste containers to be used.

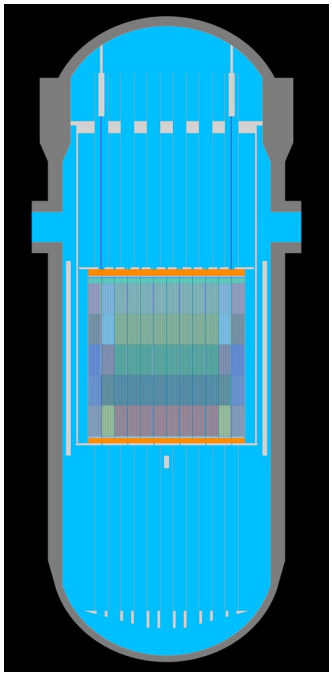


Figure 1 – Monte Carlo model of reactor of the Enrico Fermi NPP (Trino, VC)

First name: Silvio **LAST NAME**: BRANDI

Topic: Adaptive control strategies for improving energy flexibility in buildings

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

Academic context

[1] Brandi S, Piscitelli MS, Martellacci M, Capozzoli A, Deep reinforcement learning to optimise indoor temperature control and heating energy consumption in buildings, Energy and Buildings (2020) 224 https://doi.org/10.1016/j.enbuild.2020.110225.
[2] Vàzquez-Canteli J., Nagy Z. Reinforcement learning for demand response: A review of algorithms and modeling techniques. Elsevier, Applied Energy (2019) 235:1072-1089 https://doi.org/10.1016/j.apenergy.2018.11.002
[3] Wang Z., Hong T., Reinforcement learning for building controls: The opportunities and challenges, Elsevier, Applied Energy (2020) 269:115036 https://doi.org/10.1016/j.apenergy.2020.115036.

External collaborations

- Enerbrain s.r.l.
- University of Texas at Austin
- EMPA

Highlights of the research activity

Adaptive and predictive optimal control provides powerful opportunities for leveraging building properties (e.g. thermal mass, storage, renewable energy sources) to enhance energy flexibility during operation. Deep Reinforcement Learning (DRL) is a model-free control technique which does not require a model of system dynamics, rather, an agent learns an optimal control policy from past interactions with an environment through a trial-and-error approach. In order to test the capabilities of this control strategy an integrated simulation environment combining EnergyPlus and Python was developed. This tool allows the user to simulate the effect of innovative controllers on the building system overcoming EnergyPlus limitations in implementing advanced control logics. During the PhD, the environment was employed to benchmark DRL with traditional approaches such as rule-based controllers and model-based solution like Model Predictive Control (MPC). During 2021 the impact of DRL-based control strategies was analyzed for the management of integrated-energy systems in buildings. In particular, the performance of a DRL strategy coupled with a Rule-Based Control (RBC) were analyzed against a fully RBC to manage the operation of a chiller system coupled with a cold-water storage tank for an office building with on-site electricity generation and battery system. The aim of the controller was to minimize the electricity cost of the chiller and circulation pump by managing the cooling operation modes of the system. The proposed controlled proved to be capable to learn better control policy compared to baseline given the same storage capacities reducing the operating cost between 39.5% and 84.3% while improving on-site PV utilization (average increasing of Self-Sufficiency and Self-Consumption indices of 40%). The reason might be that baseline strategy employed two distinctive controllers for both BESS and TES. The baseline RBC controllers were responsible only for their relative system and did not share information between each other. The analysis carried out during the PhD aims at characterizing the applicability of DRL as an effective control technique for the management of HVAC systems in buildings. The results obtained highlighted strengths and weaknesses of this approach paving the way for future researchers and practitioners through the definition of robust guidelines and innovative methodologies.

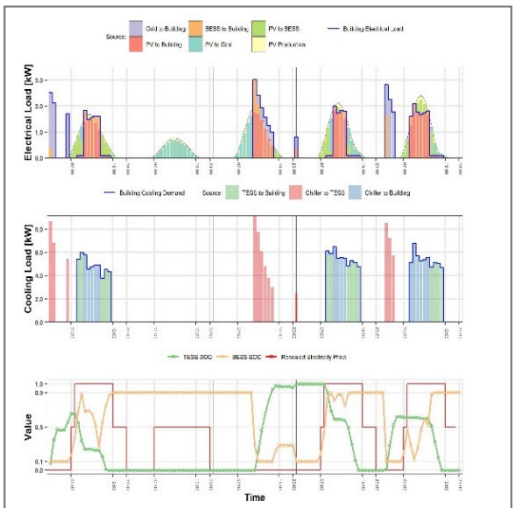
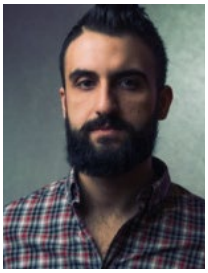


Figure 1 – Control performance of DRL strategy



First name: Luigi **LAST NAME**: CANDIDO

Topic: Lithium-lead and Tritium Technologies

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

Academic context

[1] L. Candido, et al., *HyPer-QuarCh II: A laboratory-scale device for hydrogen isotopes permeation experiments*, Fusion Engineering and Design, Volume 172, 112920, 2021.
[2] L. Candido, C. Alberghi, *Verification and validation of mHIT code over TMAP for hydrogen isotopes transport studies in fusion-relevant environments*, Fusion Engineering and Design, Volume 172, 112740, 2021.
[3] A. Aiello, et al., Determination of hydrogen solubility in lead lithium using sole device, Fusion Engineering and Design, Volume 81, 639-644, 2006

External collaborations

- ENEA C. R. Brasimone
- CEA Cadarache
- ITER Organization

Highlights of the research activity

In a liquid-metal breeding blanket of a nuclear fusion reactor, the knowledge of the Sieverts' constant, which expresses the proportionality between tritium concentration in the LiPb and the square root of its partial pressure, is mandatory in order to correctly predict tritium inventories in the LiPb, retention in the structural materials and permeation towards the environments. At ENEA C. R. Brasimone, we developed a new experimental laboratory-scale device, named Hyper-Quarch II (Hydrogen Permeation Quartz Chamber). This device is characterised by an upgraded test section in quartz and new instrumentation equipment, and has been adopted to allow the measurement of the Sieverts' constant of hydrogen solubilised in the LiPb in a temperature range from 300 to 550 °C and pressure range 0.1 to 100 hPa. Despite several experiments carried out in the past, the Sieverts' constant is characterised by significant discrepancies of up to several orders of magnitude, depending on the different methodologies adopted for its determination. With the *absorption technique*, the measure of Sieverts' constant is more than two orders of magnitude higher than with the *desorption technique*. This remarkable discrepancy may be due to some inaccuracies during the tests. One of the main objectives of HyPer-QuarCh II is to measure the same value with both absorption and desorption techniques. In the absorption tests, after the system is evacuated, the hydrogen is injected until the required pressure is reached. Then, the chamber is isolated and the hydrogen begins to be solubilized in the LiPb until equilibrium between the pressures of the gas phase and the liquid phase is reached. On the other hand, the desorption tests start from the equilibrium condition of the hydrogen partial pressure between the LiPb and cover gas, followed by a rapid pumping down of the cover gas. In 2021, the first experimental results were obtained. The incongruency of some literature measurements (see Reiter, Fauvet and Feuerstein in the picture) was found in the incorrect assumption that the pressure gradient of the desorbed isotopologues can be neglected in the first instants of the transient, whereas it is extremely high. As it can be seen, the obtained values for this work are in the range of the absorption techniques even for the desorption tests performed.

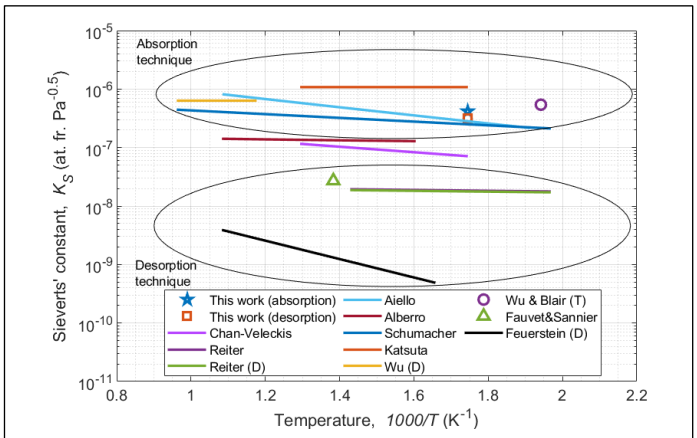
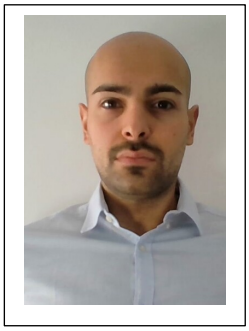


Figure 1 – Sieverts' constant of actual experimental campaign and literature.



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

Topic: Carbon Capture Utilization and Storage (CCUS)

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

Academic context

[1] G. Latini, M. et al., Unraveling the CO_2 reaction mechanism in bio-based amino-acid ionic liquids by operando ATR-IR spectroscopy, Catalysis Today, 2019, https://doi.org/10.1016/j.cattod.2018.12.050.
[2] Cannone S., Lanzini A., Santarelli M., A Review on CO_2 capture technologies with focus on CO2-enhanced methane recovery from hydrates, Energies 2021, 14, 387. https://doi.org/10.3390/en14020387
[3] Zhao Z., et al Redox Kinetics Study of Fuel Reduced Ceria for Chemical-Looping Water Splitting, J. Phys. Chem, 2016, 10.1021/acs.jpcc.6b01847

External collaborations

- Istituto Italiano di Tecnologia (IIT)
- Università di Udine
- Massachusetts Institute of Technology (MIT)

Highlights of the research activity

The proposed PhD research project aims at making scientific advances by means of test rigs located in the CO_2 Circle Lab (Environment Park) on: (a) CO_2 capture with ionic liquid, (b) CO_2 capture based on membrane separation process and (c) CO_2 valorization via chemical looping to produce renewable fuels.

CO_2 capture with ionic liquid (IL): A common test bench consisting of 2 columns i.e., an absorber and a stripper, was used to test an innovative solution based on 12.5% of [Cho] [Pro] diluted in DMSO and synthetized by IIT [1]. A loading capacity equal to 0.7 mol of CO_2/mol of IL was evaluated. This value exceeds the limit of the state of the art equal to 0.5 mol of CO_2 per mol of MEA. In the stripper column was observed that the solution can be completely regenerated at 80°C, well below the 120°C required by MEA.

CO_2 capture with membrane technology: The research activity is performed within the framework of an Italian project entitled "Methane recovery and carbon dioxide sequestration in methane hydrate reservoirs" (PRIN2017). A first preliminary work focused on techno-economic analysis of a CO_2 capture with membrane from a CO_2 emitted point and its transportation to a geological sequestration site consisting of clathrate hydrates to store the CO2 and produce methane was performed. The analysis found a cost between 50 and 60 \$/tCO_2 respectively at 50 and 500 km between source and storage site[2].

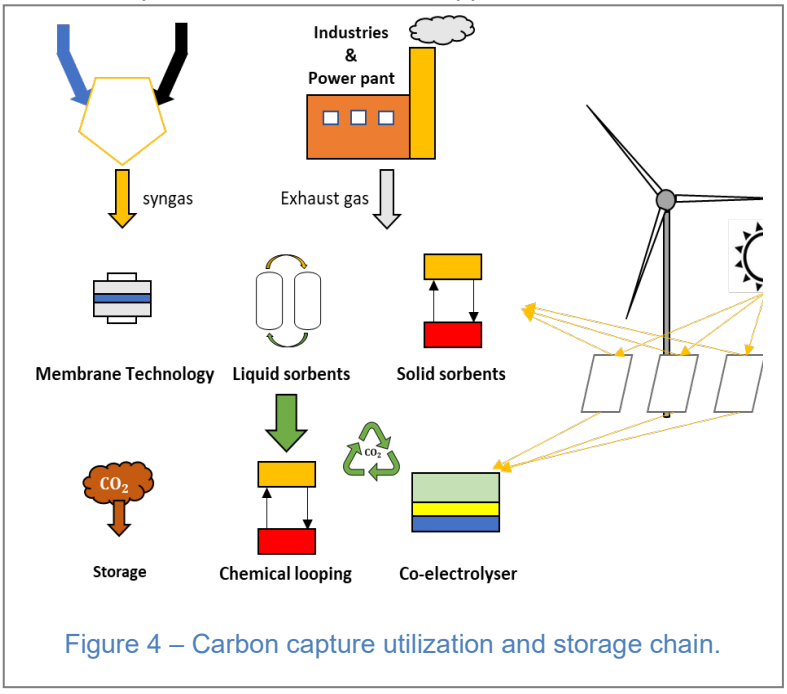


Figure 4 – Carbon capture utilization and storage chain.

CO_2 valorization via chemical looping: The performance feasibility of the chemical looping processes for syngas production using a new perovskite-based oxygen carrier (SFNM-04) for the conversion of the captured CO_2 to CO is under development taking advantage of the collaboration with Università di Udine and MIT.

First name: Martina **LAST NAME**: CAPONE

Topic: Boosting the evolution of district heating: Simulation models and optimization tools to unlock the transition of district heating towards fourth generation systems

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

Academic context

[1] H. Lund et al., "4th Generation District Heating (4GDH) - Integrating smart thermal grids into future sustainable energy systems", Energy 68 (2014) 1-11.
[2] M. Capone, E. Guelpa, V. Verda, "Optimal operation of district heating networks through demand response", International Journal of Thermodynamics 22, 25-43 (2019).
[3] M. Capone, E. Guelpa, V. Verda, "Multi-objective optimization of district energy systems with demand response", Energy 227, 120472 (2021).

External collaborations

- Iren S.p.A.
- University of Birmingham
- CEA (Commissariat à l'énergie atomique et aux énergies alternatives)

Highlights of the research activity

District Heating (DH) is a leading technology for the decarbonization of the European energy system. Lately, this technology is experiencing a gradual transition towards a new generation of systems, which are expected to be primarily based on renewable energy sources like solar, waste heat and geothermal energy. This have led to the conceptualization of the 4th generation district heating (4GDH) (Lund et al.) which is characterized by new features such as lower operating temperatures and lower grid losses, the possibility to recycle heat from low-temperature sources and to integrate renewable heat sources and the ability to be part of an integrated smart energy system. The aim of this PhD project is to develop suitable digital tools to unlock this transition, with special focus on the renovation of existing systems.

During the second year of PhD, the physical model used simulate the thermo-fluid dynamic behavior of the DH network was improved by introducing modifications to speed-up the simulation/optimization time. A key point was the rewriting of the integrated conservation equations as linear combination of pre-defined matrices. This allowed to significantly reduce the computational time for the simulation of small-scale DH networks. It also opened new research paths, e.g. the possibility of obtaining the temperature evolutions through the solution of the feasibility of a MILP optimization problem in the case of tree-shaped networks.

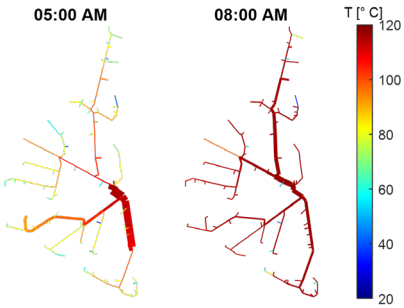


Figure 5 – Temperature distribution along a DH distribution network during the start-up transient.

In the framework of operation optimization, an effort has been paid to the improvement of the new management strategy aiming at disposing the colder water before the start-up phase (this invention was detailed in a patent application approved by the Patent Commission of PoliTo and filed); different methodologies to implement the invention have been simulated and tested. A further activity has concerned the improvement of the optimization tool developed last year and devoted to simultaneously optimize production and demand in district multi-energy systems. The original integrated optimization tool has been adapted to separately explore different sources of flexibility: the smart management of the production units, the possibility of installing a thermal storage, and the flexibility of the heating load of the customers (thermal demand side management).

Finally, some analyses on the potentials for supply temperature reductions have been successfully performed.

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

Topic: Multi-scale modeling of advanced colloid for energy applications

Course year: 1st **Tutor(s)**: Pietro ASINARI and Eliodoro CHIAVAZZO

Academic context

[1] P. de Angelis, A. Cardellini, P. Asinari, “Exploring the Free Energy Landscape To Predict the Surfactant Adsorption Isotherm at the Nanoparticle−Water Interface”, ACS central science (2019)
[2] Aiping Wang et al., “Review on modeling of the anode solid electrolyte interphase (SEI) for lithium-ion batteries”, Journal of Computational Materials (2018)
[3] Zeeshan Ahmad et al., “Interfaces in Solid Electrolyte Interphase: Implications for Lithium-Ion Batteries”, Journal of Physical Chemistry (2021)

External collaborations

- INRiM, Istituto Nazionale di Ricerca Metrologica (https://www.inrim.it/)

Highlights of the research activity

This PhD research activity involve the development of new computational approaches to describe suspensions of different nanoparticles in liquids to be used for the preparation of advaced functional materials for energy applications. During the first year of the PhD I focused the attention on the following relevant themes: 1) the evalution of phenomena at the gold nanoparticles interface in an aqueous solution; 2) the study of transport properties at the interface in colloids for electrochemical storage applications.

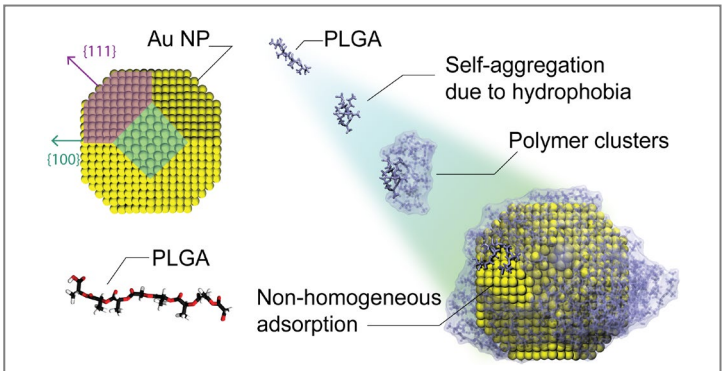


Figure 1 – Assembling biocompatible polymers on gold nanoparticles.

Regarding the first topic, gold nanopaticles have received great attention in a number of fields ranging from the energy sector up to biomedical applications. As far as the latter, it is crucial to improve and optimize the encapsulation in a biocompatible and biogradable matrix, such as polymeric poly(lactic-co-glycolic acid) (PLGA). Therefore, I combined a number of computational approaches to explore the adsorption mechanisms of PLGA polymers on a gold crystallina nanoparticles and to rationalize the PLGA coating process towards a more efficient design of the nanoparticle shape. In detail, I performed atomistic simulations supported by an unsupervised machine learning scheme by tuning the polymer concentration in solution to observe the time evolution of the PLGA self-assembly phenomenon. Then I conducted a detailed surface coverage analysis that coupled with free energy landscape calculations shed lights on the anisotropic nature of PLGA adsorption onto gold nanoparticle.
As regards the second topic, it was necessary to start with an intensive literature review activity. The problem of energy storage is a topic of great intrest, and electrochemical batteries are a rapidly growing technology. The existence of passivating layers at the interfaces affects the durability, performance, and safety of batteries. A critical passivations layer is the Solid Electrolyte Interface (SEI) which consists of a multilayer and heterogeneous structure caused by the decomposition of the electrolyte at the interface with the anode. Modeling the SEI is a challenge that has not yet been overcome due to the SEI’s chemical and structure complexity and the mechanisms involved (like elctrolyte reduction, elctron transfer, Li-ion diffusion) that occur at different lenghts and time scales. Currently, in my research activity I use atomistic simulation to understand and determine the lithium diffusion coefficient between the common components of SEI, namely lithium fluoride (LiF) and lithium carbonate (Li_2CO_3).

First name: Alessandro **LAST NAME**: COLANGELO

Topic: Thermal Energy Storage Technologies

Course year: 2nd **Tutor(s)**: Vittorio VERDA, Andrea LANZINI

Academic context

[1] Y. Dutil et al., A review on phase-change materials: Mathematical modeling and simulations, Renewable and Sustainable Energy Reviews, https://doi.org/10.1016/j.rser.2010.06.011
[2] T. Xu et al., Numerical thermal performance investigation of a latent heat storage prototype toward effective, use in residential heating systems, Applied Energy, https://doi.org/10.1016/j.apenergy.2020.115631
[3] F. Colella et al., Numerical analysis of a medium scale latent energy storage unit for district heating systems, Energy, https://doi.org/10.1016/j.energy.2012.03.043

External collaborations

- RE-COGNITION consortium (https://re-cognition-project.eu/)
- i-TES SRL (https://www.i-tes.eu/?lang=it)

Highlights of the research activity

The research activity is developed within the framework of the European project RE-COGNITION, which aims at an optimal integration of multiple storage and energy sources at the building scale through information and IoT technologies. More specifically, this research activity is centered on a shell-and-tube Latent Heat Thermal Storage (LHTS) filled with a medium/high-temperature Phase Change Material (PCM). Two main objectives are pursued: 1) development of two full-scale LHTS prototypes with two different types of fins; 2) development of a fast and reliable dynamic model able to simulate various LHTS operating conditions in order to optimally coordinate its operations within a multi-energy system. The model results will be tested and calibrated in the experimental facility available at the Energy Center.

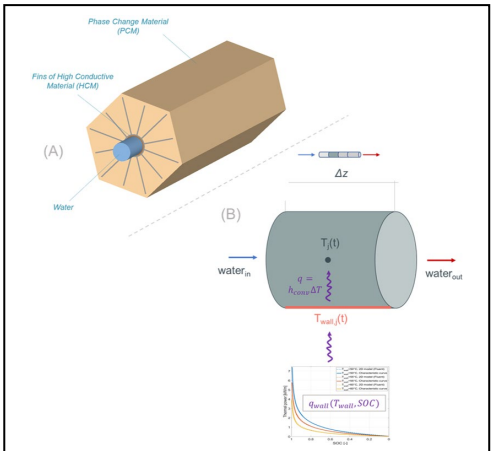


Figure 1 – (A): LHTS elementary unit; (B): LHTS reduced dynamic model.

The aforementioned goals address two main research gaps in this field. On the one hand, few real examples of multi-tube LHTS systems are reported in literature. On the other hand, a limited number of studies proposes models able to analyze the operational phase of LHTSs. In addition, these models often rely on empirical parameters to be adjusted using experimental results. Hence, a simple dynamic model entirely based on physical quantities was developed in this second year considering the LHTS prototype characterized by pipes with longitudinal fins as a reference. From a system perspective, the dynamic behavior of a thermal storage can be quantified through the temporal evolution of the temperature at which hot water is produced during the storage discharge. On the contrary, the mass flow rate circulating in the heating system and the inlet temperature towards the storage are known variables. In this context, a detailed representation of the heat transfer mechanisms inside the PCM are not necessary. Therefore, the following modelling approach was adopted. The domain of the heat transfer fluid (HTF) was decoupled from the domain of the PCM-fins assembly. The flow of the HTF was then modelled as 1D pure advection problem with a heat source term. This source coincides with the thermal power released by the PCM-fins assembly and it is evaluated through an analytical function based only on physical quantities: the equilibrium temperature at the pipe wall and the current and initial storage states of charge. The 1D pure advection problem is solved numerically relying on a finite volume discretization. Results show that this modelling approach allows to simulate the behavior of the LHTS from a system perspective with great accuracy if compared to a full 3D model, but the computational time is remarkably reduced. Validation also against experimental outcomes will be performed in the upcoming months.

First name: Alessandro **LAST NAME**: CORVAGLIA

Topic: Advanced modelling of lubricated gaps in positive displacement machines

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

Academic context

[1] Stefan Gels & Hubertus Murrenhoff (2010) Simulation of the Lubricating Film between Contoured Piston and Cylinder, International Journal of Fluid Power, 11(2), 15-24, DOI: 10.1080/14399776.2010.10781003
[2] Matteo Pelosi & Monika Ivantysynova (2012) A Geometric Multigrid Solver for the Piston–Cylinder Interface of Axial Piston Machines, Tribology Transactions, 55(2), 163-174, DOI: 10.1080/10402004.2011.639049
[3] Lars Olems (2000) Investigations of the Temperature Behaviour of the Piston Cylinder Assembly in Axial Piston Pumps, International Journal of Fluid Power, 1(1), 27-39, DOI: 10.1080/14399776.2000.10781080

External collaborations

- Casappa S.p.A.

Highlights of the research activity

In axial piston pumps, the correct design of lubricated interfaces is, timelier than ever, essential to reduce energy waste.
Considering the overall power loss by these interfaces, the piston-cylinder block mate is not the most impactful but is, by far, the most challenging to design.
The reciprocating motion of the piston and the cycling pressure in the displacement chambers generate a variable hydrostatic and hydrodynamic imbalance.
In the third year of my PhD, I focused on the dynamic resolution of this imbalance through the concept of micro-motion introduced by Ivantysynova [1999].
The idea is that the assembly gets balanced by micro-movements (order of microns) of the piston inside his bushing, which generates a pressure build-up because of the squeeze effect.
The solution of the piston's dynamics has been achieved by the Newton-Raphson iteration method, which evaluates at each time step the value of the velocity along x and y on the two edges of the gaps and updates the position for the next time step.
A particular focus has been paid on the convergence of the dynamic results in terms of the choice of: fulcrum, derivative scheme and velocity variation value for the Jacobian matrix, time step and mesh refinement.
Furthermore, to develop a simulation model up to date, the Reynolds Equation (introduced in the model during the 1st year of the PhD) has been modified with the Average Reynolds Equation. This version of the Reynolds Equation also considers some correction factors for thin gaps and one additional term for the flow rate carried by the asperity peaks.
During the first tests, aimed at evaluating the capabilities of the model, the necessity to introduce a contact/mixed lubrication module to achieve stationary results has emerged, even if the contact between bodies occurs. The model developed is fully parametric and can estimate the leakage flow rate, the friction forces and the trajectory of the piston during a full revolution. Moreover, it is possible to estimate the contact regions and the percentage of contact area if there is not a sufficient level of lubrication on the interface.

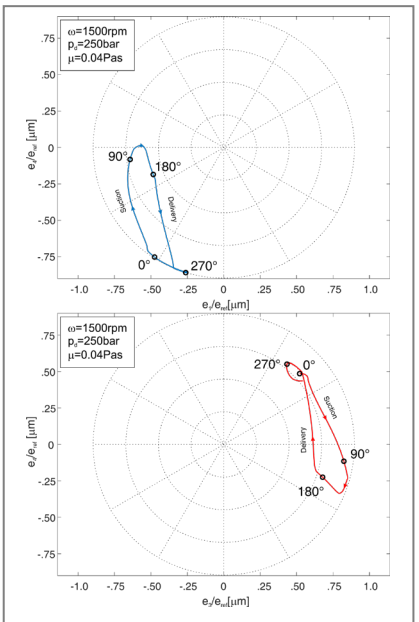


Figure 1 – Piston motion at slipper side (up) and valve plate side (down)

First name: Paolo **LAST NAME**: DE ANGELIS

Topic: Lithium-Ion Batteries (LIBs) multi-scale Modelling

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

Academic context

[1] De Angelis, P., Cardellini, A., & Asinari, P. (2019). Exploring the Free Energy Landscape To Predict the Surfactant Adsorption Isotherm at the Nanoparticle–Water Interface. *ACS central science*, *5*(11), 1804, 2019

[2] De Angelis, P., et al. (2021). Data-driven appraisal of renewable energy potentials for sustainable freshwater production in Africa. *Renewable and Sustainable Energy Reviews*, *149*, 111414, 2021.

[3] K.-S. Yun, S. J. Pai, B. C. Yeo, K.-R. Lee, S.-J. Kim, and S. S. Han, "Simulation Protocol for Prediction of a Solid-Electrolyte Interphase on the Silicon-based Anodes of a Lithium-Ion Battery: ReaxFF Reactive Force Field," *J. Phys. Chem. Lett.*, vol. 8, no. 13, pp. 2812–2818, 2017.

