MECHANICAL ENGINEERING | PHYSICS | PRESERVATION OF THE ARCHITECTURAL HERITAGE | STRUCTURAL, SEISMIC AND GEOTECHNICAL ENGINEERING | URBAN PLANNING, DESIGN AND POLICY | AEROSPACE ENGINEERING | ARCHITECTURE, BUILT ENVIRONMENT AND CONSTRUCTION ENGINEERING | ARCHITECTURAL, URBAN AND INTERIOR DESIGN | BIOENGINEERING | DATA ANALYTICS AND DECISION SCIENCES | DESIGN | ELECTRICAL ENGINEERING | ENERGY AND NUCLEAR SCIENCE AND TECHNOLOGY | ENVIRONMENTAL AND INFRASTRUCTURE ENGINEERING | INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING | INFORMATION TECHNOLOGY | MANAGEMENT ENGINEERING | MATERIALS ENGINEERING | MATHEMATICAL MODELS AND METHODS IN ENGINEERING

PhD Yearbook | 2023

DOCTORAL PROGRAM IN ENERGY AND NUCLEAR SCIENCE AND TECHNOLOGY

Coordinator:
Prof. Vincenzo Dossena

The thesis works that are presented in this Yearbook are very representative of the multi-disciplinary research activity performed within the context of the PhD educational and research program in Energy and Nuclear Science and Technology (STEN). The latter is specifically designed to provide the student with the state-of-the-art in a wide range of research fields related to:

- production, conversion and transmission of energy
- rational use of energy
- nuclear systems, nuclear fuel cycle, radioprotection
- application of ionizing radiations
- methods for safety and reliability analysis
- development of innovative materials for energy applications

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ENERGY ACCESS-DEVELOPMENT NEXUS AT NATIONAL AND LOCAL CONTEXTS

Adeleke Adedoyin - Supervisor: Prof. Emanuela Colombo

The enabling role of energy access in meeting the Sustainable Development Goals (SDGs) enshrined in the Agenda 2030 set by the United Nations largely contributes to the increasing support for the implementation of energy access projects globally, especially in developing economies. Moreover, various studies have also established linkages between energy access and the SDGs, mostly using qualitative approaches. However, assessing the nexus between energy access and the SDGs is indeed not straightforward as it involves "complex" systems, whose interactions give rise to unexpected behaviours that are far from being completely understood and characterised.

The inadequate understanding of the complexities of the energy-development nexus in designing, planning, and implementing energy policies and programmes often leads to the assumption that energy access will "automatically" facilitate development. This results in optimistic but unrealistic projections, thus, leading to inefficient, ineffective, and sub-optimal energy policies. The inherent complexities of the energy-development nexus explain the reason some energy interventions lead to significant improvement in livelihood, others only make a limited desirable impact, while some others lead to undesirable impacts. The heterogeneity of the impact of energy programmes calls for the development of tools that will facilitate holistic planning of energy projects given the promotion of their effectiveness to facilitate sustainable development. The study achieved two main objectives, namely:

i) developed a system dynamics model for investigation, evaluation and analysis of various national energisation strategies and roadmaps for an African country (Nigeria),
ii) identified and established the impact pathways between the variables of energy access and those of the other SDGs at the sub-national (rural) level.

Based on the increasing interest in the uptake of renewable energy for energy access in Africa, the study conducted a comparative analysis of renewable energy policies in Nigeria, South Africa, and Egypt, which make up the top three largest economies in Africa and the trio have huge renewable energy resources. South Africa and Egypt provide cases of transformational growth in the uptake of renewable energy driven by market-oriented policies and strategies, while, the Nigerian case typifies policy constraints that limit the optimal exploitation of renewable energy in various countries in Africa. The analysis of the Nigerian case reveals specific challenges in the policy and institutional landscape that impede the uptake of renewable energy and use in the country, which if addressed could catalyse renewable energy integration in Nigeria, among other African countries that are faced with similar challenges. By taking the cases of the three countries, the study analysed the giant strides made in the uptake of renewable energy in Africa and identifies some of the major challenges facing many African countries in developing their renewable energy sectors. Based on the experience of South Africa and Egypt, actionable recommendations that are realistic in the African context are made towards addressing the challenges.

Having gained insight into national energy policies, the study modelled the impact of energy access policies on sustainable development at the national level based on the complex interactions between energy access and other sectors of the economy. Given the multiple interconnections, interlinkages, feedback, time-dependencies, and non-linear behaviours in the energy-development nexus, a system dynamics model was developed. Being calibrated (using the World Bank data for Nigeria) and tested, the model is found to be useful for the formulation, analysis and critical evaluation of various energy policies and plausible impact on sustainable development in Nigeria.

However, national averages hide more than they reveal. Development analysis based on national averaged data is crucial to decision-making at the national level but it does not represent the reality at the sub-national level especially the conditions of rural livelihood which generally lags behind those in the urban centres. While there is a rapid rate of urbanisation in African countries, the highest share of the population in developing countries live in rural communities. The high development deficit in rural developing countries vis-à-vis the high share of their population who reside in them makes rural communities in developing countries form the largest group of people affected by the global challenges that the SDGs seek to address – 'farthest from behind'. The "leaving no one behind" operating principle of the SDGs to catalyse sustainable development 'starting from the farthest behind' , therefore, makes the case for a new momentum towards rural development in developing countries. Hence, the need for planning tools for energy access policies that would maximise their impact on the SDGs in the rural context. Nonetheless, the development of such planning tools relies on an in-depth understanding of the nexus and the interlinkages between energy access and the SDGs in a rural context.