External collaborations

- Mashayek F. and Yurkiv V. – University of Illinois at Chicago (UIC)

Highlights of the research activity

My research focuses on the study and understanding of Solid Electrolyte Interphase (SEI) degradation phenomena in Lithium-Ion Batteries (LIBs). SEI results from the degradation and deposition of organic solvents. However, uncontrolled SEI growth causes an undesirable and irreversible decrease in capacity, self-heating of the battery, and, in the worst case, thermal runaway and explosion. The highly reactive nature of SEI and the complexity of *in situ* techniques make the experimental observation of such phenomena very challenging. For this reason, we are developing a more theoretical approach. We propose a novel protocol to reconstruct the morphology of the polycrystalline layer of SEI with atomic resolution. In our approach, we combine Reactive Force Field MD - ReaxFF simulations with an in-house routine for statistical generation and placement in the computational box of different SEI crystalline grains. A consistent computational protocol was developed to impose the appropriate bulk density, allow grain boundary formation and the "welding" of the anode. After generating the SEI and SEI+Anode structures, we perform an advanced sampling simulation campaign to extract the Free Energy Landscape (FEL) and lithium transport properties. In addition, our protocol is interactively wrapped and managed with the user-friendly and easy-to-use interface of Jupyter Notebooks. Thanks to python libraries and our in-house codes, we achieved a flexible simulation environment where the user can apply major changes to the studied system with minimal effort.In conclusion, with this protocol, we aim to pave the way for a new computational platform that will enable an *in silico* experimental campaign to shed light on the mechanism of SEI formation.

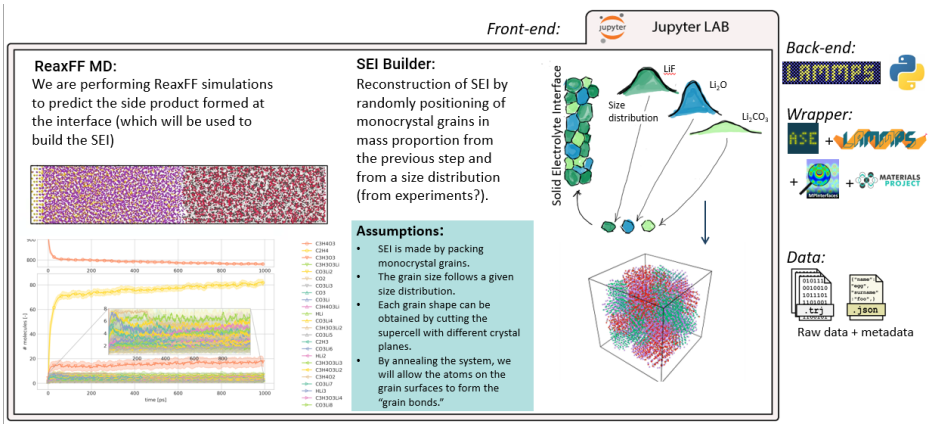


Figure 6 – Representation of the multiscale model wrapped in the user-friendly interface Jupyter Notebook.

First name: Giovanna **LAST NAME**: DE LUCA

Topic: Advanced models for the building energy performance assessment

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

Academic context

[1] van Dijk, D. EN ISO 52016-1: The new international standard to calculate building energy needs for heating and cooling, internal temperatures and heating and cooling loads. In Proceedings of Building Simulation 2019: 16th Conference of IBPSA (ISBN: 978-1-7750520-1-2). 1-4 September 2019, Rome.
[2] Crawley, D. B.; Hand, J. W.; Kummert, M.; Griffith, B. T. Contrasting the capabilities of building energy performance simulation programs. Building and Environment 2008, 43, 661-673.
[3] Bloomfield, D.P. An overview of validation methods for energy and environmental software. In ASHRAE Transactions: Symposia 1999, 105, 685–693.

External collaborations

- EdilClima Engineering & Software
- Agenzia nazionale per le nuove tecnologie, l'energia e lo sviluppo economico sostenibile (ENEA)

Highlights of the research activity

The issue of improving the energy performance of buildings has led to the rapid development of the calculation methods of energy performance (EP) assessment. Among the simplified dynamic methods, the EN ISO 52016-1 simplified hourly method (SHM) is aimed at providing a balanced accuracy and simplicity of the assessment. Whereas the application of the SHM for compliance checking with energy regulations is considered, the assessment of its accuracy and modelling assumptions is of foremost importance. Within this context, the Ph.D. research proposes an “aware” validation approach, aimed at detecting the existing modelling assumptions assumed in different calculation methods of the building EP assessment, and highlighting the expected accuracy and limitations of the SHM for different applications. Firstly, a “comparison map” was created to catalogue and compare the existing algorithms and assumptions (from research papers, and building energy simulation tools) relative to different thermal phenomena, with a specific focus on the SHM. The heat conduction through the opaque envelope, the phenomena involved in the interaction between the outdoor environment and the envelope external surfaces, and between the indoor environment and the indoor surfaces, and the solar transmission through windows, were deepened. Secondly, a single-process validation methodology was introduced, consisting in a parametric analysis, in which the SHM simplifications are tested one-at-a-time; their effect is evaluated in the prediction of the annual energy needs and hourly thermal loads/internal temperatures. The proposed methodology was applied to different case studies, considering both building archetypes and real buildings (whose energy models were calibrated against monitored data). The results of the performed analyses – reported in the attached figure for office and residential building types – show how different assumptions may be suitable for different applications. For example, the SHM simplifications on the external convection heat transfer may be applied for new buildings, while it should be preferable the use of more accurate calculation models for the existing buildings. In conclusion, the importance of a detailed knowledge of the theory behind the different heat transfer processes showed to have a key role both for the detection of inaccuracies in a calculation model, and for its possible implementations, which can be correctly addressed only after the definition of the application purpose.

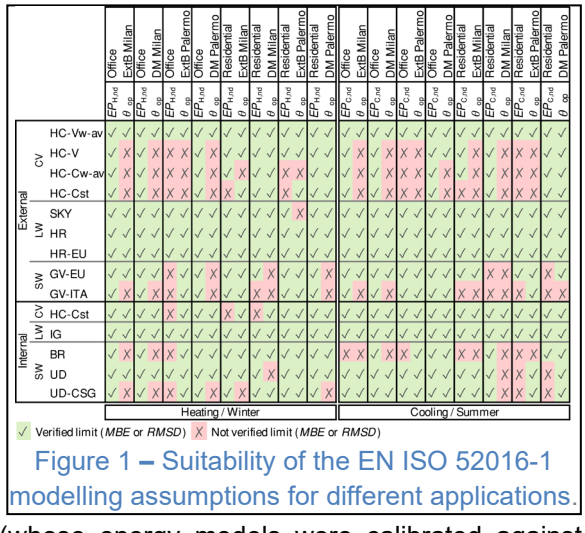
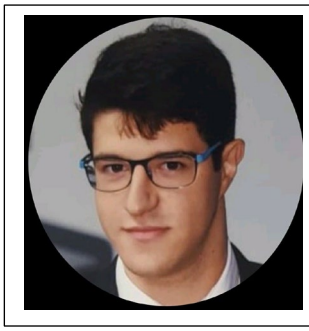


Figure 1 – Suitability of the EN ISO 52016-1 modelling assumptions for different applications.



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

Topic: Development and assessment of an innovative controller for the integrated optimization of the engine performance and of the energy flows in heavy-duty diesel hybrid electric vehicles.

Course year: 2nd **Tutor(s)**: Roberto FINESSO, Ezio SPESSA

Academic context

[1] David D., Randall et al. "Selective Catalytic Reduction". *Research Triangle Park, NC 27709* (2019): Chapter 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

During my first year, I worked in GT-suite and Matlab Simulink environments to realize the preliminary development of integrated dynamic vehicle/engine models, capable of predicting emissions and fuel consumption in transient operation.

More in detail, a longitudinal dynamic model of an IVECO Daily was developed in both Simulink and GT-suite platforms, and was integrated with a fast-running GT-power model of an FPT F1C EURO VI diesel engine. Moreover, a 1D quasi-static SCR thermal and chemical model has also been implemented. The developed simulation platform is currently under validation, on the basis of the available data.

The use of a detailed engine model makes it possible to implement and assess model-based engine control algorithms, which can be used to optimize the ICE performance and emissions in real-time by adjusting the main engine calibration parameters. In the future, the advantages obtained from the hybridization of the powertrain will also be investigated. Therefore, several hybrid architectures will be implemented, and a vehicle Energy Management System will be developed and integrated, with the aim of optimizing the vehicle energy flows, through Model-in-the-loop techniques. In the future, also the DOC and the DPF systems will be implemented in the model, compatibly with the availability of the geometric and testing data.

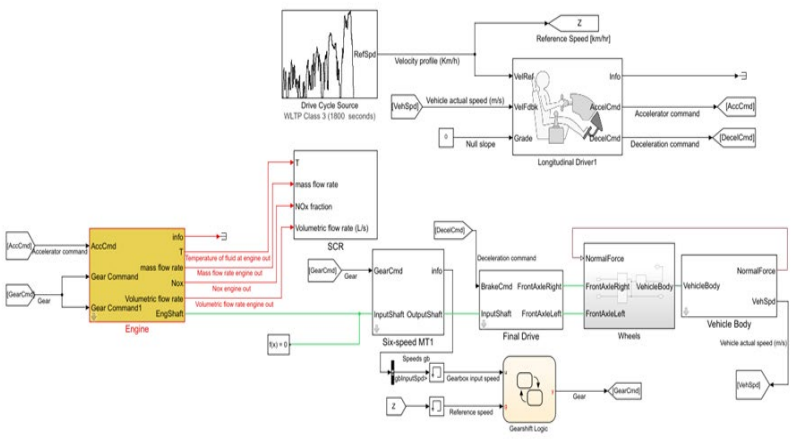


Figure 1 – A dynamic heavy-duty vehicle model, realized in the Simulink environment, is presented in the figure. A vehicle driver is also included, which is used to realize the desired vehicle mission. The yellow block is used to couple the vehicle model with the engine model developed in GT-power environment.

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

Topic: Development of a methodology for the shape optimization in high heat flux components, with application to gyrotron resonators

Course year: 1st **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] Dan Simon, "Biogegrahy-Based Optimization", IEEE Trans. Evol. Comput., vol 12, no 16, December 2008.
[3] Giles, M; Pierce, N. An introduction to the Adjoint Approach to Design Flow, Turbulence and Combustion, 2000, 65, 393-415.

External collaborations

- Karlsruhe institute for technology
- Max Planck Institute
- Thales AVS France

Highlights of the research activity

The activity carried out during this first year can be subdivided in two macro areas:
1) the development and validation of the model to simulate the performances of the new design of the cavity cooling system, based on mini-channels;
2) the study and literature research on the existing optimization algorithm and application of some of them to the case study of the cooling system of the Gyrotron cavity.

Concerning the model validation, hydraulic tests, on a mock-up equipped with mini-channels, performed in Thales AVS France allowed the choice of the better RANS model for the simulations, through a multivariate metric study. Moreover, calorimetry and thermal tests performed on another mock-up at KIT allowed to validate also the thermal part of the simulations.

To improve the heat management of cavities, to design greater RF efficiency tubes, different paths are being followed to design an optimized configuration of the mini-channels cooling system. The optimized solution should minimize the frequency shift of the radiofrequency wave, by controlling the displacements on the inner wall of the cavity, while respecting the yield strength limit. An optimization study on the cavity cooling has been developed with the aim of finding the optimal axial profile of the heat transfer coefficient (*h*) able to ensure the previous requests on displacements minimization and Yield strength constraint. A Biogeography Based Optimization algorithm has been adopted, coupled with thermo-mechanical simulations in STAR-CCM+, where the *h* profile is used for a convective boundary condition. Once the optimum *h* profile has been computed by the optimization algorithm, the second step of the work has been the attempt of reproducing the same profile implementing a cooling solution. A first solution has been designed in which the water flows through an anular section, in the axial direction. The external radius of the annulus varies along the axial direction in order to obtain the desired *h* at each point. The cooling performance of this solution has been then analysed via a CFD simulation. The results were very similar to the ones obtained with the thermo-mechanical model in terms of temperature, radial displacements and stress axial profile. The adjoint topology optimization method is also under study, applied to a cooling configuration characterized by azimuthal mini-channels.

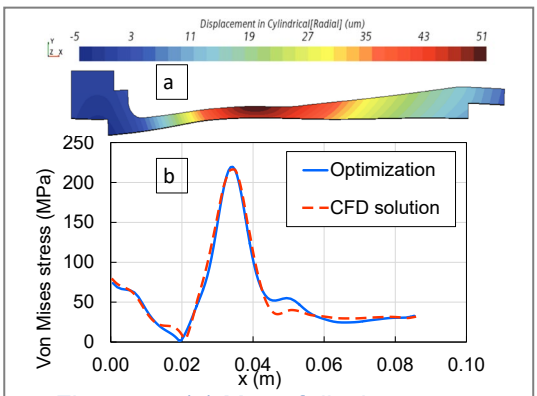


Figure 7 – (a) Map of displacements obtained after the optimization; (b) Comparison of optimization and CFD Stress profile on the resonator inner wall.

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

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

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

Academic context

[1] First Numerical Evaluation of the Thermal Performance of a Tubular Receiver Equipped with Raschig Rings for CSP Applications. ASME Power Conference 65714, V001T04A005. July 20–22, 2021Virtual, Online. Hossein Ebadi, Andrea Allio, Antonio Cammi, Laura Savoldi.
[2] Improving the overall thermal performance of parabolic trough solar collectors using porous media. Renewable Energy & Power Quality Journal 19, 571-576. Hossein Ebadi, Antonio Cammi, Laura Savoldi.
[3] Experimental and numerical investigation of a porous receiver equipped with Raschig Rings for CSP applications. Solar Energy 212 (3), 309-325. Laura Savoldi, Andrea Allio, Antonio Bonvento, Marco Cantone, Jesus Fernandez Reche.

External collaborations

- Politecnico di Milano (Italy)
- Plataforma Solar de Almeria

Highlights of the research activity

The main aim of the ongoing PhD project is to enhance the current technology of gaseous CSP absorbers using porous media. To this end, several numerical investigations were carried out using CFD codes through the implementation of commercial software Star CCM+ for simulating a solar absorber modified with Raschig Rings (RR) as the porous medium. Applying various thermal drivers helped to reveal the best working options for this design with respect to the current CSP technologies. Results showed that the inhomogeneity in the velocity field of the fluid can be attributed to the arbitrary orientation of rings where those positioned axial to the flow direction accelerate the flow through the inner holes, however, rings that are perpendicular to the flow line cause stagnation or recirculation of air. The dense structure of RR with porosity near 78%, has led to a much higher pressure drop compared to the smooth design. In terms of thermal performance, the RR presence improved the cooling effect by reducing the wall temperatures in the RR region. This difference was observed on the side of the tube where the heating is applied and nearly a 200 °C decrease was computed. The reason for such effect is attributed to the heat conduction that takes between the tube wall and RR matrix and this grows the heat transfer area to a greater extent. Thus, air could absorb a higher amount of heat passing through the heated rings and make the walls cooler. What is also evidenced in this research was the thermal mixing effect produced by the arbitrary structure of the RR. Sudden changes in the flow direction hinder the formation of thermal boundary layers and trigger turbulence and swirling flow inside the tube. As a result, when the air proceeded through the porous matrix, the azimuthal temperature difference decreased. As the next step, an equivalent porous model in macro-scale was devloped to reduce the computational cost and extend the CFD analyses for longer tube absorbers. Comaprisons showed a solid agreement between the obtained micro and macro values and this highlights the accuracy of the hydraulic and thermodynamic characteristics found in microscopic studies. The assessment of the thermal performance of the porous medium using both microscopic and macroscopic approaches demonstrated that the temperature profile of the macroscopic results is an averaged-volume representative of the fluid temperature in microscopic simulation. Future studies aim at optimization and experimental investigation of tubular receivers equipped with RR porous medium.

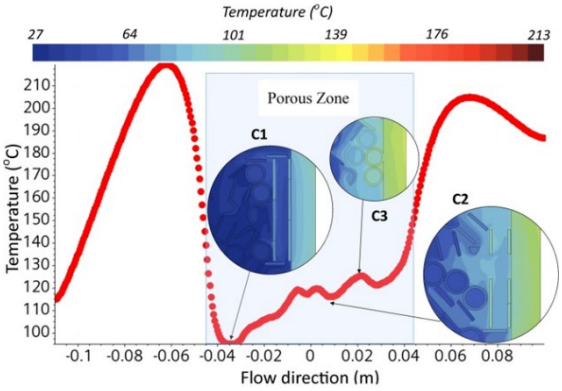
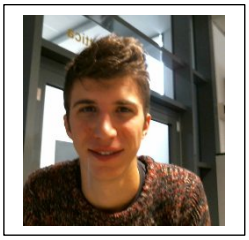


Figure 8 – Temperature distribution through the tubular solar absorber equipped with RR.



First name: Alessandro **LAST NAME**: FALAI

Topic: Li-Ion Battery Modeling and BMS Development in Electric Vehicle Application

Course year: 2nd **Tutor(s)**: Prof. Daniela MISUL, Ezio SPESSA

Academic context

[1] C. Zhang, W. Allafi, Q. Dinh, P. Ascencio, J. Marco “Online estimation of battery equivalent circuit model parameters and state of charge using decoupled least squares technique”, Elsevier, 2017, United Kingdom, doi: Energy 142 (2018) 678e688
[2] J, Lv, B, Jiang, X. Wang, Y. Liu, Y. Fu,“Estimation of the State of Charge of Lithium Batteries Based on Adaptive Unscented Kalman Filter Algorithm”, MDPI electronics, 2020, China.
[3] T. Bruen, J. Marco, M. Gama, “Model Based Design of Balancing Systems for Electric Vehicle Battery Packs”,Elsevier, United Kingdom, 2015, doi: IFAC-PapersOnLine 48-15 (2015) 395–402

External collaborations

- Danisi Engineering, Italy (IT)
- AddFor S.p.A., Italy (IT)
- AVL Italia, Italy (IT)

Highlights of the research activity

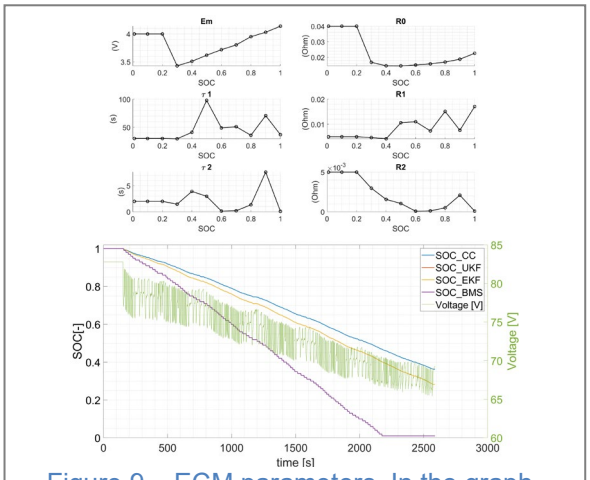


Figure 9 – ECM parameters. In the graph below, voltage response is reported with SOC trends for each estimation methods

My research activity is seeing the actual collaboration with Danisi Engeneering and AddFor and aims to model a homemade Li-Ion battery mounted on an electrid two-wheeler (motorscooter) and consequently developes the battery management system (BMS), including the most meaningful control logic in order to manage the battery. At the very beginning, an experimental tests drive were initially conducted where the electric scooter equipped with a 180 SAMSUNG INR21700-50E battery (20s9p configuration) have run a customized real driving mission. Thanks to acquired signals, second and third order equivalent circuit models (ECM) have been developed and validate over the data. Thus, the battey multiple model parameters are calculated through an optimization method based-parameter estimator which takes measured voltage signal as control variable, the current signal as input and a non-linear least squares objective function applied over measured and simulated voltage as minimization goal. The SOC is performed through the current integration over the mission and a model-based Kalman Filter method. Moreover, a two-wheeler vehicle model was developed according to forward modeling approach over selected driving missions and thanks to properly conducted coast-down tests. Finally, the models-coupled system is implemented and its performance is assessed linking the Li-Ion battery model to that of the vehicle.Thus, the development and assessment of electric vehicle model lays the groundwork of a BMS design and it provides a quick and cheap methodology for testing battery optimal control logics in Software-in-the-Loop environment. The development of Battery Management System unit is the key point to supervise the battery state of the electric vehicle in order to ensure safety and high performances. Since we are interested in developing a virtual envirommment where the Danisi simulators remotely interconnects with the battery bench theoretically presented at PoliTo, further tests have been conducted in order to test the communication from capture, transmission and processing packet of data point of views. Finally, the following tasks are computed: verification of UDP Protocol reliability on transmission data packages, battery model/simulator synchronism, network latency of comunication, bandwidth limitations. It has been verified that all previous indices are suitable for the present application.

First name: Gabriele **LAST NAME**: FALCIANI

Topic: Analysis and modelling of future emerging technologies for solar fuel generation

Course year: 2nd **Tutor(s)**: Eliodoro CHIAVAZZO

Academic context

[1] Falciani, Gabriele, et al. "A multi-scale perspective of gas transport through soap-film membranes." Molecular Systems Design & Engineering 5 (2020): 911-921.
[2] Gera, Rahul; Bakker, Huib; Franklin-Mergarejo, Ricardo; Morzan, Uriel; Falciani, Gabriele; Bergamasco, Luca; Versluis, Jan; Indraneel, Sen; Dante, Silvia; Chiavazzo, Eliodoro; Hassanali, Ali (2021) Emergence of Electric Fields at the Water-C12E6 Surfactant Interface, In: Journal of American Chemical Society, 15103-15112, 143, 37.
[3] Lewis, Nathan S. "Research opportunities to advance solar energy utilization." Science 351.6271 (2016).

External collaborations

- University of Cambridge
- International Center for Theoretical Physics - ICTP
- Teclis Scientific

Highlights of the research activity

The research activity focuses on a newly developed concept of photosynthetic soft membranes based on self-assembled functional molecules capable to convert solar energy and carbon dioxide (CO_2) directly into clean fuels within the FET OPEN H2020 project Sofia (www.sofiaproject.eu/)[1][2]. A multi-scale and multi-physics model intended to describe and predict the expected performance of a single soft photosynthetic membrane realized in the form of a soap film is proposed.

A soap film consists of two surfactant monolayers that stabilize a water core. In the case of a soap based photoreactor, these surfactants are engineered functional molecules that reduce CO_2 to CO while oxidizing water to oxygen under visible light irradiation (Fig. 1a). Studying the complete reaction envisioned in the Sofia project is a challenging task, due to the difficulties in coupling the two half reactions and the complex structure of soap films membrane. During my second year of PhD, I mainly focused on the modelling of the CO_2 reduction half reaction in monofilm photoreactors, where the photoactive amphiphilic molecules are at the interface between the solution and the CO_2 atmosphere (Fig. 1b).

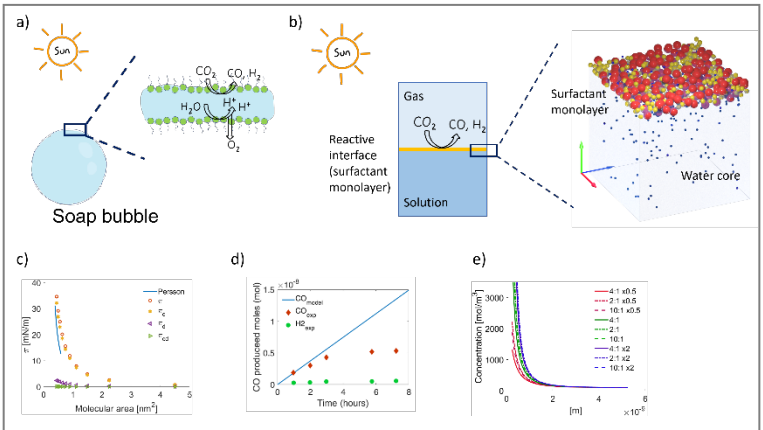


Figure 10 – a) Soap-based photoreactor. b) Monofilm-based photoreactor continuum model. Zoom in the reactive interface, self-assemble monolayer obtained from Monte Carlo simulation. b) validation of the Monte Carlo model c) Fuel production and comparison with experimental data. e) Electric double layer and charge distribution close to the reactive

A continuum macroscale model of the reactor, which accounts for the transport of species in the bulk and in gas phase, the adsorption/desorption of species and their reaction in the monolayer was developed. This model was then coupled with a mesoscale Monte Carlo code developed in house that describes how the photoactive amphiphilic molecules self-assemble at the interface. In this regard, I spent a six-month visiting period at University of Cambridge where the CO_2 reduction experiments are being performed. The experience acquired by studying monofilms photoreactors will be transferred to soap film based solar fuel production during my last year of PhD.

First name: Gabriele **LAST NAME**: FAMBRI

Topic: Energy storage and conversion technologies to improve renewable energy penetration

Course year: 3rd **Tutor**: Marco BADAMI

Academic context

[1] Badami M, Fambri G. Optimising energy flows and synergies between energy networks. Energy, 2019,173,400-412.
[2] Badami M, Fambri G, Mancò S, Martino M, Damousis IG, Agtzidis D, Tzovaras D. A Decision Support System Tool to Manage the Flexibility in Renewable Energy-Based Power Systems. Energies. 2019;13(1):153.
[3] Fambri G, Badami M, Tsagkrasoulis D, Katsiki V, Giannakis G, Papanikolaou A. Demand Flexibility Enabled by Virtual Energy Storage to Improve Renewable Energy Penetration. Energies. 2020; 13(19), 5128.

External collaborations

- VTT - Technical Research Centre of Finland, Espoo, (Finland)
- Hypertech Energy Labs, Hypertech, Chalandri (Greece)
- CERTH - Centre for Research and Technology Hellas, Thessaloniki (Greece)

Highlights of the research activity

The research activities carried out during the first, second and part of the third year of PhD was mainly performed in the framework of the EU H2020 project PLANET (Planning and operational tools for optimising energy flows & synergies between energy networks). PLANET developed a holistic Decision Support System (DSS) for the analysis of multi-energy system scenarios. In particular I worked on the development of a MQTT based co-simulation platform for the simulation of multi-energy systems. During the third year of my PhD, I used the co-simulation platform for the analysis of difference multi energy system scenarios (see Figure 1). The studies carried out can be divided into 3 categories:
1) Power-to-Gas (P2G) scenario. A scenario with a high penetration of renewable energy has been analysed in which P2G plants are used to absorb the Reverse Power Flows (RPF) on the HV/MV transformers. P2G plants offer sufficient flexibility to resolve the RPF related problems. However, large investment cost could limit the use of this technology. The results of this analysis were reported in two papers: "*Techno-economic analysis of Power-to-Gas plants in a gas and electricity distribution network system with high renewable energy penetration*" submitted to Applied Energy and "*Power-to-Gas in a gas and electricity distribution network: a sensitivity analysis of modelling approaches*" submitted to Energy Conversion and Management.
2) Localised Power-to-Heat (LP2H) scenario. The LP2H systems connected to buildings, thanks to their high efficiency, allow to reduce the energy needs and at the same time are a source of flexibility that can be exploited to optimize the use of renewable energy. This technology was analysed in an energy community contest. The flexibility enabled by LP2H technologies makes it possible to increase the self-consumption with a positive outcome also from an economic point of view. The results of this study were reported in the paper "*Flexibility of Virtual Energy Storage based on buildings thermal inertia in Renewable Energy Communities: a techno-economic analysis and comparison with Electric Batteries solution*" submitted to Applied Energy.
3) Centralised Power-to-Heat (CP2H) scenario. The CP2H technology connected to District Heating (DH) allows to reduce the overall energy cost for the production of heat, in addition, thanks to the modulation capacity of the CP2H systems, these resources can be used to offer flexibility to the electricity network. In the analysed scenario, the flexibility of LP2H plants is used to absorb the over-generations of renewable energy. The relative low cost of this well-established technology makes the investment convenient from an economic point of view, however, due to the low demand for heat in the summer months, the flexibility offered by this solution is severely limited in this season.

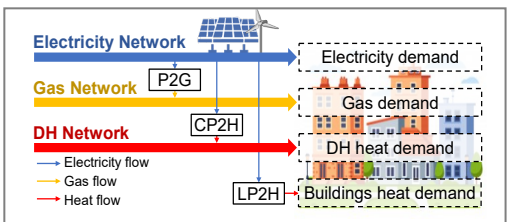


Figure 11 – Multi energy system scenario.

First name: Elisa **LAST NAME**: FENOGLIO

Topic: Opaque active multifunctional façade systems: methodologies for the energy performance assessment and design criteria definition

Course year: 1st **Tutor(s)**: Valentina SERRA, Stefano FANTUCCI

Academic context

[1] Luo Y., Zhang L., Bozlar M., Liu M., Guo H., Meggers F., Active building envelope systems toward renewable and sustainable energy, Renewable and Sustainable Energy Reviews, Volume 104 (2019).
[2] Juaristi M., Gómez-Acebo T., Monge-Barrio A., Qualitative analysis of promising materials and technologies for the design and evaluation of Climate Adaptive Opaque Façades, Building and Environment, Volume 144 (2018) 482–501
[3] Case Studies – Adaptive Facade Network, Aelenei L., Aelenei D., Romano R., Mazzucchelli E.S., Brzezicki M., Rico-Martinez J. M., TU Delft for the COST Action 1403 adaptive facade network, 2018.

External collaborations

- Instituto Pedro Nunes (IPN) – Coimbra – Portugal
- Saule Technologies – Warszawa – Poland
- Oxford Brookes University – Oxford – United Kingdom

Highlights of the research activity

The role of buildings in the energy demand reduction and the achievement of carbon neutrality level is widely recognised. To catch these goals the design of new buildings and the energy retrofit of the existing ones must be nZEB oriented. Advanced opaque envelope solutions must be developed by integrating technological solutions able to reduce energy demand and to improve thermal comfort conditions, exploit renewable sources and manage heat fluxes through the envelope. A possible solution can be represented by opaque active Multifunctional Façade Modules (MFM) that integrate different functionalities in all in one building elements. Nevertheless, since these are complex solutions, an accurate performance prediction during the design phase is needed. The goal of the research activity is to set-up methodologies for assessing active multifunctional façades and to provide tools and data to support the design process. In a first step, a comprehensive overview about the state of the art of materials and solutions to be implemented in advanced multifunctional façades, was carried out by creating a database. Then, since a preliminary evaluation on different advanced multifunctional façade configurations to correctly assess their dynamic behavior, is needed, an analysis and classification of available simulation tools was performed. Moreover, considering the complexity of these technologies, a set of preliminary guidelines for evaluating feasible/unfeasible solutions was implemented, reporting limits and risk related to the application of different functional layers. The abovementioned activities were in this first phase developed within the H2020 POWERSKIN+ project, with the aim to support the process of identification of the most promising opaque panel configurations. A relevant lab campaign was carried out in order to provide suitable data related to the equivalent properties of advanced materials. In detail, different macro encapsulated Phase Change Materials (PCMs) were analysed to evaluate their potentials related to the application in opaque MFM. The laboratory experimental results were used to select the most suitable PCM type to be integrated in slim MFMs now under development. Currently, simulations to evaluate the benefit achievable with the latent heat exploitation with different control strategies are under investigation. In parallel, a preliminary monitoring activity is ongoing on a small scale outdoor test facility (figure1).The data retrieved from the monitoring period will be later used for the validation of simulation models and to test different MFM configurations, as well as to assess their long term thermal performance.

Figure1 – Mock-up installation

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

Topic: Decarbonization of Industrial Plants

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

Academic context

[1] "Carbon footprint of a cement production system integrated with post-combustion CO2 capture and storage process", Frontiers (currently being summitted)
[2] "Carbon footprint of a steel production system integrated with calcium looping processes", Frontiers (currently being summitted);
[3] "Analisi tecno-economica di processi basati sulla tecnologia calcium looping per la decarbonizzazione di cementifici e acciaierie", Report MISE (in Italian)

External collaborations

- Ente Nazionale Energia Ambiente (ENEA)
- International Energy Agency (IEA)
- University of Natural Resources and Life Sciences (BOKU)

Highlights of the research activity

Steel and cement sectors are among the most energy-intensive and emissive heavy industries. On global scale, the steel industry is the second industry in terms of energy consumption and the first for direct CO2 emissions, contributing for about 2.6 GtCO2/year, while the cement industry is the third in terms of primary energy consumption and the second for direct CO2 emissions, contributing another 2.2 GtCO2/year. Cement and steel industries are considered hard to abate sectors as their emissions comes both from combustion and other process, such as calcination reaction, and they usually employ very carbon intensive fuels such as coal or coke. Therefore, one of the most promising solutions for the decarbonization of these sectors is the application of Carbon Capture and Storage (CCS) technologies. Between the many CCS technologies Calcium Looping (CaL) is one of the most suited to be integrated with cement and steel production processes.
The CaL process is considered by the scientific community to be one of the most promising emerging Carbon Capture technologies. This process presents some characteristics that make it particularly suitable for large-scale applications, such as: (I) the use of a CO2 solid sorbent based on calcium oxide (CaO), a low-cost mineral widely used in various industries such as cement and steel mills; (ii) the potential reuse of the sorbent that has exhausted its sorbent capacity within the cement or steel production processes; (iii) possibility of recovering the heat released by the exothermic reaction between CaO and CO_2 which can be used for the production of electricity.
The most promising configurations of CaL integration in the Cement and Steel production process for cement and steel production were modeled with the software ASPEN PLUS for the resolution of mass and energy balances. For each solution analyzed a tecno-economic analysis was performed to estimate capital (CAPEX) and operating (OPEX) costs. Energy and economic performance can, finally, be evaluated through the calculation of Key Performance Indicators (KPIs) such as: (i) CO2 emissions reduction or Avoided Carbon (AC); (ii) CO2 capture efficiency; (iii) Specific Primary Energy Consumption for CO2 Avoided (SPECCA); (iv) cost of CO2 avoided and (v) cost of CO2 captured.

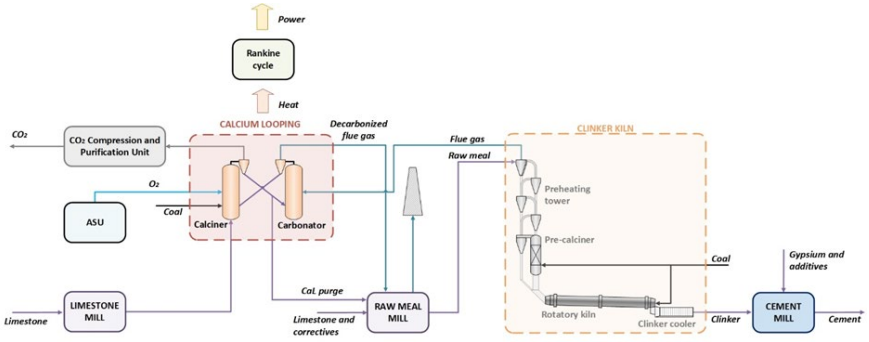


Figure 12 – Integration of CaL in the cement production process "Tail End" configuration

First name: Giovanni **LAST NAME**: GENNARO

Topic: Model-based control strategies for transparent adaptive facades

Course year: 2nd **Tutors**: Fabio FAVOINO, Marco PERINO

Academic context

[1] Catto Lucchino E., Gelesz A., Skeie K., Gennaro G., Reith A., Serra V. and Goia F. Modelling double skin façades (DSFs) in whole-building energy simulation tools: Validation and inter-software comparison of a mechanically ventilated single-story DSF, Building and Environment (119-2021).
[2] Gennaro G., Goia F., De Michele G., Perino M. and Favoino F. Embedded single-board controller for Double Skin Façade: a co-simulation virtual testbed. BS2021 Conference, 1-3 Sept 2021. Bruges, Belgium
[3] Gennaro G., Favoino F., Goia F., De Michele G. and Perino M. Calibration of DSF model for real-time control. IBPC 2021 Conference, August 2021. Copenhagen, Denmark

External collaborations

- EURAC Research (industrial partner. Tutor: Giuseppe DE MICHELE),
- Norwegian University of Science and Technology (NTNU)

Highlights of the research activity

Transparent adaptive facades (TAFs) are active building envelopes that could give a balanced behavior across different building domains such as energy use, internal comfort and IAQ. The theoretical flexibility provided by such controllable building envelope components can allow the façade to act as a climate-responsive element able to optimize everchanging building requirements with intrinsically dynamic boundary conditions. However, these dynamic features require a decision-making system able to predict the best façade configuration to ensure a certain building-level performance, as their performance strictly depends on the control strategies adopted during building operations. In addition, the control strategies implementable depend on both the complexity of the TAFs and the building control domains (energy use and comfort) which impact the computational performance of control strategies. For these reasons, a co-simulation framework [Fig.1] has been developed to design and implement different control strategies for TAFs. The co-simulation environment relies on the combination of Python and EnergyPlus, and the framework is based on the Master/Slave structure in which the Master represents the operation of the building in real conditions and the Slave model represents the controller. The framework is designed to be flexible both in terms of control strategies implemented and adaptive technologies and it has been tested for the implementation of different control strategies for two TAFs. The co-simulation framework has been used to design the Model Predictive Control (MPC) for a simpler façade consisting of electrochromic glazing (EC): the objective of the controller is to modulate the solar radiation transmitted from the façade in order to optimize the cost function which takes into account the comfort requirements over a receding horizon (6 states to the 12 control timesteps). The framework and the resulting MPC formulation were implemented and tested on a full-scale system consisting of a test cell equipped with a South-facing EC façade. The second case study is a more complex hybrid-ventilated Double Skin Façade (DSF) able to manage solar gain and ventilation in building by controlling the different actuators (ventilation openings, cavity fan and integrated blinds). The co-simulation framework was used first to design Rule-Based and Model-Based Control (RBC and MBC) and to implement them in field [2]. In particular, the MBC is based on the reduced numerical model of the DSF (whose calibration process is shown in [3]) coupled with a simplified model of the test room: the controller performs a parametric simulation by changing the DSF state and it chooses the DSF configuration which meets at each control timestep visual comfort constraint, minimizing the HVAC load.

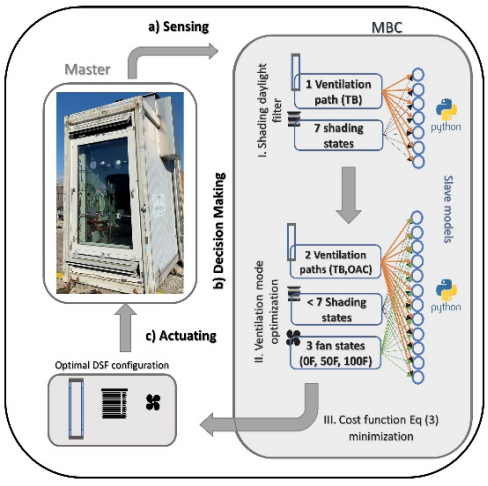


Figure 13 – Co-simulation framework for MBC.

First name: Tiziano A. **LAST NAME**: GIULIACCI

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

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

Academic context

[1] SOC Estimation with an Adaptive Unscented Kalman Filter Based on Model Parameter Optimization (Xiangwei Guo 1, Xiaozhuo Xu, Jiahao Geng , Xian Hua, Yan Gao, Zhen Liu)
[2] Generalized Characterization Methodology for Performance Modelling of Lithium-Ion Batteries (Daniel-Ioan Stroe, Maciej Swierczynski, Ana-Irina Stroe and Søren Knudsen Kær)
[3] Battery Model Parameter Estimation Using a Layered Technique: An Example Using a Lithium Iron Phosphate Cell (Robyn Jackey, Michael Saginaw, Pravesh Sanghvi, and Javier Gazzarri)

External collaborations

- Add-For S.p.a.
- Danisi Engineering

Highlights of the research activity

In the first part of this research activity, a virtual simulation ambient has been developed and tested. This will be useful to check the consistency, the affordability and the behavior of the Battery Management System control logics hereafter implemented.
This is mainly composed by a complex battery model and a vehicle dynamics model which are tuned and validated exploiting some experimental data acquired through on-road tests. Other benches-tests for a better characterization of the battery have been planned for the following year.
In the image on the side, the actual performances of global model have been represented, simulating the vehicle speed starting from the battery requested current profile. The vehicle in the case of study is a two pure electric wheeler.
As far as the battery model is concerned, an estimation of the State of Charge has been implemented too, exploiting the Kalman Filter methodology.
Furthermore, a connection through 5G technology between the site of 'Politecnico di Torino' and third parties is going to be installed to allow Hardware in the Loop real time experiments, connecting hardware form different places.

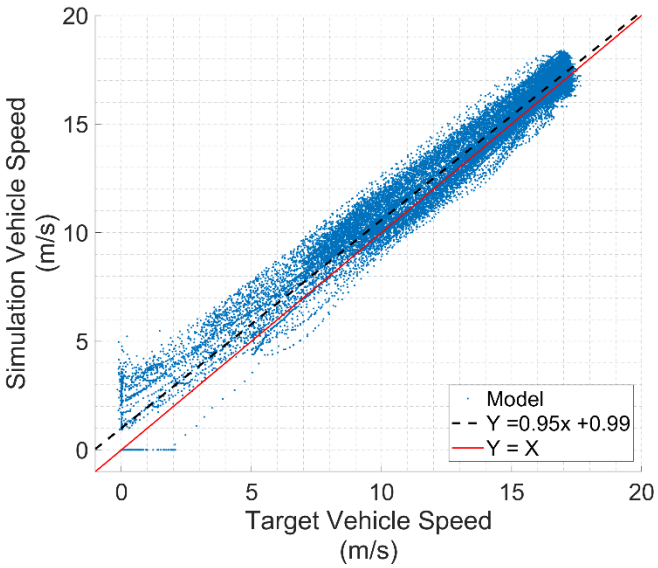


Figure 14 – Simulation vs experimental velocity profile. Root Mean Square Error = 0.96 m/s.

First name: Emerance J. C. D'A. **LAST NAME**: GOMA-TCHIMBAKALA

Topic: Application of Bioaugmentation technology for petroleum hydrocarbons remediation

Course year: 3rd **Tutor(s)**: Stefano P. CORGNATI, Stefano LO RUSSO

Academic context

[1] Xu X, Liu W, Tian S, Wang W, Qi Q, Jiang P, Gao X, Li F, Li H, Yu H (2018). Petroleum Hydrocarbon-Degrading Bacteria for the Remediation of Oil Pollution Under Aerobic Conditions: A Perspective Analysis. Front. Microbiol. 9:2885
[2] Borah Debajit and Yadav R N S. Bioremediation of petroleum-based contaminants with biosurfactant produced by a newly isolated petroleum oil degrading bacterial strain (2016). Egyptian Journal of Petroleum, 26: 181-188.
[3] Poddar Kasturi, Sarkar Debapriya, Sarkar Angana (2019) Construction of potential bacterial consortia for efficient hydrocarbon degradation. International Biodeterioration & Biodegradation 144 (2019) 104770.

External collaborations

- Eni SpA, Via Maritano 26, 20097 San Donato Milanese
- Università degli Studi di Torino, Via Pietro Giuria 5, 10125, Turin

Highlights of the research activity

Intensive use of oil for energy supply and goods manufacturing has led to massive environmental pollution threatening not only soil and aquatic ecosystems but also human health. In order to tackle this issue, conventional techniques have shifted to more eco-friendly and cost-effective strategies exploiting the natural abilities of micro-organisms to metabolize pollutants.

We aimed in this study to develop highly efficient microbial consortia usable in the decontamination of hydrocarbon-polluted environments for future reuse of the area and clean energy purposes. Specifically, the research activities were oriented towards the experimental set-up of a bioaugmentation study in contaminated soil matrix. To do so, bacteria were isolated from targeted sites with diverse contamination histories. The isolates were then assessed for their abilities to degrade hydrocarbons based on the presence of the *alkB* gene and the ability to produce biosurfactants. From there, different bacterial associations were built and the consortia efficiency was determined in microcosms. One consortium was then selected and entrapped to carry out the bioaugmentation study. Bioaugmentation was conducted during a 3 months period and the technology efficiency was assessed according to total petroleum depletion. For comparison purposes and deeper investigation of the consortium effectiveness, a natural attenuation was set up in the same conditions and a landfarming experiment was included in the study.

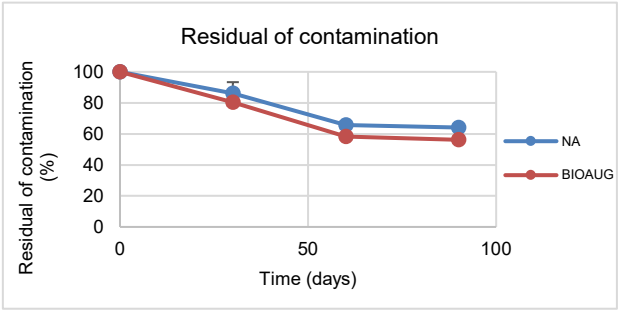


Figure 15 – Bioaugmentation efficiency compared to natural

Results showed that most of the bacterial isolates belonged to hydrocarbons degraders genera such as *Pseudomonas*, *Bacillus*, *Rhodococcus*. The amplification of the *alkB* gene showed the presence of the gene in 39% of the isolates tested while the strains exhibited good emulsification activity towards crude oil up to 76.3%. The bacterial consortium selected for bioaugmentation showed good degradation performance with the reduction of 36.7% of hydrocarbons in microcosm. Overall, the bioaugmentation was successful with almost half (56%) of total petroleum hydrocarbons depleted in the contaminated soil matrix after 3 months, therefore surpassing the natural attenuation by 10%.

Although the landfarming experiment showed better hydrocarbons degradation effectiveness with only 20% of residual contamination, the results indicate that the bioaugmentation technology developed in this study is effective and worth improvements for application in real environment.

First name: Camille **LAST NAME**: GRANIER

Topic: Magnetic reconnection and magnetic vortices in non-collisional plasmas

Course year: 2nd **Tutor(s)**: Daniela GRASSO, Emanuele TASSI

Academic context

[1] E. Tassi, T Passot, P. L. Sulem,, A Hamiltonian gyrofluid model based on a quasi-static closure, *Journal of Plasma Physics*, 86, 835860402 (2020)
[2] C. Granier, E. Tassi, D. Borgogno, D. Grasso, Impact of electron temperature anisotropy on the collisionless tearing mode instability in the presence of a strong guide field, *Physics of Plasmas* 28, 022112 (2021)
[3] C. Granier, D. Borgogno, D. Grasso,E. Tassi, Gyrofluid analysis of electron beta effects on collisionless reconnection. Submitted and waiting for review.

External collaborations

- Université Côte d'Azur, France
- Hyogo University, Japan

Highlights of the research activity

The thesis focuses on the study of magnetic reconnection modelling collision-free plasmas in the presence of a strong ambient magnetic field, such as those encountered in magnetic confinement experiments such as tokamaks or in the Sun-Earth environment. These models preserve the Hamiltonian structure, essential for the analytical techniques used and have the particularity of retaining the anisotropies of temperatures, which are known to play an important role in the dynamics of such plasmas. Here, we intend to investigate the impact that an anisotropic equilibrium electron temperature could have on the formation of magnetic islands, due to reconnection, and on their nonlinear evolution.

The concerned gyrofluid model is valid for high values of βe, whit βe being the ratio between the kinetic pressure of the electrons and the associated magnetic pressure. The consideration of a finite βe is associated with the possibility to describe phenomena taking place at a microscopic scale comparable to that of the electron thermal gyro-radius, which is a scale that is generally not described in the fluid framework.

It is known that the combination of a high βe and a high parallel pressure, only possible in the case of a strong temperature anisotropy, can make Alfvèn waves unstable. This instability is called the "firehose" instability. Our model allows us to study the possible triggering of the firehose instability during reconnection. This study can be relevant for some astrophysical plasmas as well. Indeed, in situe evidence of firehose instability during multiple reconnections have been recently reported in the magnetotail.

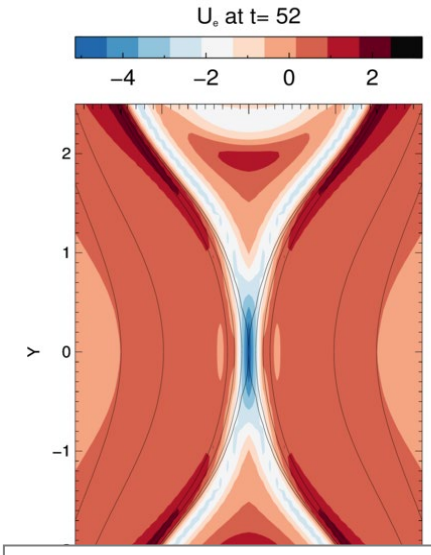


Figure 1 – Contour: Out of plane electron velocity. Black lines: Magnetic field lines that are forming two magnetic islands separated by a reconnection X-point.

First name: Giulia **LAST NAME**: GRISOLIA

Topic: Biofuels and bioplastics from micro-organisms: thermodynamic and thermoeconomic analysis of sustainability

Course year: 2nd **Tutor(s)**: Umberto LUCIA, Debora FINO

Academic context

[1] Lucia, U.; Grisolia, G. (**2021**) The Gouy-Stodola Theorem - From Irreversibility to Sustainability - The Thermodynamic Human Development Index. *Sustainability*, **13**, 3995.
[2] Lucia, U.; Grisolia, G. (**2021**) Biofuels from Micro-Organisms: Thermodynamic Considerations on the Role of Electrochemical Potential on Micro-Organisms Growth. *Applied Sciences*, **11**, 2591.
[3] Lucia U.; Fino, D.; Grisolia, G. (**2021**) Biofuels from abandoned mines: A starting point for future developments. *Atti dell'Accademia Peloritana dei Pericolanti*, **99**, SC1-SC12.

External collaborations

- Harvard Medical School; Department of Radiology, Harvard-MIT Martinos Center for Biomedical Imaging, Massachusetts General Hospital, Harvard Medical School, Charlestown, MA, United States
- Department of Physics, Georgetown University, Washington, 20057, DC, United States.

Highlights of the research activity

The present days are characterized by complex economic relationships among finance, technology, energy management, social needs, etc. All these aspects are linked with human well-being, and must be compliant with the sustainable development (SD) principles. GHG emission reduction requires technological choices, based on objective measurements of their impacts. In accordance with the UN's action plan *Agenda 21* - where indicators are identified as the main tool to evaluate and to guide policy-makers in their choices towards SD - I have improved the indicator proposed during the 1st year, based on an irreversible thermodynamic approach, and on thermodynamic optimization methods, considering both socioeconomic and environmental issues. So, the entropy production rate, $\dot{S}_g$, has been introduced, in relation to the CO_2 emission flows, and it has been related to the Income Index, *II*, in order to consider the economic and social equity, and the anthropic environmental impact, under the same useful effect, $\dot{W}$. In Figure, each bubble corresponds to a country, its condition is represented by the bubble position: the vertical axis represents the stress induced on the environment, the horizontal axis the socioeconomic condition. The dimension of the bubble is the indicator $I_T = 0.01\, T_0 \dot{S}_g / \dot{W}\ 750^{-II}$: smaller bubbles correspond to higher sustainable countries. Furthermore, I have introduced this quantity into the UN's *HDI*, that does not account the environmental domain: in this way, I have obtained the Thermodynamic Human Development Index (*THDI*). Moreover, the previously developed indicator has been used for the analysis of climate and weather changes. As concerns biofuels from micro-organisms, a thermodynamic approach has been developed, highlighting the key role of their membrane electrochemical potential in their proliferation, but also the temperature effect on the biosystem behaviour. A link among the electrochemical potential, membrane potential, pH gradient through the membrane, and temperature has been developed. The hypothesis of exploiting abandoned quarries has been evaluated in order to cultivate micro-organisms, in order to produce biofuels and create a local circular economy.

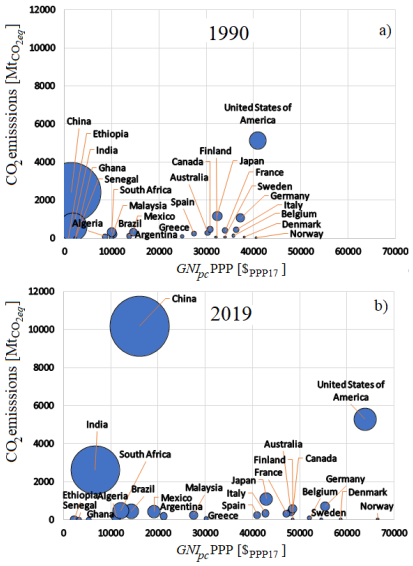


Figure 1 – Evolution (1990 -2019) of the CO_2 emissions, GNI_{pc} at PPP and I_T

First name: Fabrizio **LAST NAME**: GULLINO

Topic: Advanced Powertrain Solutions for Environmentally Friendly Hypercars

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

Academic context

[1]. Paltrinieri, S., Mortellaro, F., Silvestri, N., Rolando, L. et al., "Water Injection Contribution to Enabling Stoichiometric Air-to-Fuel Ratio Operation at Rated Power Conditions of a High-Performance DISI Single Cylinder Engine," SAE Technical Paper 2019-24-0173, 2019, doi: 10.4271/2019-24-0173;
[2]. Bozza, F., Tufano, D., Malfi, E., Teodosio, L. et al., "Performance and Emissions of an Advanced Multi-Cylinder SI Engine Operating in Ultra-Lean Conditions," SAE Technical Paper 2019-24-0075, 2019, doi: 10.4271/2019-24-0075.
[3]. Della Torre, A., Montenegro, G., Onorati, A., Paltrinieri, S., Rulli, F., Rossi, V. et al., "Calibration of the Oxygen Storage Reactions for the Modeling of an Automotive Three-Way Catalyst," Industrial & Engineering Chemistry Research 2021 60 (18), 6653-666, DOI: 10.1021/acs.iecr.0c05744

External collaborations

- Ferrari Know-How and Simulation department, www.ferrari.com
- Gamma Technologies LLC, www.gtisoft.com

Highlights of the research activity

The research activity aims to develop a quasi-dimensional virtual test rig with the objective to quantify the potential benefits in terms of greenhouse gases and criteria pollutants reduction of different engine technologies (e.g. Water injection, Turbocharger electrification, Miller cycle, Lean combustion with pre-chamber, etc...) and aftertreatment configurations over RDE cycles for high-performance SI engines.

In addition to an extensive literature review, the first year the activity was dedicated to the development of a 1D-CFD model of a Ferrari 4 liter V8 turbocharged spark ignition engine, calibrating both the gas exchange process and the combustion model (SITurb). On the other hand, during the second year, the focus shifted towards the exhaust aftertreatment system modelling. In particular, a huge amount of Synthetic Gas Bench data was exploited to define the kinetic scheme of a detailed 1D-CFD model of a Three-Way Catalyst (TWC). Once calibrated, the proposed scheme is being validated by means of an extensive experimental data set measured over different driving cycles, showing a satisfactory predictive capability for tailpipe emissions. Currently, a great effort is being devoted to the development of a methodology for the simulation of the Cat-heating transient phase, while next year will be focused on the calibration and the improvement of models for the prediction of the in-cylinder formation of unburned hydrocarbons (HC), Carbon Monoxides (CO) and Nitrogen Oxides (NOx).

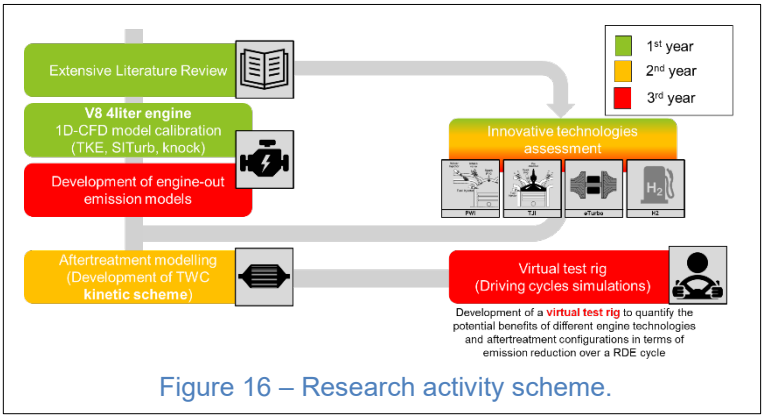


Figure 16 – Research activity scheme.

As schematized in Figure 1, the development of the predictive combustion model (SITurb) and the calibration of the TWC kinetic scheme together with reliable models for the prediction of the main engine-out pollutant species will be crucial for the main core of my PhD activity, which concerns the creation of a virtual test bench that allows to assess the benefits in terms of tailpipe emissions of several innovative engine technologies and aftertreatment configurations over RDE cycles.

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

Topic: Simulation and experimental analysis of mist sprinklers for tunnel fires applications

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

Academic context

[1] Colella F., Rein G., Borchiellini R., Torero J. (2011). A Novel Multiscale Methodology for Simulating Tunnel Ventilation Flows During Fires. Fire Technology 47(1):221-253
[2] Santangelo, P.E., Characterization of high-pressure water-mist sprays: Experimental analysis of droplet size and dispersion, Experimental Thermal and Fluid Science, 34 (2010) 1353-1366.
[3] Verda, V., Borchiellini, R., Cosentino, S., Guelpa, E., & Tuni, J. M. (2021). Expanding the FDS Simulation Capabilities to Fire Tunnel Scenarios Through a Novel Multi-scale Model. Fire Technology, 1-24.

External collaborations

- Imperial College
- NIST
- Technositaf

Highlights of the research activity

The necessity of the development of water-based fixed fire suppression systems in extinguishing tunnel fires is the main motivation of this work. My research activities are divided into two major parts. In the first part, experimental investigations on estimating the water mist characteristics and droplet sizes of water mist sprays by Phase Doppler Particle Analyzer (PDPA) are considered. Besides that, the fire behavior and the effectiveness of mist sprinklers to suppress the fire in an enclosure with the size of 2m×2m×3m are analyzed through performing fire tests. In the second part, my research studies are focused on the numerical analysis of various parameters influencing the fire in tunnels, the water mist systems, and different ventilation scenarios. The Fire Dynamics Simulator (FDS) developed by NIST is used for numerical studies.

A Comprehensive literature review has already been carried out first to carefully identify the existing gaps and second to submit it to a journal as a review paper. For my experimental section, I have already designed the measurement system and apparatuses required for the fire test room such as designing the thermocouple trees, the water flow system and so on. For the simulation section of my research work, I have conducted several simulations in FDS to study different parameters such as the fire location and the fire load and to evaluate the performance of water sprays in suppressing fires in enclosures. The sensitivity analysis to check the grid independency of the model has also been carried out. Moreover, the tunnel fire simulations to study different ventilation system scenarios, the performance of the water mist systems on extinguishing the fire, and the other parameters such as the critical velocity, the backlayering distance, and the smoke spread along the tunnel have been carried out by FDS. However, as a practical solution, I will be working on a multiscale (1D-3D) modeling to decrease the computational costs. Furthermore, the experiments mentioned above will be performed and finally the battery fires related to the electric and hybrid vehicles will be investigated.

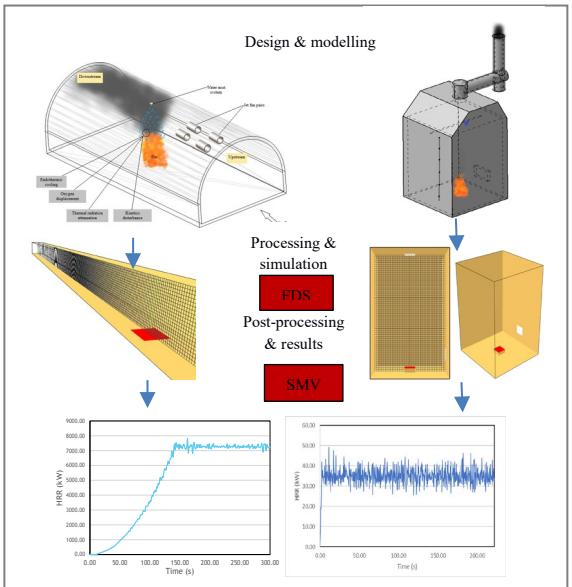


Figure 1 – Modeling approach to simulate the tunnel fire with water mist system and enclosures by FDS

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

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

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

Academic context

[1] Bhardwaj, Om Parkash, et al. "Potential of Hydrogenated Vegetable Oil (HVO) in Future High Efficiency Combustion System" SAE International Journal of Fuels and Lubricants, vol. 6, no. 1, SAE International, 2013, pp. 157–69.
[2] Federico Millo, Biplab Kumar Debnath, Theodoros Vlachos, Claudio Ciaravino, Lucio Postrioti, Giacomo Buitoni, Effects of different biofuels blends on performance and emissions of an automotive diesel engine, Fuel, Volume 159, 2015, Pages 614-627, ISSN 0016-2361.
[3] Athanasios, D., Stylianos, D., Stella, B. et al., "Emissions Optimization Potential of a Diesel Engine, Running on HVO: A Combined Experimental and Simulation Investigation," SAE Technical Paper 2019-24-0039, 2019, doi:10.4271/2019-24-0039.

External collaborations

- Università degli Studi di Perugia
- ENI
- PUNCH

Highlights of the research activity

Utilization of Hydrogenated Vegetable Oil (HVO) as a second-generation Biofuel in the current transportation fleet as an alternative to the fossil diesel is the footstone of this research activity.
A detailed analysis of the spray and injection properties of HVO was the first step, which was carried out both experimentally (in collaboration with the University of Perugia) and numerically (by developing a 3D-CFD model).
Then, a wide range of diverse tests from steady state (for both drop-in and constant calibration operation) to transient WLTC tests were carried out at ICE Advanced Laboratory of Politecnico di Torino on a light duty 4-cyl 1.6-liter displacement diesel engine.
The results demonstrated that the HVO spray and combustion properties makes it suitable to be used as a neat alternative fuel in the current fleet.
Soot and particle numbers were proved to be reduced thanks to lack of aromatics and unsaturated compounds. Also, specific HC and CO emissions were decreased likely due to improved ignition as a consequence of the higher cetane number of HVO. Mass BSFC was also reduced due to higher Lower Heating Value of HVO, which compensated for its lower density, although HVO lead, as expected, to higher volumetric fuel consumption.

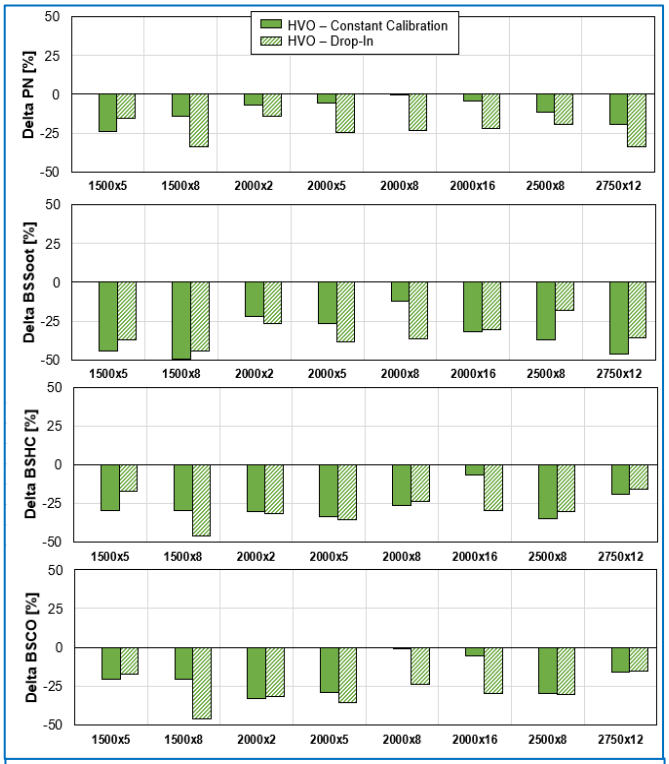


Figure 1 – Percentage of changes in specific emissions of HVO vs. Diesel in two modes: drop-in and Constant Calibration.

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

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

Course year: 1st **Tutor(s)**: Alessandro FERRARI, Zhijun WU

Academic context

[1] Investigation on spray characteristics of gasoline/water mixture based on real-time blending method
[2] Experimental investigation on diffusive combustion of fuel-water mixture
[3] Combustion simulation of ammonia mixture gas in high temperature water environment

External collaborations

- Institutions of Fuel Spray and Combustion in Tongji University
- State Key Laboratory of Automotive Safety and Energy
- Guangxi Yuchai Machinery Group Co., Ltd.

Highlights of the research activity

In the first year, I have investigated the spray characteristics of gasoline/water mixture based on an existing test bench. The spray form, spray area, spray cone angle, particle size of special mixture fuel had been tested to demonstrate spray mechanism in flash boiling conditions. Spray flash collapse mechanism had been analysed and the turning point with/ without flash boiling had been evidenced with reference to the boiling point. An experiment investigation of fuel-water mixture diffusive combustion had been designed to assess the water effect on diffusive combustion. The ignition delay period has a slightly increase with the increase of the water ratio. The flame brightness and temperature has an obvious decline in water condition.

Ammonia researches are designed for the next year. Collaborating with State Key Laboratory of Automotive Safety and Energy of China, combustion characteristics of ammonia-hydrogen mixture gas and emission mechanisms will be investigated for designing advanced ammonia engines.

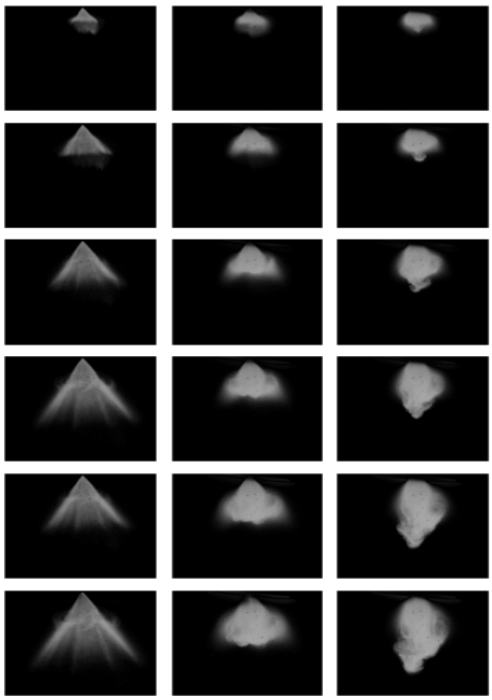


Figure 1 – Examples of gasoline spray evolutions (experimental results)

First name: Zhiru **LAST NAME**: JIN

Topic: Fluid dynamics of internal combustion engines – diesel injection systems

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

Academic context

[1] Jin Z, Vento O, Zhang T, Ferrari A, Mittica A, Ouyang L, Tan S. Numerical-experimental optimization of the Common-feeding injection system concept for application to light-duty commercial vehicles. Journal of Energy Resources Technology,143(12): 1-19, 2021.
[2] Ferrari A, Jin Z, Vento O, Zhang T. 2021. An injected quantity estimation technique based on time frequency analysis. Control Engineering Practice,116: 104910, 2021.
[3] D'Ambrosio S, Ferrari A, Jin Z. Time-frequency analysis application to the evaluation of instantaneous combustion noise. Fuel, accepted.

External collaborations

- Nanyue Fuel Injection Systems Co., Ltd

Highlights of the research activity

The activity throughout the year has been focused on the combustion noise evaluation in the design of modern diesel engines.
An innovative methodology for the evaluation of the instantaneous combustion noise related to Δp_{comb}, that is, the pressure difference between the measured in-cylinder pressure and the pseudo-motored signal has been developed. This has been realized by means of time-frequency analysis through applying the Choi-Williams distributions to the pressure signal Δp_{comb}. By evaluating the energy content of the combustion pressure signal, which has been collected on a Euro 5 diesel engine, various combustion phases have been detected and the contribution of each phase to the overall combustion noise has been obtained.
Tridimensional plots of smoothed Choi-Williams distribution have been presented to show the overall variation of combustion noise related to Δp_{comb} both in the time and frequency domain. The algorithm for the calculus of this instantaneous combustion noise contribution versus time has been realized through a home-made tool. A cause and effect analysis has been performed on the decomposed in-cylinder pressure signal for studying combustion noise. The developed procedure is validated and then applied to estimate the contribution to noise of the different phases of combustion pertaining to the single and multiple injection strategies.
The application of the time-frequency analysis technique enables a qualitative and quantitative analysis on the combustion noise contribution. The research investigation provides a hint for onboard diagnostics and real-time control of combustion noise, but the developed tool also can be provided as a practical validation tool for the refinement of the combustion models. The practical results have been submitted to Fuel and have been accepted.

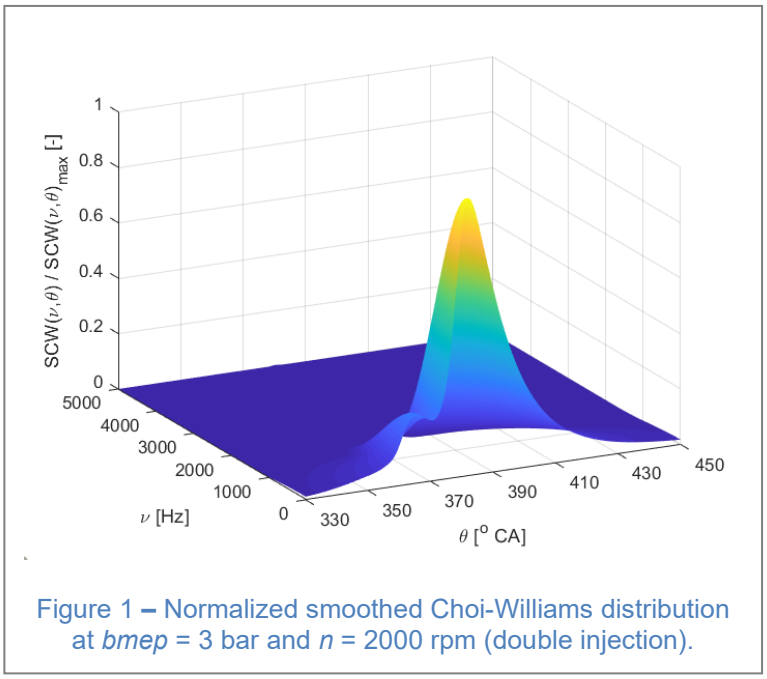


Figure 1 – Normalized smoothed Choi-Williams distribution at *bmep* = 3 bar and *n* = 2000 rpm (double injection).

First name: Daniele **LAST NAME**: LEREDE

Topic: Progressing in the assessment of the role of nuclear fusion in the future energy mix

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

Academic context

[1] D. Lerede et al., "Could clean industrial progresses and the rise of electricity demand foster the penetration of nuclear fusion in the European energy mix?", Fusion Engineering and Design, vol. 172, 112880, 2021.
[2] J. F. DeCarolis, "The case for repeatable analysis with energy economy optimization models", Energy Economics, vol. 34, pp. 1845-1853, 2012.
[3] P. Bolat et al., "Hydrogen supply chain architecture for bottom-up energy systems models. Part 2: Techno-economic inputs for hydrogen production pathways", International Journal of Hydrogen Energy, vol. 39, n. 17, pp. 8898-8925, 2014.

External collaborations

- EUROfusion
- Consorzio RFX
- ENEA

Highlights of the research activity

The research activity "Progressing in the assessment of the role of nuclear fusion in the future energy mix" is devoted to the improvement of methods for the energy modeling involving long-term projections to include nuclear fusion power plants for electricity production through an expanded modeling approach. During the second year of this PhD activity, the module for transportation technologies developed during 2020 was further expanded to consider the uncertainty related to the application of future parameters. The work was carried out coupling the EUROfusion TIMES Model (ETM) with the Stochastic Multicriteria Acceptability Analysis (SMAA) tool. As the main target of this PhD activity lays in the development of an open-source model for the European energy system including nuclear fusion as power generation option, a review of the existing open-source modeling frameworks has been carried out. The choice fell on Tools for Energy Model Optimization and Analysis (Temoa), which aims at replicating the TIMES minimum cost optimization algorithm. The translation of an energy system model in Temoa began with a case study based on TIMES-Italy, in collaboration with Dr. F. Gracceva (ENEA). In parallel, the assessment of the effects of the Covid-19 pandemic on industrial drivers for the model and the construction of an hydrogen module for energy system models were carried out. Finally, as sustainability aspects are becoming ever important and their integration in energy system models would be beneficial to comply with a broader spectrum of requirements for the evolution of the energy system in light of the current policies in act, an ex-post evaluation framework of the sustainability level of the power sector resulting from different energy scenarios obtained via TIMES models was developed. Sustainability scores were assigned to different scenarios complying with different CO2 emission targets and socio-economic developments. The activity is leading to a first-of-a-kind integration between the TIMES economic paradigm with sustainability dimensions of electricity production to better assist energy system evaluations about nuclear fusion.

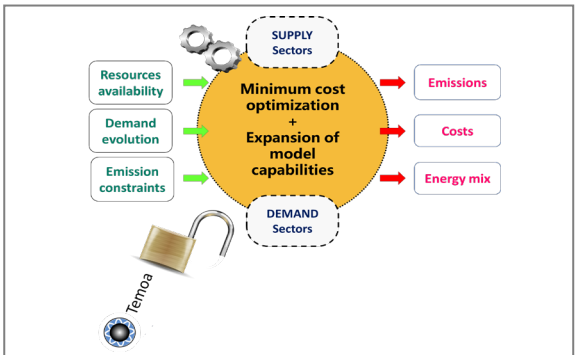
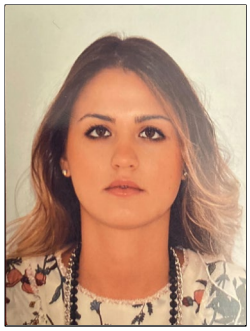


Figure 1 – Framework for the implementation of an open TIMES-like model based on Temoa to expand the modeling capabilities beyond the mere economic optimization.



First name: Carola **LAST NAME**: LINGUA

Topic: New approaches and economic-financial models to support technological innovation in the building energy sector

Course year: 2nd **Tutor(s)**: Stefano P. CORGNATI, Cristina BECCHIO, Marta C. BOTTERO

Academic context

[1] European commission 2014. Guide to Cost-Benefit Analysis of Investment Projects: Structural Funds, Cohesion Fund, and Instrument for Pre-Accession. Directorate-General for Regional Policy, Brussels.
[2] Kurnitski J., Boerstra A., et al. REHVA Covid-19 Guidance Document, version 4.1. How to operate HVAC and other building service systems to prevent the spread of the coronavirus (SARS-CoV-2) disease (COVID-19) in workplaces. April 2021.
[3] Fisk, W. and Seppanen, O., 2007. Providing better indoor environmental quality brings economic benefits. Proceedings of Clima 2007 Well Being Indoors, June 10-14, 2007, Helsinki.

External collaborations

- RHOSS S.p.A., Codroipo (UD), Italy
- ANNEX 79 community, Occupant behavior-centric building design and operation EBC

Highlights of the research activity

The outbreak of the Covid-19 pandemic has highlighted the urgency to build indoor environments that promote health and safety for occupants who spent about 90% of their time indoors. People awareness to health and well-being issues bring to an immediate impact on the market where consumers prefer technologies that can guarantee a higher level of hygiene and safety. Furthermore, moving from the occupants' health dimension to the energy efficiency of building one, it is known that it represents the key factor of the European policy actions, in order to guide the transition to a low-carbon society. In the Italian residential context, the "Recovery Decree" (D.L. 34/2020) is introduced, concerning social policies and financial support to face the economic crisis following the Covid-19 pandemic. It increased the tax incentives to 110% (so-called Superbonus), encouraging the replacement of heating systems with heat pump systems. In this context, the main objective of my Ph.D. research is to provide industrial companies with a methodological approach able to enhance their innovative technologies on the building energy sector, guiding their investment decision towards an energy transition with a view of "post-carbon" society. The research activity covered during this second year, in collaboration with the Rhoss S.p.A., focused on the development and simulation of energy models of a single-family house that allow to demonstrate the energy and environmental advantages of a green-oriented technology (air/water heat pump) over a traditional condensing boiler in three different climatic zones of Italy. In addition, in the field of energy renovation of existing buildings, the results showed that the only replacement of condensing boiler with a heat pump system makes it possible to achieve an improvement of at least two energy efficiency classes, condition required to access the Superbonus 110%.

				TURIN	ROME	PALERMO
Single-family house Category E1(1) S 150 m² (Model S)		VERY HIGH PERFORMANCE (Model A) U_{wall}= 0.15 W/m²K U_{floor} = 0.12 W/m²K U_{window} = 1.2 W/m²K	S A	Pu: 7.15 kW $Q_{h,nd}$: 31.26 kWh/m²	Pu: 5.07 kW $Q_{h,nd}$: 6.55 kWh/m²	Pu: 3.80 kW $Q_{h,nd}$: 2.44 kWh/m²
			S B	Pu: 8.42 kW $Q_{h,nd}$: 47.75 kWh/m²	Pu: 5.98 kW $Q_{h,nd}$: 14.34 kWh/m²	Pu: 4.48 kW $Q_{h,nd}$: 6.81 kWh/m²
		HIGH PERFORMANCE (Model B) U_{wall}= 0.28 W/m²K U_{floor} = 0.21 W/m²K U_{window} = 1.4 W/m²K	S C	Pu: 16.61 kW $Q_{h,nd}$: 163.8 kWh/m²	Pu: 11.82 kW $Q_{h,nd}$: 82.35 kWh/m²	Pu: 8.87 kW $Q_{h,nd}$: 46.59 kWh/m²
			S D	Pu: 19.01 kW $Q_{h,nd}$: 183.2 kWh/m²	Pu: 13.54 kW $Q_{h,nd}$: 87.84 kWh/m²	Pu: 10.16 kW $Q_{h,nd}$: 50.42 kWh/m²
L 220 m² (Model L)		LOW PERFORMANCE (Model C) U_{wall}= 0.86 W/m²K U_{floor} = 0.5 W/m²K U_{window} = 2.2 W/m²K	L A	Pu: 9.38 kW $Q_{h,nd}$: 33.39 kWh/m²	Pu: 6.65 kW $Q_{h,nd}$: 8.81 kWh/m²	Pu: 4.98 kW $Q_{h,nd}$: 4.03 kWh/m²
			L B	Pu: 10.92 kW $Q_{h,nd}$: 47.95 kWh/m²	Pu: 7.74 kW $Q_{h,nd}$: 16.41 kWh/m²	Pu: 5.81 kW $Q_{h,nd}$: 8.22 kWh/m²
		VERY LOW PERFORMANCE (Model D) U_{wall}= 0.86 W/m²K U_{floor} = 0.5 W/m²K U_{window} = 4.5 W/m²K	L C	Pu: 22.43 kW $Q_{h,nd}$: 160.9 kWh/m²	Pu: 16.02 kW $Q_{h,nd}$: 83.66 kWh/m²	Pu: 11.96 kW $Q_{h,nd}$: 47.65 kWh/m²
			L D	Pu: 25.3 kW $Q_{h,nd}$: 176.9 kWh/m²	Pu: 18.06 kW $Q_{h,nd}$: 87.46 kWh/m²	Pu: 13.51 kW $Q_{h,nd}$: 50.52 kWh/m²

Figure 1 – Definition of modelling scenarios

First name: Claudio **LAST NAME**: MAINO

Topic: (P)HEV Optimal Design

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

Academic context

[1] Maino, C. *et al.* (2021). Optimal mesh discretization of the dynamic programming for hybrid electric vehicles. *Applied Energy*. Elsevier Ltd, 292(March), p. 116920. Doi: 10.1016/j.apenergy.2021.116920.
[2] Maino, C. et al. (2021). A deep neural network based model for the prediction of hybrid electric vehicles carbon dioxide emissions. Energy and AI. Elsevier Ltd, 5, p. 100073. Doi: 10.1016/j.egyai.2021.100073.
[3] Cannavacciuolo, G. *et al.* (2021). A model for the estimation of the residual driving range of battery electric vehicles including battery ageing, thermal effects and auxiliaries. *Applied Sciences (Switzerland)*, 11(19). Doi: 10.3390/app11199316.

External collaborations

- FPT Industrial
- AVL Italia S.r.l
- Addfor S.p.a

Highlights of the research activity

Optimal mesh discretization of the Dynamic Programming for hybrid electric vehicles

Dynamic Programming (DP) represents one the most popular approaches for the global optimization of offline control problems related to (plug-in) hybrid electric vehicles ((P)HEVs). Nevertheless, the curse of dimensionality phenomenon affects the possibility of employing the DP when large computational grids have to be taken into account. In [1], a model for the selection of a smart refinement of the DP grid has been developed considering the typical offline control optimization of parallel HEVs (i.e. selection of the optimal power-split between the engine and the battery). Specifically, a self- adaptive statistical approach based on a proper management of any admissible battery energy variation has been developed to significantly improve the calculation times required for HEV architectures while still attaining the best possible accuracy in terms of CO_2 emissions. Relevant reductions of the machine time have been demonstrated ranging around 90% for a passenger car and 80% for a heavy-duty vehicle while introducing irrelevant accuracy losses in the computed CO_2 of roughly 1%.

Deep Neural Networks for the prediction of the carbon dioxide emissions produced by hybrid electric vehicles

A model for the prediction of the tank-to-wheel CO_2 emissions of different HEV architectures has been developed and tested on data generated within a design optimization procedure. Specifically, a pipeline of Deep Neural Networks (DNNs) has been trained at predicting both the possibility of simulating a specific HEV layout ("feasible layout") and eventually its related emissions on a given driving mission calculated by a DP algorithm. The DNNs learn the correlations underlying between the values assumed by the main HEV design variables and the results produced by the DP on a specific driving mission. The pipeline have shown significant performances when tested on three different parallel HEV architectures and have proved the capability of being integrated within a design optimization procedure for HEV fleets ([2]).

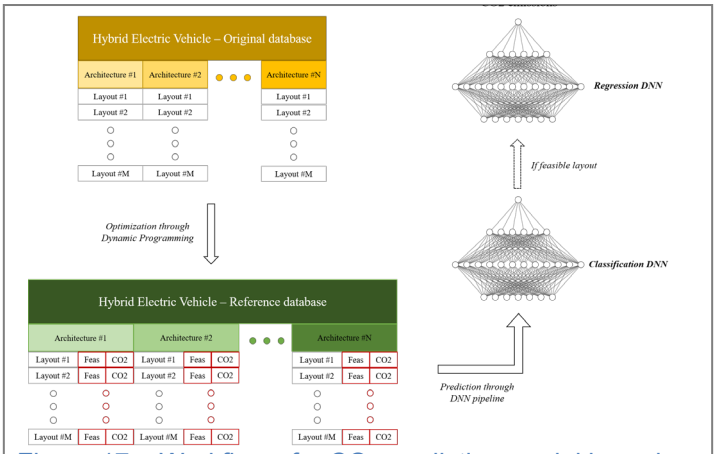


Figure 17 – Workflow of a CO_2 prediction model based on DNNs

First name: Andrea **LAST NAME**: MANELLI

Topic: Engine technologies for reduction of fuel consumption and pollutant emissions in light-duty diesel engines with model-based and sensor-based controllers

Course year: 3rd **Tutors**: Stefano D'AMBROSIO, Roberto FINESSO

Academic context

[1] Experimental analysis on the effects of multiple injection strategies on pollutant emissions, combustion noise, and fuel consumption in a premixed charge compression ignition engine / d'Ambrosio, S.; Mancarella, A.; Manelli, A.; Mittica, A.; Hardy, G. - In: SAE INTERNATIONAL JOURNAL OF ENGINES. - ISSN 1946-3936. - 14:5(2021). [10.4271/03-14-05-0037]
[2] Ventura, Loris; Manelli, Andrea; Malan, Stefano, "Diesel Engine Cycle to Cycle Feed-forward plus Closed-loop Combustion Control". In: 6th IFAC Conference on Engine and Powertrain Control, Simulation and Modeling, Tokyo, August 23-25, 2021, pp. 119-125.
[3] Ventura, Loris; Malan, Stefano; Manelli, Andrea, "Cycle to cycle closed-loop combustion control through virtual sensor in a diesel engine". In: 29th Mediterranean Conference on Control and Automation (MED 2021), Bari, Puglia, Italy, June 22-25, 2021.

Highlights of the research activity

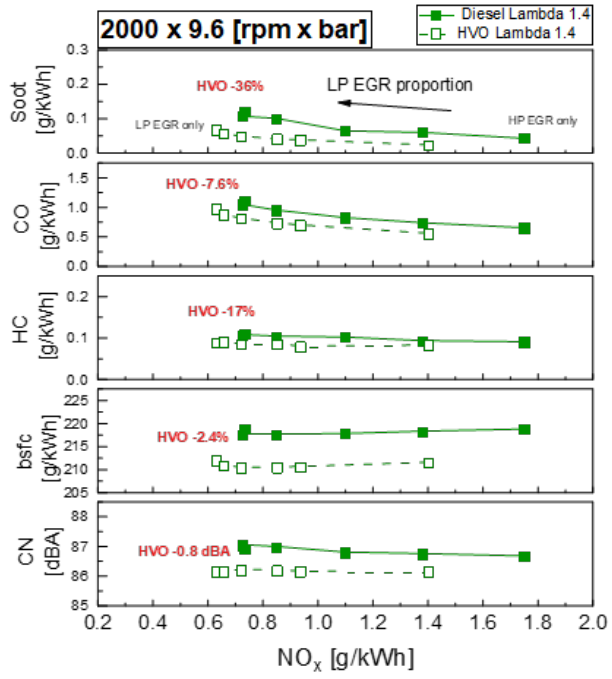


Figure 2 – Pollutant emission trends for Diesel and HVO

During this year, my research activity has been focused on the testing of an alternative fuel, HVO, comparing its performances with standard diesel oil.
The experimental tests were performed on a FPT 2.3L Euro VI F1A prototypal diesel engine. Preliminary experimental tests have been carried out on 5 engine operating points, representative of the behavior of the application of the engine to a light-duty commercial vehicle along a WLTC. Starting from their baseline calibrations, the lambda value has been kept fixed, while exploring different combinations of HP and LP EGR actuators: from the graphs of figure 1 can be seen an important reduction of HC and CO (especially significant at low load) and of soot (especially significant at high load). A minor variation in CN is also measured. Starting from these tests DoE plans have also been tested with final optimizations considering second order polynomial models, with constraints chosen in order to minimize the engine-out pollutant emissions (e.g. NOx, CO for low load or soot for high load). Finally, an open-loop compensator plus cycle to cycle closed-loop controller has also been developed and tested in Model-in-the-Loop phase, coupling it with a fast-running GT-Power model of a FPT Euro VI 3.0L diesel engine. In this strategy, both model-based open-loop compensator and closed-loop controller employ a virtual sensor realized through a predictive combustion model calibrated on real measurements at the test bench. Injected fuel quantity and start of injection of the main pulse are regulated to target the desired engine load and NOx respectively.

First name: Mohsen **LAST NAME**: MANSOURKIAEI

Topic: Optimization of control strategies of degradation management for power to power systems

Course year: 3rd **Tutor**: Prof. Massimo SANTARELLI

Academic context

[1] M. Carmo, D.L. Fritz, J. Mergel, D. Stolten, A comprehensive review on PEM water electrolysis, Int. J. Hydrogen Energy 38 (2013) 4901-4934.
[2] S. Siracusano, N. Van Dijk, R. Backhouse, L. Merlo, V. Baglio, A.S. Arico, Degradation issues of PEM electrolysis MEAs, Renewable Energy 123 (2018) 52-57
[3] H Javed, AG Sabato, M Mansourkiaei, D Ferrero, M Santarelli, K Herbrig, Glass-Ceramic Sealants for SOEC: Thermal Characterization and Electrical Resistivity in Dual Atmosphere, Energies v13, (2020) p 3682.

External collaborations

- SINTEF (Stiftelsen for industriell og teknisk forskning), Trondheim, Norway
- CNR-ITAE, Messina, Italy
- KTH Royal Institute of Technology, Stockholm, Sweden.

Highlights of the research activity

The goal of my research is to have a thorough control on the performance of novel technologies of power to power (P2P) storage by studying the degradation of a system's elements i.e. Electrlolyser/Fuel cell, batteries and H_2-based energy storage system. For in depth analysis of degradation a test rig was built at Environmental park of Turin aiming at the characterization and performance evaluation of electrochemical devices for the production and utilization of hydrogen. It is designed to test low temperature (T) electrolytic devices up to 150°C under pressures (P) up to 30 bar both with anionic and cationic electrolyte. It can also test both individual electrolytic cells and small assembled cells called stackes.

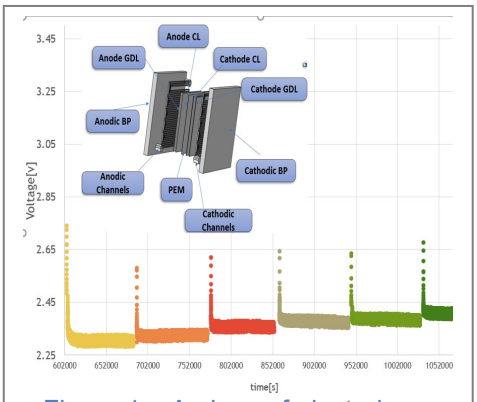


Figure 1 – A piece of electrolyser degradation graph, voltage[V] vs time [s]; and 3D geometry for simulation in COMSOL Multiphysics

To be able to deeply study the degradation phenomena starting from the technology level in each P2P system component, accelerated experimental degradation tests were designed and a series of tests have been arranged on low-T PEM cells to create semi-empirical degradation models coming from the collected data. After cell characterization in different physical conditions, an array of open vs closed cathode experiments were done to compare the difference between the performance in these cases at variable temperature or pressure conditions. Also, a MATLAB model has been developed which can predict the behaviour of the cell in different conditions as well as giving the possibility to study the effect of various electrochemical and physical variables -such as T, P and current densities- on the cell performance. Lastly a series of accelerated degradation tests with the scope of modelling the degradation have been performed on the cells with constant current profiles and specificly designed dynamic current profiles that mimic the load of a real case study with frequent variations and shutdowns. During all experiments, the circuit demineralized water was continuously analysed for its thermal conductivity and fluoride ion quantities. Electrochemical impedence spectroscopy have also been used to investigate the changes in cell characteristics, and electrical equivalent circuits were developed to model the behaviour of the cells. After the degradation tests on the mentioned cells, post-mortem analysis using SEM-EDS was performed to have a complete overview about the degradation mechanisms. Furthermore, using COMSOL Multiphysics®, 2D and 3D Single Phase and Multi-phase Models (Bubbly Flow, k-ω) of PEM electrolytic cell were developed to simulate the main involved physics with special consideration on biphase anodic mixture interactions within the system; and the effect of different variables such as temperature gradient at anode and cathode, bubbles overpotential and O_2 and H_2 concentration at electrode interface on the system were modelled.

First name: Antonino **LAST NAME**: MELI

Topic: Advanced Material application in Nuclear Fission Reactor Industry

Course year: 2nd **Tutor(s)**: Massimo ZUCCHETTI, Mariano TARANTINO (ENEA)

Academic context

[1] Tarantino, M. et al., Overview on Lead-Cooled Fast Reactor Design and Related Technologies Development in ENEA, Energies 2021,14, 5157. https://doi.org/10.3390/en14165157
[2] NEA 2015 Edition Handbook on Lead-bismuth Eutectic Alloy and Lead Properties, Materials Compatibility, Thermal-hydraulics and Technologies
[3] Bassini, S. et al. Material Performance in Lead and Lead-Bismuth Alloy, Comprehensive Nuclear Materials 2nd edition, vol. 4, pp. 218–241.

External collaborations

- Research center ENEA of Brasimone, (Bo)

Highlights of the research activity

The research topic of this PhD thesis was in the frame of radiation damage evaluation in advanced materials adopted in nuclear fusion industry, with related development of a material science comprehensive model aiming to predict it and possibly reduce the time required to develop and qualify novel alloys for fusion applications. After an initial stage of the PhD characterized by a literature review on radiation damage and on the most promising alloys, a reactor case study concerning the ARC reactor design (developed at the MIT-PSFC) has been taken as reference. Once further details concerning the superconducting materials adopted in the reactor design have been defined, the PhD candidate has developed a model in order to study the behavior of high temperature superconductors (HTS) adopted in the design in the ARC reactor's toroidal field coils for the confinement of the plasma in nominal working conditions. The aim was to estimate their radiation damage and how it would have affected their superconductive properties. The results of the model have been collected and discussed in a paper submitted in the third quarter of second academic year. Meanwhile, since the second quarter of the same academic year, the PhD candidate has established a collaboration with the Dr. Tarantino from the research center ENEA of Brasimone (Bo): here he is currently carrying experimental tests in order to characterize the behavior of advanced alloys with eventual coatings when exposed in liquid lead environment. He has already monitored some experimental campaigns, and then approached with the analysis of the exposed samples at the SEM (Scanning Electron Microscope) and EDX (Electron Diffraction X-ray). According to his first results, base material 15-15Ti austenitic steel suffered from some minor lead corrosion on its surface, when exposed in liquid lead at 550°C, for 2600h and $5*10^{-5}$Ox wt.%, while the bulk resulted unaffected. From the same experimental campaign, the same alloy has been tested with alumina coatings, adopting different coating techniques. The samples with PLD (Pulsed Layered Deposition) alumina coating have validated the coating effectiveness, meaning that no lead permeation or corrosion has occurred in the alumina layer nor in the bulk of the alloy. The sample coated with alumina through DG (Detonation Gun) has shown slightly different results: as a matter of fact, the alloy beneath the coating layer resulted to be unaffected by the lead exposure, although some lead infiltration has occurred in the alumina coating; since this might depend on the porosity of the deposition, further studies concerning the deposition technology and validation is foreseen for afore mentioned coating technique. Other alloys such as the AISI 316L (with and without coating), AFA (Alumina Forming Austenitic) steels, have been exposed in lead environment, although their composition and morphology analysis is not ready yet.

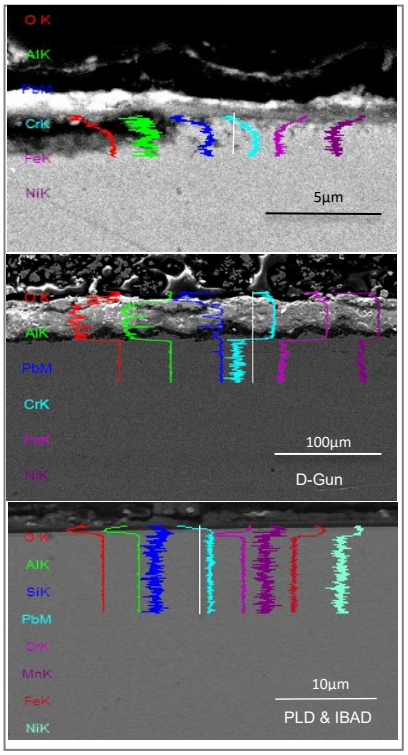


Figure 18 – EDX line scans of the sample exposed in lead

First name: Samuele **LAST NAME**: MESCHINI

Topic: Preliminary safety assessment and safety-oriented design of ARC fusion reactor

Course year: 2nd **Tutor(s)**: Massimo ZUCCHETTI, Raffaella TESTONI, Eliana DE MARCHI (ENI).

Academic context:

[1] Meschini, S., et al. "ARC reactor: A preliminary tritium environmental impact study." Fusion Engineering and Design 167 (2021): 112340.
[2] 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.
[3] Zucchetti, M., Hartwig, Z., Meschini, S., Segantin, S., Testoni, R., & Whyte, D. (2021). ARC reactor: Radioactivity safety assessment and preliminary environmental impact study. Fusion Engineering and Design, 162, 112132.

External collaborations

- Massachusetts Institute of Technology (MIT)
- ENI
- DTT S.c.a.r.l.

Highlights of the research activity

During the 2nd year of PhD the following activities on ARC FLiBe loop have been carried out: functional analysis and FMEA; development of a tritium transport, system-level model for inventory quantification; development of a thermal-hydraulics, system-level model to simulate transients in nominal operations or in accidental scenarios; probabilistic-deterministic coupling of the aforementioned model by means of a Monte Carlo (MC) failure injection engine and post-processing by means of machine learning algorithms. First, the FLiBe loop model sketched during the 1st year has been extended by means of a functional analysis that allowed to identify minor components required for operations and control. A FMEA has been carried out to identify possible criticalities in the preliminary design – no major issues have been found. Also, the FMEA identified possible initiating events with the corresponding frequency. LOFAs look as the most probable accidental scenario for ARC FLiBe loop. Hence, a tritium transport, system-level model has been developed by taking advantage of EcosimPro. The model quantifies the time-dependent tritium inventory in the main components, providing a precise source term for safety analyses. The thermal-hydraulics model has been developed on OpenModelica environment. Standard components such as pumps and heat exchangers have been extended from the *ThermoPower* library, whereas fusion relevant components (blanket, vacuum vessel channels, vacuum vessel structural layers, plasma and heaters) have been defined on purpose. In this respect, the model accounts for nuclear heating, plasma transients and decay heat due to materials activation. A suitable control logic has been developed in such a way that it is possible to "inject" components failure as the simulation proceeds. This allows to explore system transients that arise "naturally" from system nominal operations. Specifically, a MC routine samples components failure according to their failure probability. A Python wrapper handles the pre-processing and post-processing. During pre-processing, the failures times and failure magnitude sampled by the MC routine are passed to OpenModelica as simulation inputs. No user-defined input is therefore required, removing the "expert judgment" from the analysis. During post-processing, each transient is classified according to the system end state (failure, near miss and safe state). More than 2000 transients have been analysed until now. Machine learning algorithms are then trained on the results to extract relevant system features and to provide possible online failure detection strategies.

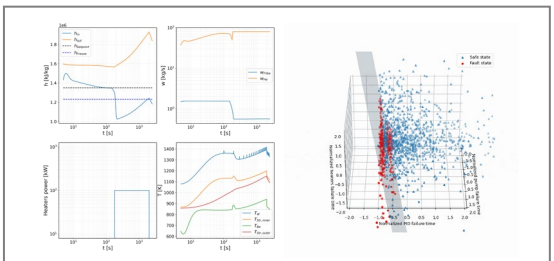
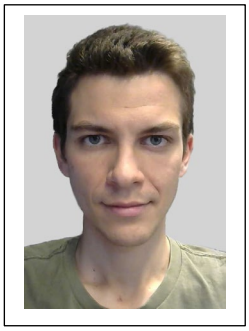


Figure 19 – Left: system evolution following multiple failures in ARC FLiBe loop. Right: decision boundary for online failure detection computed with logistic regression.



First name: Federico **LAST NAME**: MIRETTI

Topic: Integrated ICE-ATS management in (P)HEVs

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

Academic context

[1] Miretti, F.; Misul, D. & Spessa, E., DynaProg: Deterministic Dynamic Programming solver for finite horizon multi-stage decision problems, *SoftwareX*, *Elsevier BV*, 2021, *14*, 100690
[2] Jacobson, D. H. & Mayne, D. Q., Bellman, R. (Ed.), Differential dynamic programming, *American Elsevier Publishing Company,* 1970, 24
[3] Anselma, P. G.; Belingardi, G.; Falai, A.; Maino, C.; Miretti, F.; Misul, D. & Spessa, E., Comparing Parallel Hybrid Electric Vehicle Powertrains for Real-world Driving, *2019 AEIT International Conference of Electrical and Electronic Technologies for Automotive (AEIT AUTOMOTIVE), IEEE*, 2019

External collaborations

- FPT industrial
- IVECO
- ENI

Highlights of the research activity

My research activity starts from the following engineering problem: to ensure that the decarbonization benefits of hybrid-electric vehicles are not jeopardized by an increase of pollutant emissions.
To reduce emissions, catalytic after-treatment systems are employed which, in order to work properly, must be heated up using the engine's exhaust gases. The more electrical part of the hybrid powertrain gets involved to reduce CO_2 emissions, the more the effectiveness of the ATS is at risk.
Sophisticated optimal control techniques are therefore needed to maximize CO_2 reduction while minimizing cancerous pollutant emission.
The first main topic was to develop a multi-objective optimal control tool based on *Dynamic Programming* to obtain an optimal energy management strategy to minimize CO_2 and pollutants.
This optimal control tool was then embedded in a powertrain optimal design tool for heavy-duty hybrid electric vehicles which was previously developed by the research group; the tool, developed for the industrial partner *FPT industrial*, compares hybrid powertrain layouts fuel consumption and/or pollutants emissions over a given driving mission and the vehicle total cost of ownership over its lifespan.
As a first step of this activity, the first year's work has been focused on physical modelling of the ATS components, with particular focus the SCR of a diesel-hybrid architecture.
Since the optimal design tool requires analyzing many simulations, simulation time is vital to the tool's impact on the industrial partner's research and development activities. Thus, as a second step, numerical, coding and physical modelling aspects have been engineered to cut down simulation time while maintaining modelling accuracy. As a result, individual simulation time has been reduced by two orders of magnitude.

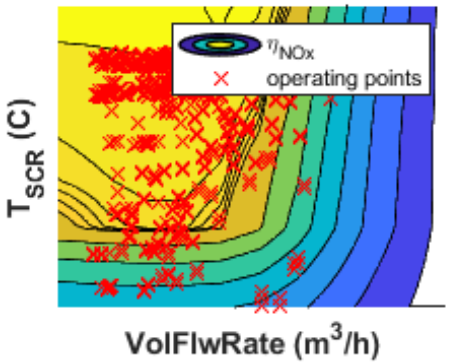


Figure 1 – The SCR deNOx efficiency is mapped as a function of SCR temp and exhaust gases flow rate

The second main topic was to develop a new optimal control algorithm based on *Differential Dynamic Programming* which retains the same benefits of Dynamic Programming (mainly, ensuring truly optimal control trajectories) but without suffering from the same computational complexity pattern (the so-called *curse of dimensionality*). Similarly to Dynamic Programming, this algorithm would be suitable for off-line design of EMSs, but it would be able to handle more complex models with higher-dimensional state spaces.

First name: Alberto **LAST NAME**: MOSCATELLO

Topic: CFD simulations and experimental validation of industrial accidents and environmental pollution

Course year: 2nd **Tutor(s)**: Andrea CARPIGNANO

Academic context

[1] Paté-Cornell, M.E., 1993. "Risk analysis and risk management for offshore platforms: lessons from the piper alpha accident", *J. Offshore Mech. Arctic Eng*. 115 (3),179–190.
[2] Moscatello, A. et al., 2021, "A novel approach to high-pressure gas releases simulations", *Journal of Loss Prevention in the Process Industries*, 72(May), 104531.
[3] Moscatello, A. et al., 2020, "Scaling procedure for designing accidental gas release experiments", *Engineering Computations*.

External collaborations

- Ministero dello Sviluppo Economico (MiSE)
- École Central de Lyon (AIR – Atmosphère, Impact & Risk group)

Highlights of the research activity

The proposed research activity is part of a large project, founded by the Italian Ministry of Economic development (MiSE) since 2015, which aims at enhancing the safety of Oil & Gas plants and guarantee a sustainable transition towards a low carbon future.
During this second PhD year, the research activity was mainly focused on the validation of the Computational Fluid Dynamics (CFD) model proposed in [2] based on ANSYS Fluent. This model, called Source Box Accident Model (SBAM), aims at handling complex accidents in complex geometries with a reduced computational cost. The validation campaign has been carried out in the SEASTAR-WT wind tunnel, realized at the Environment Park in Turin (Italy). A 1:10 scaled Oil & Gas platform mock-up, equipped with flow and gas concentration sensors, was built and installed inside the wind tunnel, in order to reproduce an accidental gaseous release in dynamic similarity conditions with some real cases. A set of gas releases were performed, and the predicted concentrations were compared to the observed ones in order to validate the CFD model. An example of results comparison, related to one of the case studies, is shown in the picture. This direct comparison of the values is useful to qualitatively estimate the behavior of the model, on the other hand, a more robust methodology was followed to assess the model validity. This methodology uses several statistical measures to quantify the CFD model error with respect to the experimental values, accounting for both systematic and random errors.
Results showed that, in most of the cases, acceptance criteria for the statistical measures were met and a good consistency between experimental and numerical values is found. Furthermore, an overestimating tendency of SBAM is observed, suggesting that it is a conservative tool for consequences estimation.
In parallel to the experimental activity, a further improvement of the CFD model was carried out. To speed-up the simulation time, a non-intrusive reduced order model (NIROM) was developed and tuned to reproduce the CFD behavior. A set of training and validation CFD simulations were realized to adequately refine the NIROM.
Results showed that the surrogate model can reproduce the output results with an error below 10% on the interest quantities. This outcome will lead to a strong computational time reduction, since the NIROM performs calculations in few seconds, instead of the ~24 h needed by CFD.

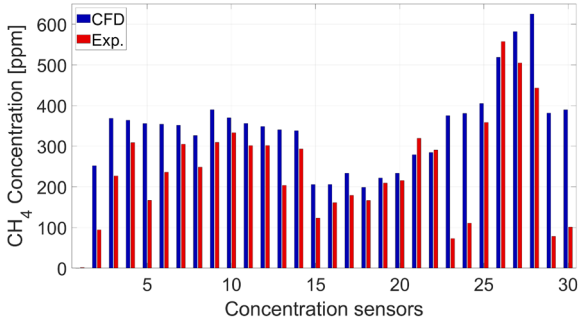


Figure 20 – Comparison of numerical and experimental concentrations obtained for 30 sensors among the domain.

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

Topic: Multiscale modeling of smart materials for energy applications

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

Academic context

[1] Srivastava, et al. *Carbon-Based Smart Materials*, **2020**, 33-80
[2] Marrink, et al. *The Journal of Physical Chemistry B*, **2004** 111 (27), 750-760
[3] Plimpton, et al. *Journal of Computational Physics*, **1995** 117 (1), 1-19

External collaborations

- ITAINNOVA (Zaragoza, Spain)
- FORTH (Patras, Greece)
- NTUA (Athens, Greece)

Highlights of the research activity

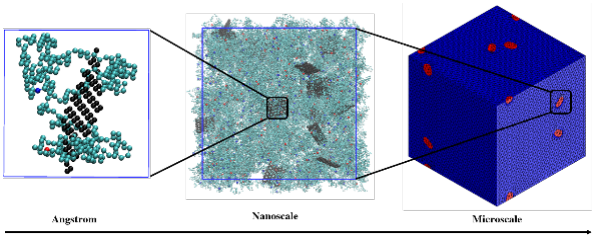


Figure 21 – Multi-scale description of a carbon-reinforced polymer composite

Over the last years, smart polymer nanocomposites are expected to play an increasing role in sustainable technologies for energy conversion, storage, automotive, and electronics. Recently, polymer nanocomposites have been reinforced with nanostructured fillers, e.g., graphene, graphene oxide, reduced graphene oxide, and carbon nanotube, because of their exceptional mechanical, thermal, and electrical capabilities. The technological development of nanocomposites with desired properties strongly depends on understanding the structure-property relationship, which requires advanced multiscale modelling. In this PhD activity, a multiscale modelling framework that incorporates data spanning from atomistic to mesoscopic to continuum techniques is employed. In detail, I have investigated the thermo-physical properties (such as density, glass transition temperature, elastic constant, Poisson's ratio, and thermal conductivity) of neat polymers (thermoplastic: polypropylene (PP), polylactic acid (PLA); thermoset: epoxy resin), nanofillers (graphene (Gr), graphene oxide (GO), and reduced graphene oxide (rGO)) and the resulting carbon reinforced polymer composites. The model results have been verified and experimentally validated as well.

Initially, the Coarse-Grained (CG) potentials of neat polymers (PP, PLA and epoxy resin) are determined by upscaling the atomistic information. The CG potentials are used to develop the most suitable mesoscopic model that imitates the thermo-physical properties determined experimentally. The coarse-grained force field used for the neat Gr is based on the Tersoff CG potential. The determination of CG potentials of neat polymers and optimization of the graphene model have been made by our research partner (ITAINNOVA). After determination of potentials, CG MD simulations have been performed to determine the thermo-physical properties of neat polymers (PP, PLA and epoxy resin), nanofiller (Gr) and nanocomposites (PP/Gr, PLA/Gr and Epoxy/Gr). Benchmark force fields (MARTINI) [2] available in the literature have been also utilized to verify the thermo-physical properties of neat polymers (PP and PLA), fillers (Gr, GO and rGO) and nanocomposites (PP/Gr, PP/GO, PP/rGO, PLA/Gr, PLA/GO and PLA/rGO). CG MD simulations are run with a time step of 1 fs in the NPT and NVT ensembles using LAMMPS package [3]. To upscale the results of CG MD simulations of nanocomposites, macroscopic simulations have been also carried out. Continuum modelling is used to predict the thermal and mechanical behaviour of the nanocomposites using mean field (MF) and finite element (FE) modules. The input parameters in MF and FE models are taken from benchmark CG model (in case of PP and PLA) and developed model (in case of epoxy resin). The results obtained from the finite element simulation are compared against the benchmark forcefield CG simulations and experimental results. The results reveal that the Young's modulus, Poisson's ratio, and thermal conductivity of nanocomposite predicted using FE model shows similar trend with the CG simulation results, therefore verifying them. An experimental thermo-mechanical characterization of neat polymers (PP and PLA) and nanocomposite (PP/Gr and PLA/Gr) has been also done to validate the results of simulations in collaboration with our research partners (FORTH and NTUA).

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

Topic: Predictive control for energy saving, safety and comfort enhancement for connected and ADAS-equipped vehicles

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

Academic context

[1] Musa, A.; Pipicelli, M.; Spano, M.; Tufano, F.; De Nola, F.; Di Blasio, G.; Gimelli, A.; Misul, D.A.; Toscano, G. A Review of Model Predictive Controls Applied to Advanced Driver-Assistance Systems. Energies 2021, 14, 7974. https://doi.org/10.3390/en14237974
[2] Kazemi, H.; Mahjoub, H.N.; Tahmasbi-Sarvestani, A.; Fallah, Y.P. A Learning-Based Stochastic MPC Design for Cooperative Adaptive Cruise Control to Handle Interfering Vehicles. IEEE Trans. Intell. Veh. 2018, 3, 266–275, doi:10.1109/TIV.2018.2843135
[3] Capuano, A.; Spano, M.; Musa, A.; Toscano, G.; Misul, D.A. Development of an Adaptive Model Predictive Control for Platooning Safety in Battery Electric Vehicles. Energies 2021, 14, 5291. https://doi.org/10.3390/en14175291

External collaborations

- Teoresi S.P.A.
- Università degli Studi di Napoli Federico II
- Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili (STEMS)

Highlights of the research activity

This research activity aims at the development and assessment of predictive control solutions for energy saving, safety and comfort enhancement for connected and ADAS-equipped vehicles. The first year of the research activity focused on a comprehensive review of Advanced Driver-Assistance Systems. It has been found that although a variety of algorithms can be used to control the vehicle and achieve the different automated strategies (cruise control, path following and lane keeping), most of the studies exploit algorithms based on model predictive control. Together with Università degli Studi di Napoli Federico II, STEMS and Teoresi S.P.A. a comphensive review on model predictive controls applied to advanced driver-assistance systems has been presented. Moreover, two different application based on CACC have been considered. The former refers to a neural network-based CACC in V2V scenario. More specifically, due to the temporal nature of the problem under consideration, a particular type of recurrent neural network has been considered, namely the gated recurrent unit. On the other hand, the second application refers to model predictive applied to CACC and unexpected manoeuvres. Based on the research work proposed by Kazemi et al. [2] the safety analysis during a cut-in maneuver has been considered. The effectiveness of the proposed methodology was assessed for in different driving scenarios such as diverse cruising speeds, steep accelerations, and aggressive decelerations. The research activity has been carried out in collaboration with other colleagues from DIMEAS department within the CARS@PoliTO centre.

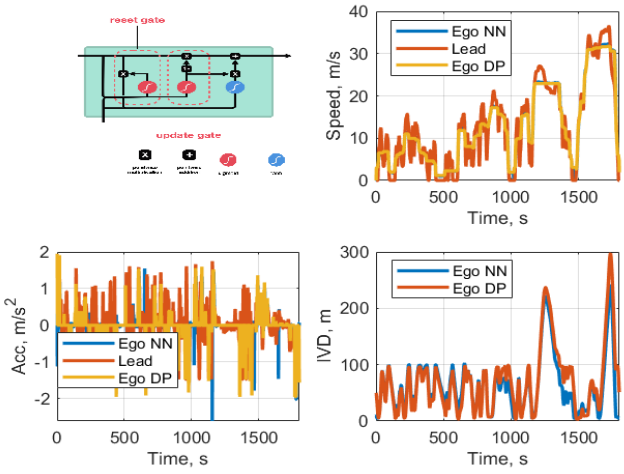


Figure 1 – Gated recurrent unit scheme (top left); comparison between the speed (top right), acceleration (bottom left) and IVD (bottom right) profiles for the lead vehicle and ego vehicle obtained through two different controllers, namely dynamic programming and gated recurrent unit.

First name: Francesco **LAST NAME**: NEIROTTI

Topic: Decarbonization of Urban Areas: electrical and thermal grid integration

Course year: 3rd **Tutor(s)**: Marco SIMONETTI, Michel NOUSSAN

Academic context

[1] IEA (2018), The Future of Cooling, IEA, Paris https://www.iea.org/reports/the-future-of-cooling. https://www.iea.org/reports/the-future-of-cooling
[2] Connolly, D. (2017). Heat Roadmap Europe: Quantitative comparison between the electricity, heating and cooling sectors for different European countries. *Energy*. https://doi.org/10.1016/j.energy.2017.07.037.
[3] Jarre, M., Noussan, M., & Simonetti, M. (2018). Primary energy consumption of heat pumps in high renewable share electricity mixes. *Energy Conversion and Management, 171,* 1339-1351. https://doi.org/10.1016/J.ENCONMAN.2018.06.067.

External collaborations

- IEA annex 50 – Heat Pump Technology in multifamily building
- Partners of the ReCognition EU project

Highlights of the research activity

Electrification of final uses is probably the main driver for decarbonization of urban areas, and more in general of final energy consumption. Electrification is especially related to the heating sector and the mobility one. On the other side, electricity consumption is becoming an important issue as cooling systems are expected to put strong pressure on the electrical grid with the exponential increase of cooling demand around the world, also due to increasing temperatures. For this reason, in the future, we will see cooperation more than a competition between full electrification and traditional technologies. The variability of the emission factor for key electrical technologies, such as HPs and EVs, can have important variations with respect to the yearly national average. At the nowadays penetration level, RES have a minimal impact during the winter period. This difference increases as looking for cooling AC units operating during the summer season where, due to the high impact of solar technologies, the RES shares present wider fluctuations. AC units are becoming a predominant part of the electricity consumption share and the main driver of summer peak demand. Latent load handling strategies are key factors to decrease the peak request and adsorption technologies are part of it. Within the ReC framework, the HySun prototype has been developed: it is a particular type of adsorption chiller based mainly on solar thermal energy to drive the regeneration and on an efficient HP to cool down the adsorption battery and air stream and, if needed, to drive the regeneration. The adsorbent coated heat exchanger allowed to dehumidify the air stream using higher temperature with respect to the traditional chiller cycle, resulting in energy savings and increase energy efficiency. Moreover, the thin coating layer allowed a fast regeneration of the material even at low temperatures (50-60°C) which are easily reachable with RES technologies and state of the art heat pump machines.

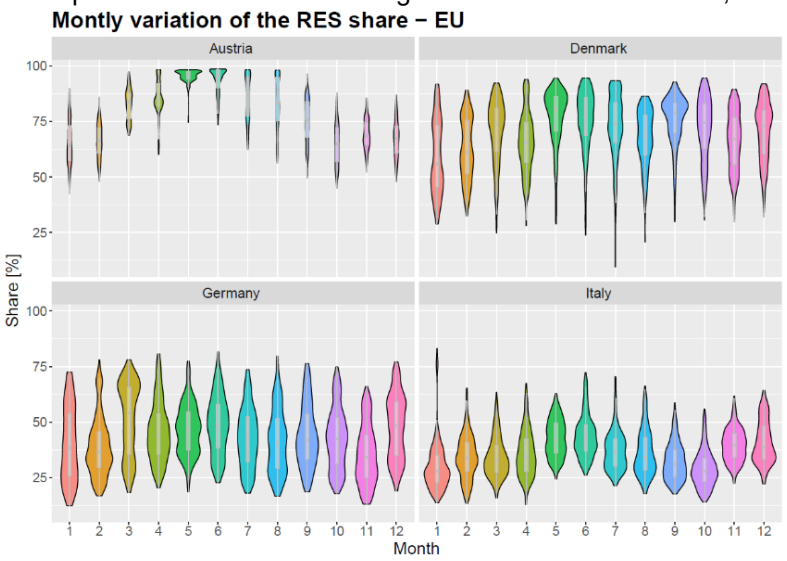


Figure 22 – Monthly RES share variation in different area in the EU (2019 data)

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

Topic: Strategic roadmap for district cooling development

Course year: 1st **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

Highlights of the research activity

Residential cooling demand has increased in the last decades and is continuing to rise, having an impact on the environment in terms of emissions and causing grid instabilities due to large shares of peak demand. More efficient technologies are therefore needed and district cooling can be a feasible alternative to conventional cooling systems, especially in areas characterized by large energy densities. However, with respect to district heating, the temperature difference between supply and return is much lower. Consequently, to transfer the same amount of thermal power, larger mass flow rates are required and therefore larger diameters and pumping power as well. As a consequence, if these systems are not properly designed and managed, the benefits with respect to other technologies could be limited or inexistent. In this context, it was implemented a 1D thermal fluid dynamic model for the thermal, economical, environmental and exergy analysis of district cooling networks. From the results, it emerged that the thermal losses are negligible in these systems, due to the small temperature difference with the ground. On the other hand, pumping cost is significant and represents about 10% of primary energy consumption.

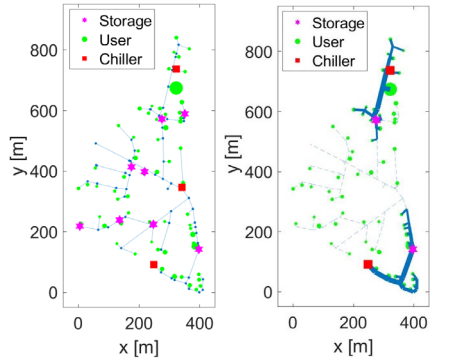
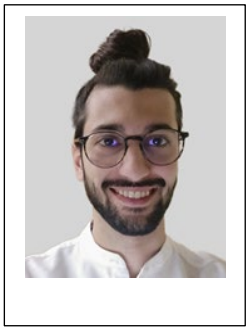


Figure 23 – Design optimization of a district cooling network. The optimal solution consists in two independent smaller networks.

Most of the activities of the first year of my PhD were focused on the design optimization of district cooling networks. Firstly, a Mixed Integer Linear Programming (MILP) was developed for the optimization of the topology and the set of users to connect to a district cooling network. The objective of the model is to minimize the total costs characterized by piping, pumping, energy transfer stations and chillers capital and operational costs. The non-linearity of pressure drops and pumping power has been handled rigorously by using two linearization techniques: reformulation linearization and the cutting plane method. A heuristic model was also developed to solve the same problem by means of a genetic algorithm. The MILP model proved to be slightly more precise, but the heuristic is more than 90% faster. The heuristic approach was further improved by clustering the users on the base of their position, hence reducing the number of variables. The model was then enhanced by including also the possibility to optimize the size and position of chillers and storages in a district cooling network. In addition, a comparison was made between centralized and decentralized storages. Although decentralized storage is more expensive than centralized one, it is more convenient thanks to a better sizing of energy transfer stations.
Lastly, the developed model has been used to evaluate the minimum linear energy density, such that a district cooling is more convenient than traditional technologies. It resulted that this threshold increases with the dimension of the network, therefore smaller district cooling networks are generally more feasible than larger ones.



First name: Giuseppe **LAST NAME**: PINTO

Topic: Enhancing Energy Flexibility in Cluster of Buildings through Coordinated Energy Management

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

Academic context

[1] Huang P., Fan C., Zhang X., Wang J. **A hierarchical coordinated demand response control for buildings with improved performances at building group**. *Elsevier, Applied Energy (2019)* https://doi.org/10.1016/j.apenergy.2019.03.148.
[2] Hu M, Xiao F, Wang S. **Neighborhood-level coordination and negotiation techniques for managing demand-side flexibility in residential microgrids**. Renew Sustain Energy Rev 2021;135:110248. https://doi.org/10.1016/j.rser.2020.110248.
[3] Vázquez-canteli JR, Nagy Z. **Reinforcement learning for demand response : A review of algorithms and modeling techniques**. Appl Energy 2019;235:1072–89. https://doi.org/10.1016/j.apenergy.2018.11.002.

External collaborations

- University of Texas at Austin
- University College of Dublin
- Lawrence Berkeley National Laboratory

Highlights of the research activity

Building energy management can enable energy flexibility by enhancing on-site renewable energy exploitation and storage operation, reducing energy costs and providing services to the grid. However, when the energy management is faced shifting from a single building to a cluster of buildings, individual demand-side management may have negative effects on the grid reliability. The first year was devoted to identifying different ways of harmonizing the control of multiple buildings, with particular attention on Reinforcement Learning (RL). RL agent directly learns an optimal control policy through a trial-and-error interaction with the environment. The main outcome of the first year was the development of a framework able to exploit a model-free Deep Reinforcement Learning (DRL) controller for the energy management of a cluster of buildings. The second year was devoted to the comparison of two multi-agent reinforcement-learning architectures: a centralised (coordinated) controller and a decentralized (cooperative) controller, which have been benchmarked against a rule-based controller. The research formulated the energy management of four buildings equipped with thermal energy storage and PV systems as a multi-agent problem. The DRL controllers were designed to act on building active thermal storage systems, with the aim to exploit energy flexibility, minimising the energy cost for both individual buildings and the entire district. The two controllers outperformed the rule-based controller by 3% and 7% respectively for cost, and 10% and 14% respectively for peak demand, assessing the effectiveness of handling the district of building as a whole rather than just the sum of individual buildings. The last part of the second year was devoted to the development of a framework able to simulate the building dynamics to integrate occupant comfort into the control problem. Using Long Short-Term Memory (LSTM) neural network, building internal temperature variation was considered, with the twofold advantages of exploiting building thermal mass and consider thermal comfort for users. This module was then coupled with the framework developed during the first year, creating a framework called 3DEM (Data-Driven District Energy Management), used to perform coordinated energy management of multiple buildings considering internal temperature evolution, providing computational cost advantages, and increasing the performances of the district of buildings.

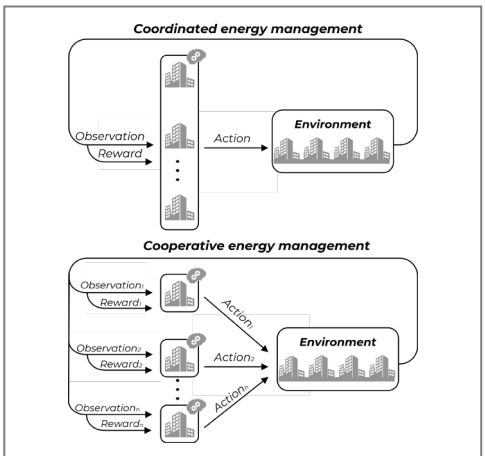


Figure 3 – Control architectures.

First name: Mamak **LAST NAME**: POURABDOLLAHTOOTKABONI

Topic: Towards climate resilient nearly zero energy buildings; A comparative study on energy related components, adaptation strategies and whole building performance.

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

Academic context

[1] ZHANG, Chen, et al. Resilient cooling strategies – A critical review and qualitative assessment. Energy and Buildings. 2021, 251, 111312. ISSN 0378-7788
[2] RAHIF, Ramin, et al. Simulation-based framework to evaluate resistivity of cooling strategies in buildings against overheating impact of climate change. Building and Environment, 2021, 108599.
[3] Pérez-Andreu, Víctor, et al. "Impact of climate change on heating and cooling energy demand in a residential building in a Mediterranean climate." Energy 165 (2018): 63-74.

External collaborations

- Institute of building research & innovation, Vienna, Austria (Operating agent of IEA EBC-Annex 80)
- Italian National Agency for New Technologies, Energy and Sustainable Economic Development

Highlights of the research activity

Climate change and heatwaves cause overheating of buildings, increase cooling energy consumption and bring about energy shortage due to excess demand. The existing literature neglects the impacts of future scenarios on building stock on a regional scale for assessing and developing an adaptation and mitigation framework. Hence, the main objective of the Ph.D. research is to investigate and optimize energy performance and thermal comfort of buildings in a changing climate (long-term assessment) and in the case of summer heatwaves (short-term assessment) in Italy. The first observed methodological gap dealt with the lack of knowledge on robustness and reliability of future weather files, which led to investigate their relative advantages for building future performance simulation. Consequently, it was found out that the dynamical downscaling provides physically consistent datasets by better representing the spatial and temporal variability of the local climate. Therefore, a typical meteorological year (TMY) was created using a high-quality regional climate model database (from Euro-CORDEX) applying the dynamical downscaling. It was then applied to analyze the effect of climate change on nearly zero-energy buildings (NZEBs) in three different Italian climatic zones (cities of Milan, Rome, and Palermo). Overall, it was shown that buildings would miss the nearly zero-energy target in the future, so a new configuration is needed to meet the NZEB requirements. The following goal was to assess the resilience of several categories of cooling strategies by dynamic simulation (Fig.1). In this regard, in synergy with IEA-Annex 80 Weather Data Task, using bias adjusted REMO-2015 regional climate model, TMYs and heatwave files were created for the city of Rome. Case studies in this step are the three representative residential building types (SFH, MFH, and AB) beside the retrofitted scenarios to verify the NZEB requirements in Italy, and a medium office from DOE prototype buildings. Followingly to reach adaptation measures, sensitivity analysis is performed for the annual net energy need for cooling, the maximum cooling load, and the annual electrical energy use in relation with correlated parameters, such as window area, opaque envelope insulation, color of the external wall surface, etc. Variance-based sensitivity analysis was used due to its capability to measure the sensitivity across the entire input space as opposed to local methods. However, to better reach convergence of the sensitivity indexes, more samples are still needed, which is being provided in collaboration with the IEA-Annex 80 simulation subtask that aims to generate Resilient Cooling 'Technology Profiles'.

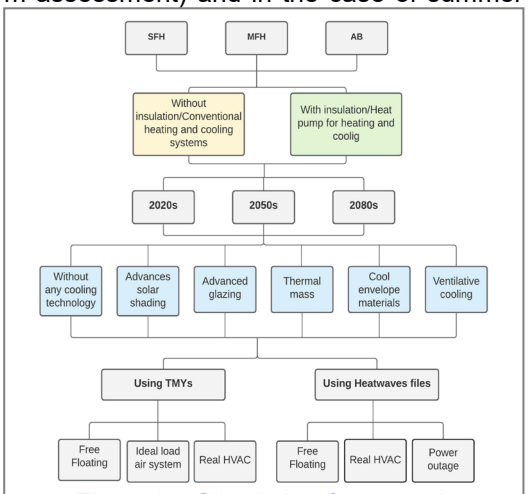
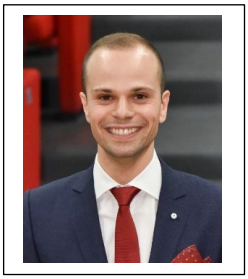


Figure1 – Simulation framework



First name: Luca **LAST NAME**: PULVIRENTI

Topic: Exploiting V2X connections and advanced energy management strategies to achieve maximum CO_2 reductions from HEVs

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

Academic context

[1] S. Doulgeris, A. Dimaratos, N. Zacharof, Z. Toumasatos, D. Kolokotronis, Z. Samaras, "Real world fuel consumption prediction via a combined experimental and modeling technique", Science of The Total Environment, Vol. 734, 2020, 139254, ISSN 0048-9697, https://doi.org/10.1016/j.scitotenv.2020.139254.

[2] Olin, P., Aggoune, K., Tang, L., Confer, K. et al., "Reducing Fuel Consumption by Using Information from Connected and Automated Vehicle Modules to Optimize Propulsion System Control," SAE Technical Paper 2019-01-1213, 2019, doi:10.4271/2019-01-1213.

[3] Xu, B., Malmir, F., Rathod, D., and Filipi, Z., "Real-Time Reinforcement Learning Optimized Energy Management for a 48V Mild Hybrid Electric Vehicle," SAE Technical Paper 2019-01-1208, 2019, doi:10.4271/2019-01-1208.

External collaborations

- Stanford University
- FEV Italy
- Powertech Engineering

Highlights of the research activity

Last-generation vehicles can be connected with the surrounding environment. The aim of this research activity is to assess, through numerical simulation, the potentialities coming from the integration of Vehicle-to-Everything (V2X) information into the powertrain control strategy of Hybrid Electric Vehicles (HEVs). The case study which was initially selected is a P2 diesel Plug-in Hybrid Electric Vehicle (PHEV) available on the European market. An experimental campaign was carried out on the real vehicle, and a virtual test rig was built in the GT-SUITE software environment and validated against experimental results (methodology and results published on SAE International Journal of Electrified Vehicles).

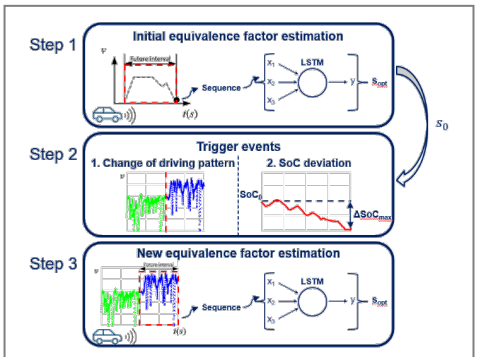


Figure 1 – Driving pattern identification to adapt the equivalence factor of an Equivalent Consumption Minimization Strategy (ECMS) based on V2X info

The virtual test rig was then used for testing several innovative optimization strategies. In the first part of the activity, driving pattern identification was employed to predict future driving conditions and, in turn, to adapt the equivalence factor of an Equivalent Consumption Minimization Strategy (ECMS) when a change in the driving patterns occurred. Long Short-Term Memory (LSTM) deep neural networks were properly trained for choosing the optimal value of equivalence factor for a specific sequence of data (i.e., speed, acceleration, power, and initial SoC). The results obtained were presented at the 2021 FISITA World Congress, and awarded with the 1st Prize Student Award. In a second phase of the activity, an eco-driving optimization was performed by simulating the vehicle in a connected environment. The associated control problem was formulated and solved by means of Dynamic Programming (DP), aiming to assess, through numerical simulation, the maximum benefits in terms of energy consumption reduction, which could be achieved by means of a synergic use of global optimization techniques and Vehicle-to-Everything (V2X) information. Finally, in a third and last phase of the activity, the EMS of the vehicle was redesigned by exploiting deep learning techniques, after training off-line the Artificial Intelligence (AI) models on a wide range of driving and traffic scenarios by providing the optimal solutions given by Dynamic Programming (DP).

From the 1st of November 2021, I am a Visiting Student Researcher at Stanford University invited by Prof. Simona Onori. This appointment will last 10 months, and my research activity is focused on the state of health estimation of battery packs combining electrochemical modeling and data-inspired algorithms.

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

Topic: Aerosol technology – Generation, diffusion, and mitigation of biologically active aerosols

Course year: 1st **Tutor(s)**: Paolo TRONVILLE, Marco SIMONETTI

Academic context

[1] Hinds, William C. Aerosol technology: properties, behavior, and measurement of airborne particles. John Wiley & Sons, 1999.
[2] Buonanno, Giorgio, Luca Stabile, and Lidia Morawska. "Estimation of airborne viral emission: Quanta emission rate of SARS-CoV-2 for infection risk assessment." Environment international 141 (2020): 105794.
[3] Wang, Chia C., et al. "Airborne transmission of respiratory viruses." Science 373.6558 (2021): eabd9149

Highlights of the research activity

The research activity carried out during the first year is divided into two subsets:

1- Literature review and experimental tests related to the performance of different types of masks
2- Investigation and simulation of the aerosol, particle tracking, and airflow in a closed area that is equipped with a bio stopper

For the first case, in the literature review, many references according to the mechanics of airborne particles were studied. After that, performances of different types of masks, including respirators, surgical masks, and community face covers (CFC), were investigated experimentally. Through precise use of devices and appropriate methodology, the factors of fractional efficiency and breathability were obtained, and after that, the quality factors of the samples were calculated. A comprehensive range comparison between the same type of masks was conducted according to the experimental data. For instance, a comparison was made between masks made with Spunbond and Meltblown layers. The result of this comparison is shown in the following figure. Concerning the test results, having had a layer of Meltblown was an obligation to have an acceptable performance. Also, as was expected, the more layers, the higher the efficiency and the lower the breathability. Other comparisons are related to the masks made with at least one layer of cotton material, the combination of different materials, investigating the effect of washing on the performance of the samples, and the impact of airflow velocity on the mask efficiency. For the second case, after studying different types of modeling for the simulation of airborne particles, a simple geometry was first chosen to model particle tracking by the Lagrangian method. Then, modeling the bio-stopper device – a device for circulating the air and controlling the path of airborne particles manufactured, patent-pending – and locating it in that simple geometry. The second step was to investigate the device performance in more complex geometry. This geometry included a desk and two persons sitting on chairs in a closed area. The simulation has been compared with qualitative results done by the group. The results prove the presence of bio-stopper could significantly prevent the pass of aerosol particles released by an infected to the other person.

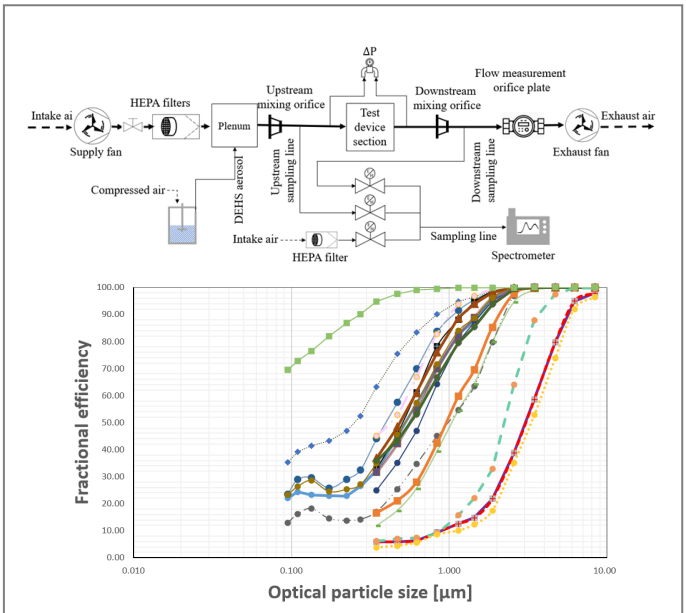


Figure 1 – The schematic of the mask setup and the results of comparing the masks made with Spunbond and Meltblown materials.

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

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

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

Academic context

[1] 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.
[2] M. Fasano et al., Thermal transmittance of carbon nanotube networks: Guidelines for novel thermal storage systems and polymeric material of thermal interest, Renewable and Sustainable Energy Reviews 41 (2015), 1028-1036.
[3] R. Pal Singh *et al.*, Thermal performance enhancement of eutectic PCM laden with functionalised graphene nanoplatelets for an efficient solar absorption cooling storage system, Journal of Energy Storage 33 (2021), 102092.

External collaborations

- Centro Ricerche ENEA Portici

Highlights of the research activity

A literature review about phase change materials (PCM), phase change slurries, phase change nanocomposites, polymeric nanocomposites, heat transfer at nanoscale, molecular dynamics simulations, percolation in composites, solid to solid phase change materials and barocaloric materials has been performed. As output of this review, an advanced draft of a review paper about the impact of additivation of different nanofillers in phase change materials has been generated. In the context of the collaboration with ENEA, a model to estimate the thermal conductivity of phase change materials nanocomposites using finite element simulations has been developed. A validation of the numerical model has been obtained through a comparison with the experimental measurements performed during the period as a visiting fellow at the center of ENEA Portici. Furthermore, an optimization of a heat storage tank for a real case application has been carried out to obtain an estimation of the optimal amount of nanofiller to add to the phase change material.

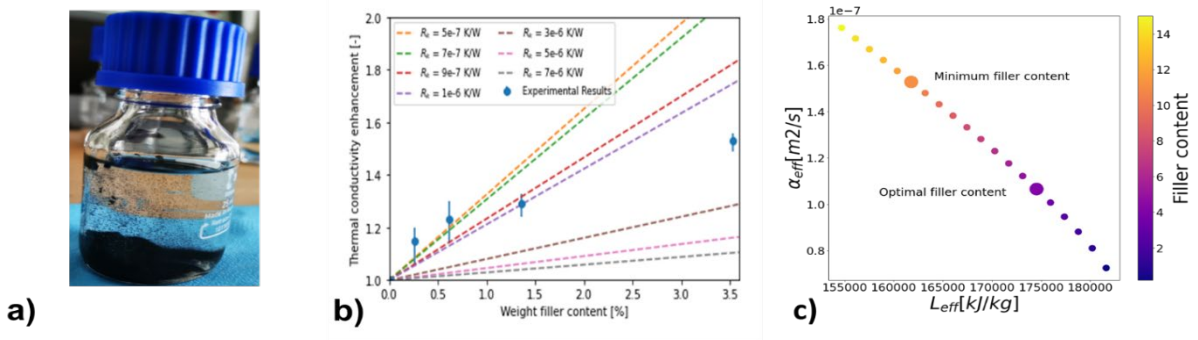


Figure 1 – a) Sample of PCM additivated with graphene nanoplatelets before the mixing process, b) Comparison between numerical simulations, performed with different interface resistances, and experimental measurements, c) Pareto front of PCM additivated with different filler content to obtain the optimal concentration (i.e. maximizing specific power and specific energy) and the minimum concentration ensuring melting of the whole PCM.

First name: Antonio **LAST NAME**: RICCIO

Topic: Exhaust after treatment systems (EAS) modelling for off road diesel engines

Course year: 2nd **Tutor**: Federico MILLO

Academic context

[1] Lafossas, F., Matsuda, Y., Mohammadi, A., Morishima, A. et al., "Calibration and Validation of a Diesel Oxidation Catalyst Model: from Synthetic Gas Testing to Driving Cycle Applications," SAE Int.J.Engines, 2011.
[2] Onorati, A.; Montenegro, G. "1D and Multi-D Modeling Techniques for IC Engine Simulation", ISBN 978-0-7680-9352-0, SAE International, 2020.
[3] Millo, F., Longhi S., Mallamo, F., International Journal of Engine Research, VOL.15, N. 8, pp.965-979, http://dx.doi.org/10.1177/1468087413492526.

External collaborations

- Lombardini S.r.l. (www.kohlerpower.com)
- CNR - Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili (STEMS) (www.stems.cnr.it)

Highlights of the research activity

The research activity is part of a wider research program carried out in Lombardini Srl, in close collaboration with Politecnico di Torino and CNR - STEMS, aiming to the development and to the deployment of advanced simulation methodologies to support the exploitation of new technologies for the control of pollutant emissions from diesel engines for off-road applications.

During this second year my activity focused on the development of a methodology for building and calibrating the kinetic scheme for the 1D-CFD model of an off-road Diesel Oxidation Catalyst by means of a Genetic Algorithm (GA) approach. The methodology consists of a preliminary experimental activity followed by a modelling process in GT-Suite environment. The tested aftertreatment component presents two zone coating with different Platinum Group Metal (PGM) loadings. Reactor scale samples representative of each coating zone were tested on synthetic gas bench (SGB). SGB test protocols were defined with the aim to decouple the effects of different mechanisms, by feeding the catalyst sample with controlled species concentrations, flow rates and temperatures, thus facilitating the model calibration process. On the modelling side, a 1D-CFD model of the component was built in GT-Suite environment and a global kinetic scheme was defined, based on the available literature, expressed in the Arrhenius form.

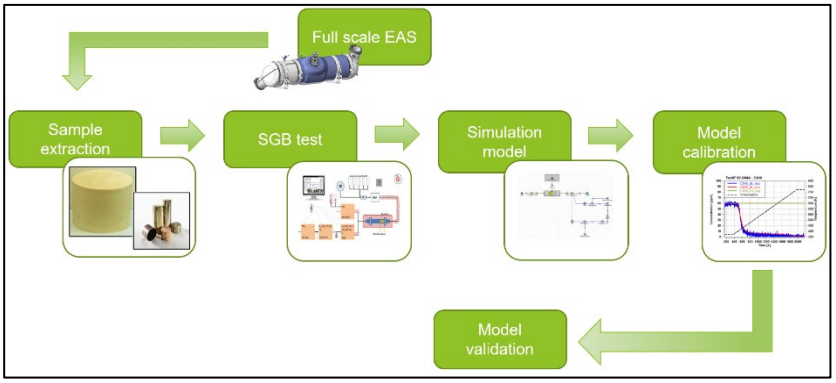


Figure 24 – 1D EAS model development and calibration protocol, from SGB to full size validation

A Genetic Algorithm optimization tool was then used to calibrate reaction rate parameters by means of a sequential calibration strategy, categorizing the reaction model into several steps according to the experimental test protocol. In each step of the calibration, the number of independent variables was reduced as much as possible, and the reactions could be isolated using primary single species tests, moving then to more complex gas mixtures to calibrate the mutual interaction of different species. The model was finally validated over experimental data, showing satisfactory results.

First name: Salvatore **LAST NAME**: ROGGIO

Topic: Study of Ultra-low NOx Diesel Combustion Systems by Synergetic Application of 3D-CFD and Single-Cylinder Engine

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

Academic context

[1] Millo, F., Piano, A., Roggio, S., Bianco, A. et al., "Numerical Investigation on Mixture Formation and Combustion Process of Innovative Piston Bowl Geometries in a Swirl-Supported Light-Duty Diesel Engine," SAE Int. J. Engines 14(2):247-262, 2021, https://doi.org/10.4271/03-14-02-0015.
[2] Millo, F., Piano, A., Roggio, S., Bianco, A. et al., "Numerical Assessment of Additive Manufacturing-Enabled Innovative Piston Bowl Design for a Light-Duty Diesel Engine Achieving Ultra-Low Engine-Out Soot Emissions," SAE Int. J. Engines 15(3):2022, https://doi.org/10.4271/03-15-03-0022.
[3] Millo, F., Piano, A., Roggio, S., Pastor, J.V. et al., "Mixture formation and combustion process analysis of an innovative diesel piston bowl design through the synergetic application of numerical and optical techniques," Fuel, 2022, 309:122144, https://doi.org/10.1016/j.fuel.2021.122144.

External collaborations

- PUNCH Torino S.p.A (formerly General Motors Global Propulsion Systems)
- CMT- Motores Térmicos (Universitat Politècnica de València)
- Powertech Engineering Srl

Highlights of the research activity

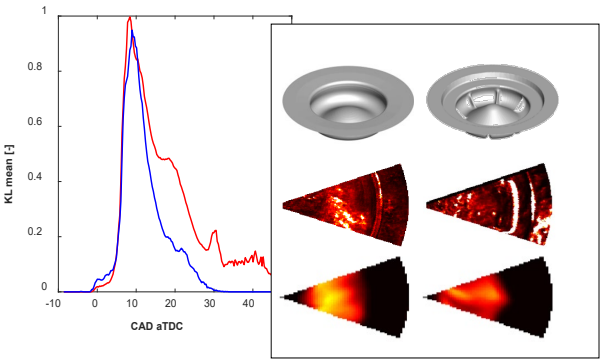


Figure 25 – Left: experimental mean soot-KL; Right: experimental and 3D-CFD soot-KL distribution. Partial load engine working point.

The research activity aims to develop innovative diesel combustion systems for the next generation of low-emissions engines by means of a synergetic approach based on 3D-CFD simulations and experiments. For the scope, a predictive combustion model based on detailed chemical kinetic mechanism and the Particulate Mimic (PM) soot model were adopted. Firstly, a stepped-lip and a radial-bumps bowls for a high-swirl light-duty diesel engine were assessed. These combustion systems have shown significant reduction of both fuel consumption and engine-out soot with respect to a conventional re-entrant bowl. Then, in order to understand if there are synergies between these abovementioned designs, a hybrid piston bowl was proposed. This innovative profile combines both a highly re-entrant sharp-stepped bowl and a number of radial bumps in the inner bowl rim equal to the injector nozzle holes. The combustion simulations highlighted for the hybrid bowl a remarkable soot reduction (up to -70% at partial load) compared to the re-entrant bowl, without any efficiency worsening. The numerical results were finally compared against experimental data from an optical access engine, in the framework of a collaboration with CMT-UPV. The combustion image velocimetry (CIV) and OH* chemiluminescence experimental techniques were used to evaluate the kinematic analysis of the flame and to qualitative analyse the oxidation rate, respectively. Then, the 2-color pyrometry technique was adopted to obtain the optical soot density (KL) and the temperature of the soot surface. To directly compare the numerical results with the experimental KL distribution, a numerical methodology was developed. The comparison between 3D-CFD results and experiments showed a good agreement in terms of soot distribution. This analysis confirmed that the hybrid bowl strongly mitigates the flame-to-flame interaction leading to lower soot formation in the flame collision area. Moreover, faster flame propagation toward the cylinder axis is highlighted with a consequent higher soot oxidation rate. Future analysis will be focused on additional piston geometry optimization enabled by Additive-Manufacturing techniques which guarantee extremely complex geometry and the durability request for a diesel engine.

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

Topic: Unsteady interaction in High Pressure Turbine Stages

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

Academic context

[1] Fluid machines

External collaborations

- University of Purdue

Highlights of the research activity

An extensive activity related to the performance of numerical models in the prediction of the thermal performance of cooling holes on a simplified test rig was performed reproducing the experimental setup studied at the University of Karlsruhe during the TATEF project. The activity was majorly devoted to the assessment of RANS and Scale Adaptive Simulation models for a cylindrical cooling hole at various blowing conditions in a compressible regime (Ma=0.6) with a Reynolds number equal to 3*10^4.
The activity was divided into 3 different steps:

1. Steady RANS modelling
2. Unsteady RANS modelling
3. Hybrid modelling

Steady RANS modelling highlighted the inability of RANS closure to correctly predict the mixing occurring at inertial scale of motion between the hot gas and the cooling flow
Unsteady RANS simulations proved to be able to capture integral unsteady interaction between the two flows. Nevertheless, the mixing was still underpredicted and time-averaged results are comparable with the steady approach. This does not justify increased time resources necessary to obtain unsteady convergence when compared to a steady RANS approach.
SAS model allows for a better matching between the numerically predicted temperature maps and the experimental counterpart thanks to an improved prediction of the mixing. Still the penetration of the cold jet is still underestimated, confirming previous results of the literature. The final part of the activity will be dedicated to the analysis of coherent time-space modes due to the hot-cold flow interaction.

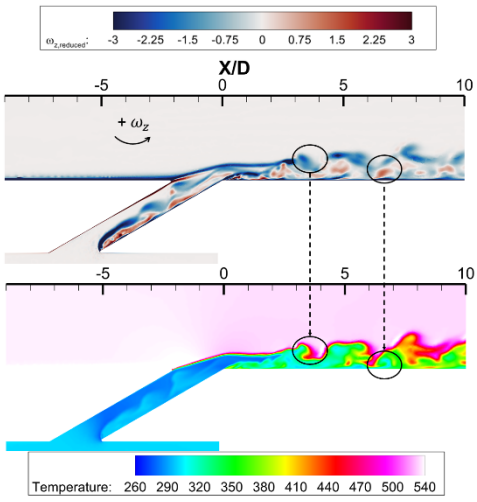


Figure 2 – Hot gas - coolant interaction

The second major topic, in collaboration with the University of Purdue is focused on the analysis of the impact of rim-seal flow on the aerodynamics and heat transfer of a transonic high-pressure turbine stage.
Three main configurations are under analysis:

1. Nominal rotational speed with flow purge
2. Nominal rotational speed with flow ingestion
3. Low rotational speed with flow purge

The first part was devoted to the validation of the numerical setup versus experimental data regarding the rotor blade load, hub pressure distribution and outlet radial traverses for total pressure and temperature.
The numerical simulations were able to reproduce experimental results and trends at various blowing conditions, highlighting the impact of flow purge over the pressure distribution at the stator outlet and the stage degree of reaction.
The second part is mainly focused on the study of secondary flows redistribution, also compared with steady approaches (such as Frozen Rotor), and to the study of the heat transfer of the stage.

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

Topic: Urban energy atlas for a sustainable development

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

Academic context

[1] "An Energy Community for Territorial Resilience. The Measurement of the Risk of Energy Supply Blackout", Mutani G., Santantonio S, Brunetta G., Caldarice O., Demichela M., Energy and Buildings, Vol. 240 (110906), 2021, DOI: https://doi.org/10.1016/j.enbuild.2021.110906.
[2] "Urban-Scale energy models: the relationship between cooling energy demand and urban form", Mutani G., Todeschi V., Santantonio S., Journal of Physics: Conference Series, 38th International Conference on Heat and Mass Transfer (UIT), June 21st-23rd, 2021, Gaeta.
[3] "Evaluation of ventilation loads in buildings energy modelling at urban scale", Mutani G., Santantonio S., Todeschi V., IEEE Cando Conference 2021, November 17-18, 2021, Budapest.

External collaborations

- Idiap Research Institute, Martigny, CH

Highlights of the research activity

The building stock in urban areas accounts as a major source of climate changing emissions. Here, higher degrees of liveability are related to energy security and affordability, the reduction of GHG emissions and the resilience in case of unexpected events. Sustainable energy policies are required at every context and scale, with local energy planning relying on place-based and holistic approaches. Data spatialisation allows to supply energy where it is required, having identified energy supply options and explored energy efficiency solutions [1]. Urban-Scale Energy Models allow to obtain lower energy demand by optimizing the morphology of the built environment and local energy production. The definition at a larger scale of the energy-related variables, used in validated models and standards, allows to assess energy consumption and productivity at district, urban or territorial scale. Relying on available databases, a simplified, flexible methodology has been validated by our research group. A GIS-based engineering model consists in the dynamic energy balance of buildings at urban scale, ensuring reliable results with short-time simulation and its adaptability to different case studies. During the first PhD year, my research activity focused on the calibration of the GIS-based model to assess the hourly space cooling energy consumption of residential building [2]. The re-scaling of the input parameters (local climate, urban morphology, building characteristics) has allowed to apply the model at the block of building scale, investigating the relationship between the urban morphology and their cooling energy demand. The same input parameters have been also considered to assess a monthly variation of ventilation load and number of air changes per hour (ach) at buildings scale [3]. This first results encourage me to pursue my research in the validation of a methodology at neighbourhood scale able to exploit the GIS tools potential and to implement our model by investigating: i) the influence of microclimatic conditions, building orientation, shape and permeability, and urban morphology on hourly variability of ach; ii) how the air flow rates affect the overall energy performance of buildings, analysing loads of the thermal balance, iii) how urban morphology influences the ventilation rate impacting on energy consumption and thermal comfort.

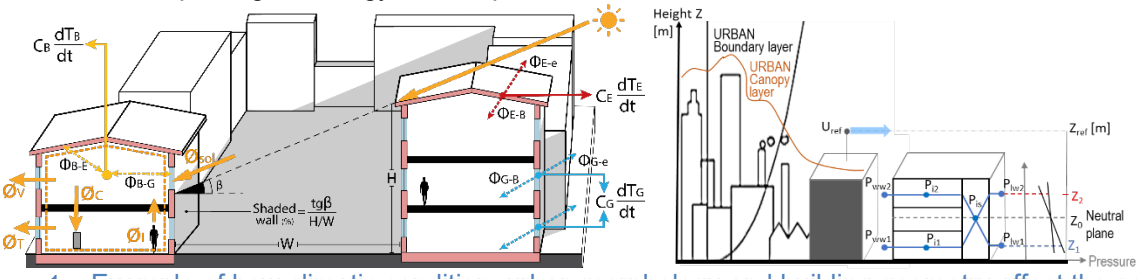


Figure 1 – Example of how climatic condition, urban morphology and building geometry affect the solar exposition (left) and the ventilation loads (right) at block of buildings scale.

First name: Daniele S. **LAST NAME**: SCHIERA

Topic: A holistic methodology, software platform and toolset for modelling and simulation of Cyber-Physical Multi-Energy Systems

Course year: 3rd **Tutor(s)**: Romano BORCHIELLINI, Carlo CAMBINI

Academic context

[1] D. S. Schiera, F. D. Minuto, L. Bottaccioli, R. Borchiellini, A. Lanzini, "*Analysis of Rooftop Photovoltaics Diffusion in Energy Community Buildings by a Novel GIS- and Agent-Based Modeling Co-Simulation Platform*," in IEEE Access, vol. 7, pp. 93404-93432, 2019;
[2] D. S. Schiera et al., "*A Distributed Multimodel Platform to Cosimulate Multienergy Systems in Smart Buildings*," IEEE Transaction on Industry Application, vol. 57, no. 5, pp. 4428–4440, 2021;
[3] L. Barbierato, D. S. Schiera, E. Patti, E. Macii, E. Pons, E. F. Bompard, A. Lanzini, R. Borchiellini, L. Bottaccioli, *"GAMES: A General-Purpose Architectural Model for Multi-energy System Engineering Applications,"* in Proceedings of. 2020 IEEE 44th Annual Computers, Software, and Applications Conference (COMPSAC), Madrid, Spain, 2020, pp. 1405-1410.

External collaborations

- European Project H2020 PLANET (https://www.h2020-planet.eu/).
- TU Delft
- OFFIS - Institute for Information Technology

Highlights of the research activity

The PhD research activities focus on developing a holistic methodology, software platform and toolset for modelling, simulation, control and optimization of Cyber-Physical Multi-Energy Systems, such as the Urban Energy System (UES). In particular, the proposed methodology aims to integrate energy planning and operational dimensions, exploiting the synergies of energy sector coupling, automation and digitalization, as modern energy systems increasingly rely on communication and information technology to combine smart controls with hardware infrastructure, operating on different spatial and temporal scales and often across different engineering domains. The methodology consists of adoption of Model-Based Engineering (MBE) by proposing an architectural model called GAMES (General purpose Architecture for Multi-Energy System) [3] to support the system design of UES use case, and a hybrid multi-modelling co-simulation platform [1, 2] that can integrate different domain-specific models in a plug-and-play fashion and Real-Time Hardware-In-the-Loop (Fig. 1). GAMES extends the well-known Smart Grid Architecture Model by adding more functionalities, i.e., description and integration of other energy networks with the electricity grid, analysis and simulation tools through the co-simulation infrastructure, composition and automation of use cases throughout the MBE process. The software platform exploits Mosaik, a Python-based Co-simulation Orchestrator Engine capable of managing multi-model time synchronization and their data exchange. Mosaik has been extended, including: i) Scenario Builder that composes the UES use case developed in GAMES through an effective cross-domain scenario configuration procedure that establishes a common understanding among the co-simulation expert and the model domain experts, ii) Functional Mock-up Interface (FMI) to couple heterogeneous domain-specific models (e.g. MATLAB, Simulink, Modelica, Energy Plus), and iii) VILLASframework to provide interfaces with Digital Real-Time Simulation and Hardware-In-the-Loop.

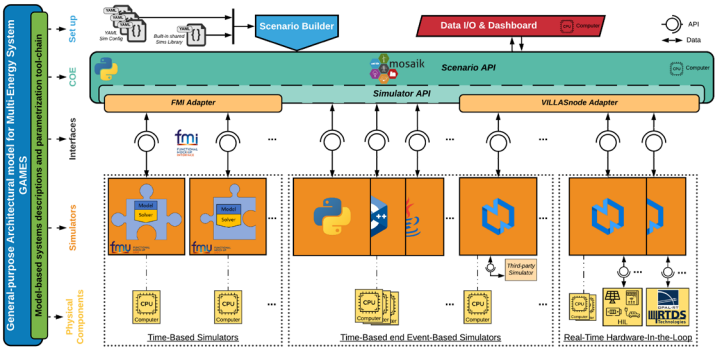


Figure 1 – Hybrid Multi-Modelling Co-Simulation Platform for Cyber-Physical Multi-Energy Systems

First name: Sonja **LAST NAME**: SECHI

Topic: Multi-scale energy and materials modelling for the decarbonisation and sustainability of the industrial sector

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

Academic context

[1] Pauliuk, S., Arvesen, A., Stadler, K. et al. Industrial ecology in integrated assessment models. Nature Clim Change 7, 13–20 (2017)
[2] Neves, A., Godina, R., Azevedo, S. G., & Matias, J. C. O. (2020). A comprehensive review of industrial symbiosis. In *Journal of Cleaner Production* (Vol. 247). Elsevier Ltd.
[3] Stefan Pfenninger, Adam Hawkes, James Keirstead, "Energy systems modeling for twenty-first century energy challenges", *Renewable and Sustainable Energy Reviews*, Volume 33, 2014, Pages 74-86

External collaborations

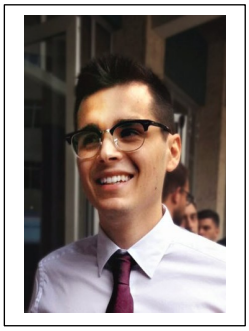
- Imperial College London
- Engie
- Enea

Highlights of the research activity

During the first months* of the second year of my PhD, the research investigated the possibility to introduce a new industry module in the framework of a selected Integrated Assessment Mode (IAM). This kind of models are widely used and well-known for energy and climate future scenario [1]. The IAM chosen for the analysis is able to simulate the heterogeneity of agents such as investors or consumers. Moreover the open source code developed in Python and framework allows to expand the model and to try to answer to new research questions.
In particular, the research questions we are trying to explore and indagate with the model concern the following three main aspects:
1)The modelling of industrial clusters both as an independent module but also as a part of regional models. Hence, the goal is the application of the module in geographical context where these structures are diffused and representative of a relevant share of the energy consumption and the greenhouses emissions. A first mapping of the industrial clusters (Fig.1) linked by a common demand of hydrogen was carried out for Europe and the North Africa, but other characteristics of the industrial districts will selected in order to define some cluster archetypes, to generalize the methodology and to extend the module at a regional level;

Figure 26 – Industrial clusters linked by hydrogen demand.

2) The modelling of industries as prosumers (including distributed power production) and as possible actors of the flexibility market capacity. In fact the contribution of renewable heat and electricity in heavy industries is still scarse (less than 1% of the combined energy demand in 2018 according the REN21 report) and energy models should add more details to this aspect to identify appropriate policies for industry sector and hence to make industrial solutions competitive too;
3) the modelling of a module for circular economy and industrial symbiosis [2],[3], between different industry sectors and/or different sectors exploring also the possibility to enlarge the environmental aspects through the introduction of specific indicators based on the specific sector.
The on-going analysis and its scale depends to some extent on the availability of industrial data with the appropriate granularity. The industrial collaborations should facilitate the access of companies data.



First name: Stefano **LAST NAME**: SEGANTIN

Topic: Development of radiation resistant materials for compact tokamak cores

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

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] Segantin, S., et al. "ARC reactor–Neutron irradiation analysis." *Fusion Engineering and Design* 159 (2020): 111792.
[3] Jin, M., et al. "Thermodynamic mixing energy and heterogeneous diffusion uncover the mechanisms of radiation damage reduction in single-phase Ni-Fe alloys." *Acta Materialia* 147 (2018): 16-23.

External collaborations

- Massachusetts Institute of Technology (MIT), Cambridge, MA, US
- ENI – San Donato Milanese (MI), Italy

Highlights of the research activity

The aim of the third year of PhD was to provide general design guidelines for radiation resistant materials for compact tokamak applications. In this framework, the main issues identified are the irradiation primary damage and the swelling rate. Figures of merit for the primary damage have been identified as the defect production and the size of the defect clusters that show up with high energy radiation in ordered systems such as transition metals. Figures of merit for swelling are the defect clusters size and the gas transmutation. Evaluations on primary damage usually require complex molecular dynamics simulations modeled specifically for the material of interest. Studies of the third year of PhD determined the primary damage modeling strategies targeting a wide range of materials. In addition, an explanation linking the thermodynamic properties of each material and its radiation resistance is provided. Materials chosen were pure metals and some solid solutions based on the same pure metals. The potential energy landscape of each system has been characterized in terms of average potential energy (U) and defects Migration Energy Barriers (MEB). Irradiation damage has been modeled as subsequent collisional cascades to the systems up to defect saturation. It has been found that there is a strong linear correlation between the defect production in a system and the MEB-U ratio (MUR) of the system itself for pure metals, effectively linking material thermodynamic properties to its radiation resistance. Furthermore, mixed systems stand below the uncovered line of pure metals. Mixed systems can have similar radiation damage of pure metals. Lastly, at equimolar concentrations of mixed systems a minimization of the defect clusters size has been recorded. Mixed systems at equimolar concentrations made up by low MUR and low gas transmutation elements have the potentialities to hold high radiation resistance and minimized swelling rates. Lastly, these findings seem to have a wide range of validity on materials, which can accelerate the design of future radiation resistant alloys.

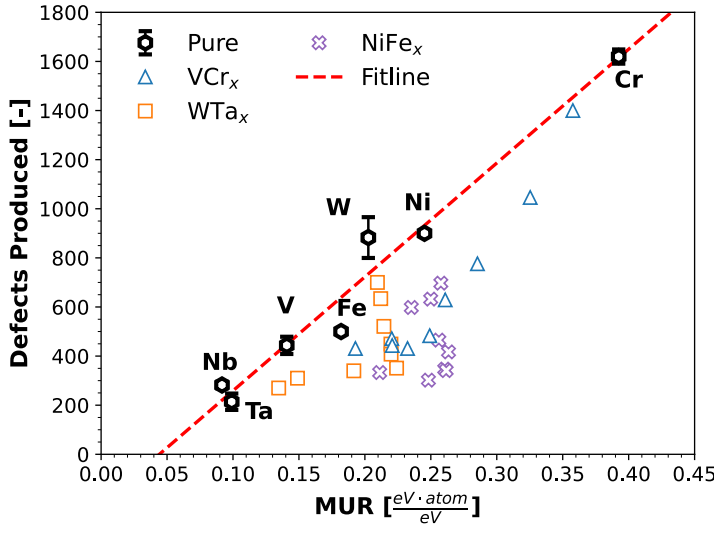


Figure 1 – Radiation damage vs MUR of pure metals and mixed systems after primary damage saturation

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

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

Course year: 1st **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," *Appl. 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] Millo, F., Piano, A., Peiretti Paradisi, B., Segatori, C. et al., "Ducted Fuel Injection: A Numerical Soot-Targeted Duct Geometry Optimization," *SAE Int. J. Engines* (2022), doi:10.4271/03-15-02-0014.

External collaborations

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

Highlights of the research activity

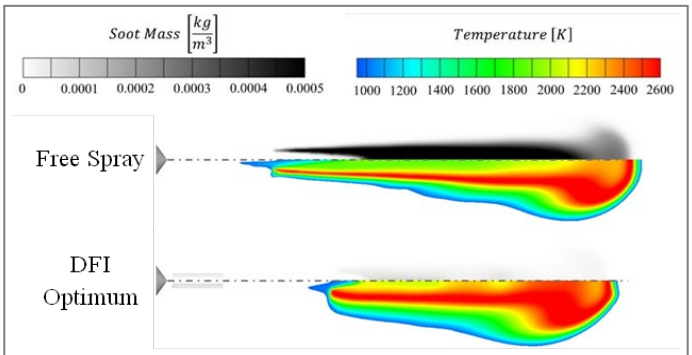


Figure 27 – Soot mass and temperature distributions on a section of the spray flame for free spray (top) and DFI (bottom) featuring the optimized duct configuration.

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 important 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, 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 the light of this, the present research activity aims to cover several key knowledge gaps for the complete success of this new concept. A 3D-Computational Fluid Dynamics (CFD) high-fidelity virtual test rig, calibrated and validated against spray experimental data, was developed as mean to investigate the DFI-related physics in constant-volume conditions. DFI showed a dramatic enhancement of the air entrainment into the fuel spray and the turbulent mixing, leading to a leaner and more homogeneous air/fuel mixture in the auto-ignition zone. Furthermore, the impact of the main duct geometrical features (length, diameter, shape, etc.) was studied, allowing to figure out an optimal duct geometry (Fig.1), able to reach a soot mass reduction of about 94% compared to the free spray configuration. DFI ability in soot mitigation was also demonstrated over a wide range of engine operating conditions. On-going activities include an accurate analysis of DFI physical mechanisms through more detailed and computationally expensive CFD simulations (i.e., LES) and exploration of DFI potential benefits on a series production PUNCH propulsion system, highlighting the factors which can limit or facilitate its integration in existing combustion chambers.

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

Topic: Modeling of concentrated solar power systems

Course year: 1st **Tutor(s)**: Roberto ZANINO, Mattia CAGNOLI

Academic context

[1] 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.
[2] 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.
[3] Forristall, R., 2003. Heat Transfer Analysis and Modeling of a Parabolic Trough Solar Receiver Implemented in Engineering Equation Solver. Technical Report, NREL/TP- 550-34169. National Renewable Energy Laboratory.

External collaborations

- ENEA, Casaccia, Italy

Highlights of the research activity

- Two main activities have been followed during the first year of my PhD program: optimization of the photo-thermal efficiency applied to a parabolic trough plant, and comparative economic and thermal analysis of the Parabolic and Fresnel technology using encapsulated and evacuated tubes.
- For the parabolic trough system, the developed Modelica code was first validated by means of experimental data provided by ENEA.
- The best photo-thermal performance of the system was found using 3 different coatings along the absorber tube. Such a strategy increased the photo-thermal efficiency nearly 1% in average, compared to the single-coating tubes, and consequently decreased the required tube length by around 190 m. Hence, it was proven that using a coating suitable for low temperature in most of the receiver length could be economically advantageous.
- For the Fresnel system, a 2D CFD model was developed to obtain the relevant heat transfer coefficient between the glass envelope outer surface and the ambient air. In fact, in the Fresnel configuration a secondary reflector is mounted over the receiver acting as a shield against the wind and, consequently, the correlations available in literature for cylinders in cross flow are not applicable here.
- The CFD model was first validated by available correlations for the isothermal cylinder in the case of natural convection and parallel (forced) flow.
- The model has been then exploited to determine the new Nusselt number correlations for the Fresnel receiver unit, considering the presence of the secondary reflector, which have been then implemented in the Modelica code to make this model able to simulate also the Fresnel systems.
- A parametric analysis was carried out comparing the evacuated and non-evacuated tubes. The thermal performance of the evacuated tube is much better than the non-evacuated one.
- The comparative economic analysis of the two configurations is in progress.

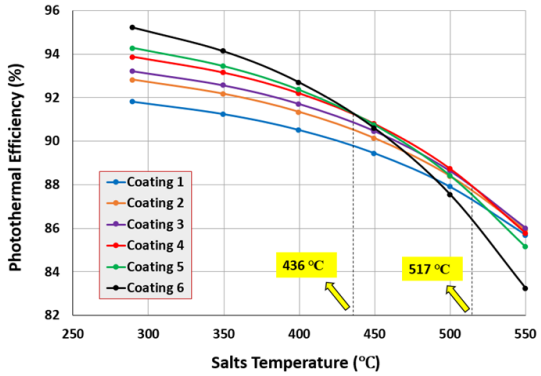


Figure 1 – Optimization of photo-thermal efficiency for the six absorber tubes

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: 1st **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

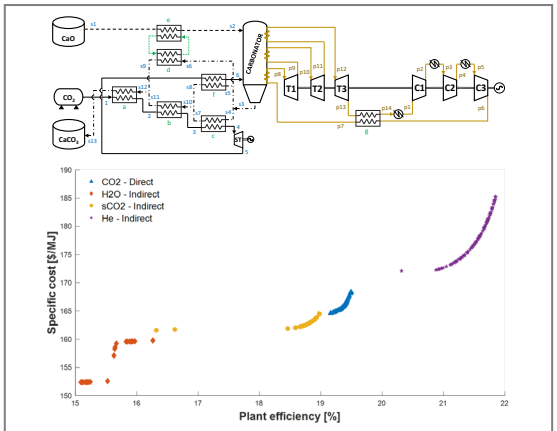
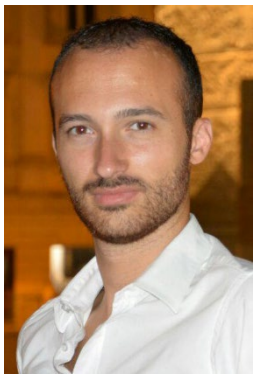


Figure 28 - Plant layout for indirect He cycle integration and composite Pareto curve of power blocks integration in a CaL-CSP plant.

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 a literature review as detailed as possible. 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. Despite most of the fundamental features of energy systems have been implemented, there are still some important elements that require a proper treatment. Among these are the uncertainties affecting the inputs, the thermal inertia of heating/cooling networks and a reliable modelling of energy storages. In light of the works found in the scientific literature, I have written a review paper that is intended to be published on an international journal. The scope is to provide an overview of the research in the sector of the energy systems, guiding the implementation of the optimization problem by giving the mathematical formulation of the most simple and effective methodologies currently available. In the meanwhile, I started the development of an optimization model for the operation of an energy system in the framework of a collaboration with the research center of an international company. As an attempt to deal with one of the unsolved issues characterizing energy hubs, the effect of the thermal inertia of the heating network has been implemented.
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, a paper regarding integrations comparison is now under drafting.



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

Topic: Towards sustainable biofuel production for aviation, marine and heavy duty

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

Academic context

[1] Chiaramonti, David; Talluri, Giacomo; Vourliotakis, George; Testa, Lorenzo; Prussi, ... (2021) Can Lower Carbon Aviation Fuels (LCAF) Really Complement Sustainable Aviation Fuel (SAF) towards EU Aviation Decarbonization?. In: ENERGIES, vol. 14. ISSN 1996-1073
[2] 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
[3] 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

- RE-CORD (https://www.re-cord.org/)
- EXERGIA (https://exergia.gr/)
- FAO (https://www.fao.org/)

Highlights of the research activity

The research activity is framed in the field of biofuels production through thermochemical conversion processes and is thus strictly connected to refineries and renewables.
I worked on the JRC project "*Analysis of the potential impact of Lower Carbon Aviation Fuels (LCAF) in the European alternative fuel sector"*, mainly aimed to identify of the production potential for LCAF technologies and practices, and to estimate the potential market share of LCAF in the EU context. A paper in this matter has been written and published on the scientific journal "Energies".
The main endeavor of my research is the H2020 BIKE *("Biofuels production at low Iluc risK for European sustainable bioeconomy")*, which supports the implementation of the RED II of the EC in the matter of low ILUC-risk biofuels. The activities of BIKE are organized around two value chain types: (a) cultivation in unused, abandoned or severely degraded land, and (b) productivity increases from improved agricultural practices. The value chain I am involved in is (b), more specifically the production of biogas through Biogas Done Right model (BDR) in decentralized plants, injection of biomethane into the grid, and further processing in centralized biomethane-to-liquid conversion plants for Fischer-Tropsch fuels or MeOH production. In this matter, I carried out a review of the Italian "Decreto Biometano 02/03/2018", focusing on its applicability to the aforementioned value chain. Moreover, I am working on a review article and the construction of an Aspen Plus model simulating the production chain from biomass to FT fuels and MeOH.

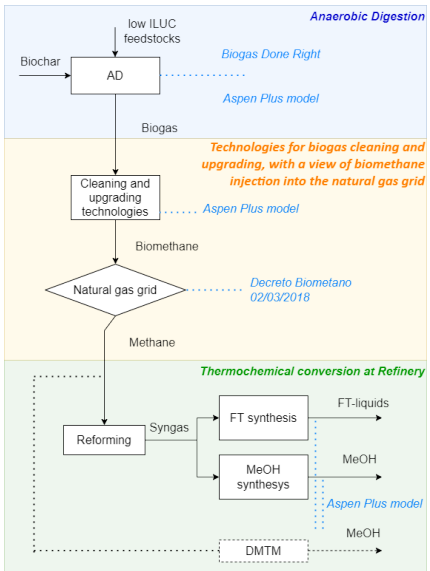


Figure 29 – Research activity flowchart

The processes involved are: (1) Anaerobic Digestion for biogas production, (2) cleaning and upgrading, (3) reforming, (4) Fischer-Tropsch synthesis, (5) methanol synthesis, (6) DMTM. Additionally, I am involved in other BIKE tasks, i.e. a technology review to assess the present EU biofuels production sites, and a technology innovation assessment of low ILUC-risk system in the EU biofuels sector.

First name: Valeria **LAST NAME**: TODESCHI

Topic: Smart energy solutions for sustainable cities and policies

Course year: 3rd **Tutor(s)**: Guglielmina MUTANI, Marco MASOERO

Academic context

[1] "Energy consumption models at urban scale to measure energy resilience", G. Mutani, V. Todeschi, S. Beltramino, in: *Sustainability*, Vol. 12, No. 14, 5678 (2020) DOI: 10.3390/su12145678
[2] "Evaluation of Urban-Scale Building Energy-Use Models and Tools—Application for the City of Fribourg, Switzerland", V. Todeschi, R. Boghetti, G. Mutani, J.H. Kämpf, in: *Sustainability,* Vol. 13, No. 4, 1595 (2021) DOI: 10.3390/su13041595
[3] "Optimization of Costs and Self-Sufficiency for Roof Integrated Photovoltaic Technologies on Residential Buildings", G. Mutani, V. Todeschi, in: *Energies*, Vol. 14, No 13, 4018 (2021) DOI: 10.3390/en14134018

External collaborations

- Ecole Polytechnique Fédérale de Lausanne (EPFL), CH
- Idiap Research Institute, Martigny, CH
- Joint Research Centre (JRC), Ispra (VA), IT

Highlights of the research activity

The buildings sector in the EU accounted for about 38% of total energy-related CO_2 emissions, and buildings play a central role in the clean energy transition. To achieve energy sustainability in urban contexts, two main actions are needed: the improvement of energy efficiency level of buildings and the exploitation of the available renewable energy sources (RESs). The development of Urban-Scale Energy Modelling (USEM) is currently the goal of many research groups due to the increased interest in evaluating the impact of energy efficiency measures in city environments. USEMs are useful to explore energy efficiency solutions at district or city scales and to quantitatively assess retrofit strategies and energy supply options on the real built environment.
A review of the literature reveals that USEMs only consider a few of the variables that influence energy consumption, especially as regards the urban context. Research should be dedicated to the construction of engineering models that consider several possible factors to describe the urban environment, to develop a process-driven model that is flexible and can easily be applied to different contexts.
The aim of my PhD research is to investigate and create new energy models at urban scale to drive a smarter use of energy, and to match the energy demand with more efficient available energy sources, especially to help public administrations in defining policies adapted to existing and future built environment, population and climate. In the three years of my PhD, data-driven and process-driven energy models at urban scale that use top-down and bottom approaches were designed for different European cities [1, 2]. Using Geographic Information System (GIS) tools, these models can estimate energy consumption, energy production and energy productivity from RESs related to a specific territory, considering their spatial distribution and the local environmental impact [3]. The novelty of these place-based models is that they add a number of variables to the energy balance of the built environment to take the urban context into account. These models were applied in future climate scenarios, to evaluate the impact of climate change in the energy demand/supply of buildings, as well as in the potential retrofit scenarios. These models were also used to evaluate the feasibility of energy communities, grouping users and prosumers to improve self-sufficiency and self-consumption (Figure 1).

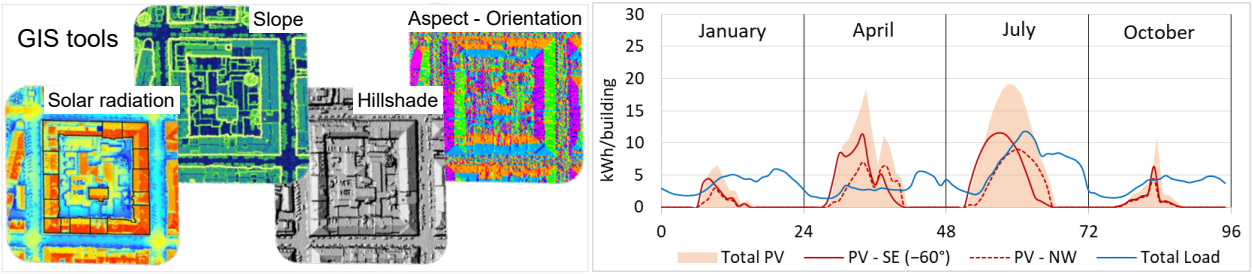


Figure 1 – Solar PV potential analysis at block of buildings scale (left), and hourly electrical consumption and PV potential at building level for typical days (right).

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

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

Course year: 1st **Tutor(s)**: Eliodoro CHIAVAZZO, Matteo FASANO, Luca BERGAMASCO

Academic context

[1] Trezza, Giovanni, et al. "Minimal set of crystallographic descriptors for sorption properties in hypothetical Metal Organic Frameworks: Role in sequential learning optimization." *arXiv preprint arXiv:2111.09602* (2021).
[2] Boyd, Peter G., et al. "Data-driven design of metal–organic frameworks for wet flue gas CO2 capture." *Nature* 576.7786 (2019): 253-256.
[3] E. Brochu, et al. "A tutorial on bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning", *arXiv preprint arXiv:1012.2599* (2010).

External collaborations

- École Polytechnique Fédérale de Lausanne
- IBM Zurich

Highlights of the research activity

I mainly focused on the investigation of relatively new compounds, namely Metal Organic Frameworks (MOFs), by means of Machine Learning (ML) techniques. In particular, those materials are employable in the Energy field by exploiting physisorption phenomena, which can be accompanied by significant amount of energy exchange. In this work, I considered adsorption/desorption-based heat pumps as possible application. In such a context, this activity aimed at understanding which properties, at the elementary cell level, influence the performances of a heat pump based on MOFs allowing adsorption/desorption of water. Another target of this work was to achieve a comprehensive comparison of algorithms for sequential MOFs optimization, assuming to ignore the values of relevant properties. In such cases, efficient exploration algorithms are provided by Sequential Learning (SL), aiming at reducing the number of evaluations to be performed. In order to achieve those targets, I have first featurized the Crystallographic Information Files (CIFs) of roughly 8000 potential MOFs, ending up with 1557 crystallographic-based descriptors for each one. Furthermore, for three available DFT-computed properties, i.e., Henry coefficient for CO_2, Working capacity for CO_2, Henry coefficient for H_2O, I have trained the corresponding regression ML models, identifying the relevance of each descriptor over the models outputs. Thus, I investigated the use of those potential MOFs for closed water sorption thermal energy storage application. More specifically, over the database above, I identified the material maximizing the released heat – dependent on the Henry coefficient for H_2O - under specific operating and environmental conditions. Finally, for the SL procedure, I have compared more methodologies for efficiently choosing the next material to be tested, aiming at the maximization of the three DFT-based properties above; as result, it turned out that employing the subset of the most important features, in general does not ensure a faster convergence of the SL methodologies.

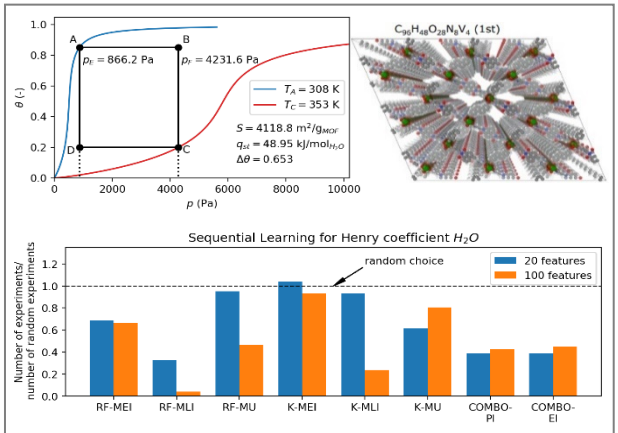


Figure 1 – TOP: adsorption/desorption based heat pump ideal cycle for the optimal potential MOF in the database, with the related CIF. BOTTOM: number of evaluations before the convergence to the maximum for SL over the H_2O Henry coefficient.

First name: Daniel **LAST NAME**: URIBE

Topic: Understanding the behavior of PCM glazing and evaluating its impact on occupants' comfort and the energy performance of open-plan office buildings

Course year: 1st **Tutor(s)**: Marco PERINO, Sergio VERA

Academic context

[1] F. Goia, M. Perino, and M. Haase, "A numerical model to evaluate the thermal behaviour of PCM glazing system configurations," Energy and Buildings, vol. 54, pp. 141-153, 2012/11/01/ 2012.
[2] L. Giovannini, F. Goia, V. R. M. Lo Verso, and V. Serra, "A Comparative Analysis of the Visual Comfort Performance between a PCM Glazing and a Conventional Selective Double Glazed Unit," Sustainability, vol. 10, no. 10, pp. 1-20, 2018
[3] M. Pomianowski, P. Heiselberg, and Y. Zhang, "Review of thermal energy storage technologies based on PCM application in buildings," Energy and Buildings, vol. 67, pp. 56-69, 2013/12/01/ 2013

External collaborations

- Pontifical Catholic University of Chile
- Center for Sustainable Urban Development CEDEUS (Chile)
- Lodz University of Technology (Poland)

Highlights of the research activity

Open plan office buildings have poor thermal inertia in the envelope because they are built using columns and slabs, then they used to present overheating problems. Double-glazed windows filled with Phase Change Materials, or PCM glazing, can increase the thermal inertia of the envelope, taking advantage of the energy storage of the PCM. In addition, PCM glazing has advantages regarding low cost and solar heat gains control. From the literature, a numerical heat transfer model and a daylight transfer model of a PCM glazing were developed and experimentally validated. The numerical heat transfer model was integrated into EnergyPlus to perform energy performance simulations. The daylight transfer model was developed in Radiance. The energy and occupants' comfort performance analysis of office buildings with PCM glazing in different climates were assessed. An optimization process is carried out to determine the best PCM glazing disposition on the buildings.

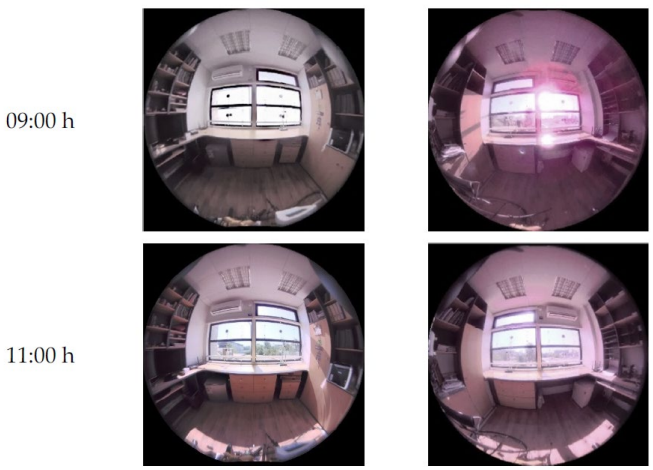


Figure 1 - Pictures of the experimental setup of two offices with PCM glazing (left) and double-clear glazing (right).

First name: Domenico **LAST NAME**: VALERIO

Topic: Multi-physics modelling of liquid metals in Advanced Nuclear Systems

Course year: 3rd **Tutor(s)**: Sandra DULLA, Roberto BONIFETTO

Academic context

[1] F. Papa, D. Valerio et al., "Engineering design of a Permeator Against Vacuum mock-up with niobium membrane," *Fusion Eng. Des.*, vol. 166, no. February, p. 112313, 2021, doi: 10.1016/j.fusengdes.2021.112313
[2] R. Bonifetto, M. Utili, D. Valerio, and R. Zanino, "Conceptual design of a PAV-based tritium extractor for the WCLL breeding blanket of the EU DEMO : effects of surface-limited vs . diffusion-limited modeling," *Fusion Eng. Des.*, vol. 167, no. February, p. 112363, 2021, doi: 10.1016/j.fusengdes.2021.112363
[3] M. Massone, G. F. Nallo, D. Valerio, S. Dulla, and P. Ravetto, "Code-to-code SIMMER / FRENETIC comparison for the neutronic simulation of lead-cooled fast reactors," *Submitt. to Ann. Nucl. Energy*, 2021.

External collaborations

- ENEA
- Karlsruhe Institute of Technology (KIT)
- EUROfusion

Highlights of the research activity

The main outcome of the fusion activities consists in the development of a new model for the permeation of hydrogen/tritium from a liquid-metal carrier to the vacuum across a metallic membrane. With respect to a model where only the mass flux diffusion across the membrane is considered, capable to deal only with diffusion-limited permeation regimes, the surface phenomena are also accounted for here, encompassing adsorption, desorption, absorption, and de-absorption mass fluxes on each side of the membrane. The model has been verified and compared to purely diffusion-limited approach, showing that it can model both the diffusion-limited regime and the surface-limited regime (where permeation is driven by the above-mentioned surface phenomena) if proper conditions are applied. It has therefore been used to design the mock-up of the EU DEMO tritium extraction system (TES) based on the permeator against vacuum (PAV). Moreover, FEM have been used to calculate the mechanical stresses and CFD analyses have been performed to verify if the mass flow distribution in the mock-up could ensure sufficient turbulence to promote the hydrogen/tritium transport towards the membrane [1]. The new model has then been used to size the PAV of the TES at DEMO scale [2].

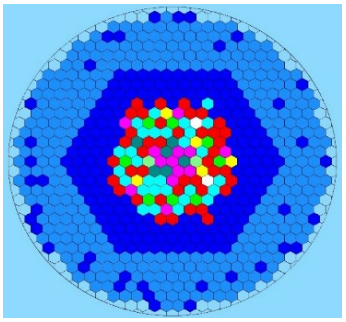
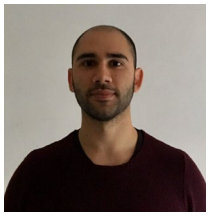


Figure 1 – Radial mesh of full-core EBR-2 simulation performed in Serpent 2.

Concerning the fission activities, the validation of the photon diffusion module of FRENETIC has been carried out by means of a simulation on an experimental case, specifically SHRT-45R test of the EBR-2 sodium-cooled reactor. A new set of nuclear libraries have been calculated with Serpent-2 (Figure 1). A further activity regarded the benchmark of the FRENETIC code with the SIMMER code on the ALFRED core design. This work has been carried out with PhD Student N. Abrate, Dr. G. F. Nallo and Dr. M. Massone (KIT) [3]. Optimised axial/radial meshes have been adopted to reduce this effect in both codes. With this setup, a 3D comparison of the total thermal power (purely neutronic) has been performed, showing satisfactory agreement between the two tools when the control rods are extracted. Moreover, the preliminary development of a sub-channel level code for the thermal-hydraulic analyses of deformed fuel assemblies in lead-cooled fast reactors has been started within the European project PASCAL. This tool, called EFIALTE, is still under development and will become part of the suite of the ENEA design-oriented code for lead fast reactors. With respect to the previously developed ANTEO+ code, which accounts only for the mixing in non-deformed condition in the axial direction, EFIALTE must assess also the transverse mixing of the coolant due to a deformation of the i^{th} sub-channel.



First name: Loris **LAST NAME**: VENTURA

Topic: Development and assessment of model-based and sensor-based algorithms for air path, combustion, and emission control in diesel engines.

Course year: 3rd **Tutor(s)**: Roberto FINESSO, Stefano MALAN
Stefano D'AMBROSIO

Academic context

[1] Malan, S. A., Ventura, L. (2020) A Systematic procedure for engine air-path procedure, In: International Journal of Mechanics and Control, JoMaC, Vol. 21, No. 01, pp. 127-138, 2020.
[2] Ventura, L., Malan, S. A. (2020) NLQR-Iteration control of High Pressure EGR in Diesel Engine, ICCAS 2020, 13-16 Oct. 2020.
[3] Ventura, L., Manelli, A., Malan, S. A. (2021) Diesel Engine Cycle to Cycle Feedforward plus Closed-loop Combustion control, 6th IFAC Conference on Engine and Powertrain Control, Simulation and Modeling, Tokyo, August 23-25, 2021, pp. 119-125.

Highlights of the research activity

My research activity is focused on the development and assessment of model-based and sensor-based algorithms for air path, combustion and emission control in diesel engines. The key points of the research are summarized as follows:

1. Exploration of variables correlation to define the input-output pairs.
2. Development of a test procedure in order to collect the data needed to the identification process of the black-box and NN models.
3. Investigation of input-output (black box) models for the air-path of diesel engines.
4. Development of an air path control system for a diesel engine that handles the intake O2 concentration and the boost pressure.
5. Design of a closed-loop control system for the management of injection parameters in a diesel engine.
6. Build-up of a reference generator for the management of the engine by the two developed controllers.

The systems developed in points 4, 5 and 6 have been tested through Model-in-the-Loop procedure both separately and coupled together.

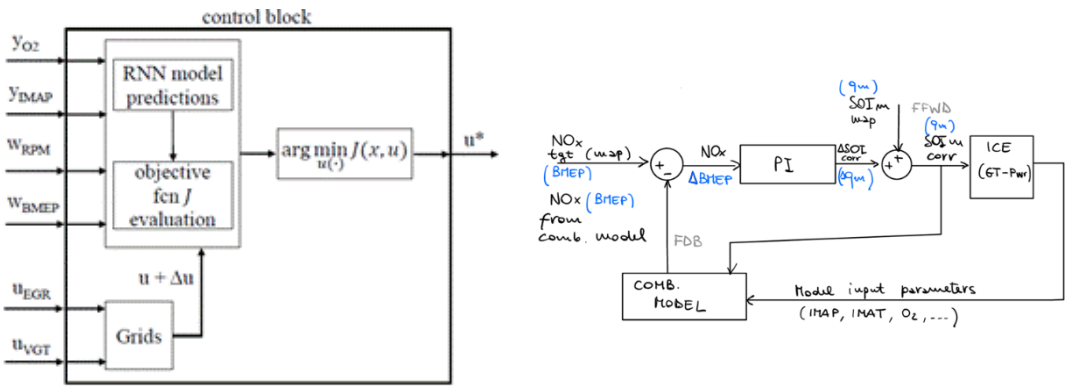


Figure 30 – a) NLQR air path control architecture. B) Closed loop combustion controller architecture.

First name: Giulia **LAST NAME**: VERGERIO

Topic: Balancing energy demand and supply in post carbon cities and societies

Course year: 3rd **Tutor(s)**: Stefano CORGNATI, Giulio MONDINI

Academic context

[1] Fisk W. J., Black D., Brunner G. (2011). Benefits and costs of improved IEQ in U.S. offices. Indoor Air 21: 357-367.
[2] IEA (International Energy Agency), EBC (Energy in Buildings and Communities Programme), Statistical Analysis and prediction methods, Annex 53, Volume V, 2013. ISBN: 978-4-9907425-6-0.
[3] Becchio C., Bottero M., Bravi M., Corgnati S. P., Dell'Anna F., Mondini G., Vergerio G., Integrated Assessments and Energy Retrofit: The Contribution of the Energy Center Lab of the Politecnico di Torino. Chapter in book: Values and Functions for Future Cities, 2020.

External collaborations

- H2020 Mobistyle project consortium
- Enel foundation
- Compagnia di San Paolo (CSP)

Highlights of the research activity

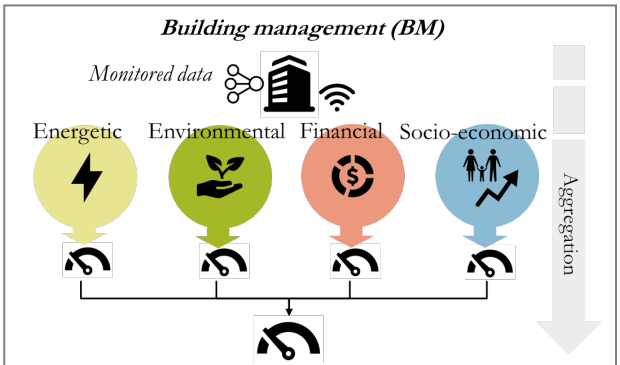


Figure 1 – Multi-domain evaluation model for BM.

It is well recognized that cities are the main actors towards a sustainable society and that buildings are key contributors to reaching the European targets on energy efficiency and emissions reduction. Being the place where people spend 90% of their time, buildings can also contribute to meeting Sustainable Development Goal on people's health and well-being. However, there are non-technical barriers to the transition to more performing buildings. One of these barriers is that the market value of building does not yet fully account for an increase in energy performance and non-monetary benefits due to building intervention, like the improvement of health and well-being of occupants. Thus, there is the need for an integrated approach addressed to occupants and decision makers to make these benefits quantitative, tangible and understandable. Accordingly, the aim of the PhD project (connected to the Energy Center goals and founded by the Energy Center Lab) is to support building design and management processes through the definition of multi-disciplinary methodologies for building performance assessment, defining innovative metrics and indicators, starting from available data at different scales, namely simulated, billed and monitored data. The first ones are treated to support scenarios evaluation of interventions, deploying energy models of archetypes to represent a portion of the stock. This traditional approach is applied overcoming the boundaries of the energy domain, defining parametric costs and emission savings as support to the preliminary evaluation of building design alternatives. Unlike simulated data, billed data are referring to real consumptions of buildings. Methodological insights are offered to use them to set priorities of interventions according to energy, financial and environmental criteria based on real performances. Finally, monitored data collected at the building level are treated to build evaluation models for building management, based on innovative indicators accounting for indoor environmental quality and its impact on health and well-being. The proposed models are based on Cost-Benefit Analysis and Multicriteria Analysis. They allow to measure the performance of buildings through aggregated figures (monetary or non-monetary, respectively), easy to understand and possibly translated into information services. Thus, they represent integrated tools to support building management towards more performing and sustainable buildings.

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: 1st **Tutor(s)**: Laura SAVOLDI, Fabio FRESCHI

Academic context

[1] H. Jones, "Superconductors in the transmission of electricity and networks," *Energy Policy*, p. 4, 2008.
[2] M. Ciotti, A. Nijhuis, P. L. Ribani, L. S. Richard, and R. Zanino, "THELMA code electromagnetic model of ITER superconducting cables and application to the ENEA stability experiment," *Supercond. Sci. Technol.*, vol. 19, no. 10, pp. 987–997, Oct. 2006.
[3] E. P. A. van Lanen and A. Nijhuis, "JackPot: A novel model to study the influence of current non-uniformity and cabling patterns in cable-in-conduit conductors," *Cryogenics*, vol. 50, no. 3, pp. 139–148, Mar. 2010.

External collaborations

- Ricerca sul Sistema Energetico S.p.A. (RSE)
- ENEA

Highlights of the research activity

The main activity carried out throughout the year regards the development of an object-oriented open-source flexible tool for modelling low temperature (LTS) and high temperature (HTS) superconducting cables, in collaboration with Ing. Daniele Placido: the OPENSC^2, developed to simulate thermal-hydraulic and electromagnetic transients in forced-flow superconducting cables for fusion and power applications.
The thermal-hydraulic module for the superconductors modelling has been implemented in Python, thanks the help of the colleague Daniele Placido, and benchmarked against the 4C code. The electro-magnetic model, envisaged for the current-carrying elements, describes the current distribution accounting for the transient losses whenever present and the interaction between the different strands or tapes. The mathematical model is based on lumped equivalent circuit, see Figure 1., which accounts for the interactions between the current carrying elements through longitudinal electrical resistances, transverse conductance and self and mutual inductance, according to the cable layout. The equivalent set of equations takes the form of an integral formulation of the magneto quasi-static approximation of Maxwell's equations with 1D elements, whose solution has been implemented in Python, in stationary and transient conditions. Proper functions have been implemented for the evaluation of the self-induced magnetic field and the characterization of the critical current density, as a function of the temperature and the magnetic field (through suitable definition of the material properties for LTS and HTS). The electrical resistivity of superconducting material depends on the operational current and the critical current through a power law, so the problem is strongly non-linear. The electric module and its solution have been verified and validated against experimental measurements and numerical simulations, obtained from available results found in literature. The comparison shows a good agreement with the reference. The coupling with the thermal module, already developed and benchmarked against other tools, and the coupling validation are ongoing.

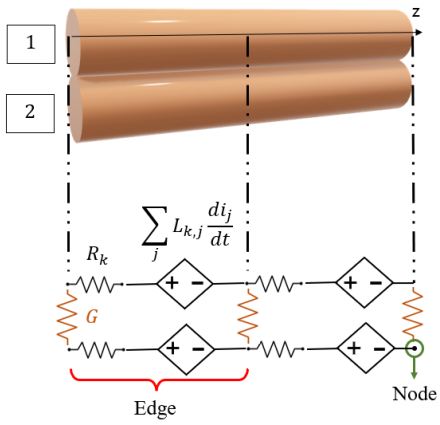


Figure 31 – Example equivalent circuital model for two superconducting strands, where R and L, respectively, represent the equivalent resistance and mutual and self-inductance on k-th edge, and G represents the traversal conductance.