To provide conceptual tools for modelling the impact of rural energy polices on rural development, the study conducted a detailed analysis of scientific literature on the nexus of energy access and each of the themes of the SDGs. The study presents a detailed descriptive analysis, developed 16 comprehensive causal loop diagrams and crystalises 85 feedback loops of the interlinkages and the impact pathways between energy access and 16 SDGs in the rural context of developing countries. The feedback loops represents the conceptualisation framework for the modelling of system-dynamic models for holistic rural energy planning towards facilitating the realisation of the SDGs in rural contexts of developing countries. Based on the literature analysis, causal loop diagrams and feedback loops, recommendations are made on policies and strategies for energy access towards maximising the impact of energy access on the realisation of the SDGs in a rural context.

EVALUATING TECHNO-ECONOMIC SCENARIOS FOR LOW-TEMPERATURE DISTRICT HEATING AND COOLING NETWORKS AND CONVENTIONAL SOLUTIONS

Selva Calixto - Supervisor: Prof. Giampaolo Manzolini

Neutral temperature district heating and cooling (NT-DHC) is a relatively new concept in the district heating (DH) sector. A missing aspect in current literature is the ability to model the performance of NT-DHC systems and draw master plans (even for traditional DH systems). Experimental data are scarce, preventing the development of validated models. The energy modeling for systems of this kind is also more complex than for conventional systems due to the multiple energy sources and the higher complexity of decentralized heat pumps (HPs) compared to conventional heat exchanger substations.

Objectives and scope of the thesis

The scope is to develop an innovative and reliable model for the technical, economic, and environmental performance of NT-DHC systems. In this context, the present work aims to achieve the following specific objectives:
To develop a new methodology for the techno-economic scenario analysis of NT-DHC systems and validate it on a case study.
To apply an optimization model to identify transition pathways for the network extension and its application to the case study.
The findings from this research are intended to contribute to the planning of potential network expansions by identifying the transition pathways from an initial phase to a final stage.

Model methodology and novelty

A model is developed for the analysis of techno-economic scenarios in DHC systems. The simulations are executed with hourly resolution, enabling the integration of multiple waste heat sources, thermal availability, and temperature. The network control allows for the implementation of specific operational strategies based on sources' merit order. Spatial and heat density inputs are sourced from an open-source mapping tool. Additionally, the thesis discusses the key aspects to consider when planning a network expansion, including load aggregation through clustering. A comparison of clustering algorithms is presented, and a test was conducted to find the most suitable for this type of application. The network model proposes two types of network components: the intra-cluster distance, corresponding to the service pipes required to connect buildings within a cluster; and the inter-distance, the primary network backbone that connects the sources with the loads. In this framework, the first category is calculated using literature-supported methods, whereas the second (star-like approach) is a novel addition to the whole methodology. Hydraulic and network sizing calculations are supported by previous research in the DHC sector.
This methodology provides a comprehensive techno-economic assessment suitable for scenario analysis, utilizing a cost database. The thesis presents the main equations for estimating the energy and investment costs of both NT-DHC and individual heating and cooling benchmark solutions. Additionally, a knapsack approach is proposed to solve the optimal expansion problem of an NT-DHC system, with a mathematical formulation of the 0-1 knapsack problem in the DHC context. This methodology goes beyond the state of the art by modeling decentralized HP substations, accounting for economic aspects that DH physical models do not possess and incorporating optimization for selecting the best system extension.

Verification and calibration

In Ospitaletto, Italy, monitoring data from an NT-DHC network is used to improve the model's reliability. The first step was to compare the technical outputs from the lumped approach of the proposed model with a physical model, which showed reasonable agreement with a 15% difference in overall electricity consumption by the HPs. According to the lumped and detailed models, uninsulated pipes caused estimated thermal losses to the ground of 46% and 40%, respectively. Electric consumption of decentralized HPs, heat absorbed by the HPs from the network, and average COP are all closely linked, and discrepancies between the two models are explained by the different temperature values. The computational performance of both models was also reported, with the lumped model being immediately executable, while the detailed model takes about 30 minutes to solve the whole network (about 50 vertices) for an entire year with an hourly time step. The impracticality of the detailed model for parametric analysis or optimization is evident, as intermediate approximation levels can be chosen.
The second step involved calibrating the upgraded lumped model (implemented in Python) with experimental data. An integrated approach was used to analyze the overall network performance, with 2019 data used for the annual analysis and selected 2020 data used for the detailed analysis (e.g., daily profiles and thermal losses).
The network relies on source temperatures between 15 and 25 °C and exhibits an SPF of 3.11. Large portions of the network pipes are not insulated, resulting in thermal losses of about 30%. Electric pumping consumption is approximately 4% of the users' thermal consumption. The lumped model provides proper order of magnitudes for these values, even with simplified default estimates. However, for a good agreement, two simple phenomenological coefficients must be calibrated.
Based on this analysis, it was concluded that a lumped approach seems appropriate for such a simple network and offers a quick tool for scenario analysis, a needed application for this innovative NT-DHC network strongly coupling electrical and thermal consumptions.

Model application and results

The method can be applied to any city if the necessary heat density data is available. However, the approach was applied to the case study in Ospitaletto for simplicity. Additionally, a sensitivity analysis was conducted to determine the extent to which the NT-DHC concept is competitive with individual heating and cooling (H&C) solutions under various energy price conditions and subsidies.
The model's results are in alignment with qualitative expectations. The optimization algorithm determines which combination of potential extensions maximizes the overall economic value. The NT-DHC solution is more convenient for dense urban zones, while air-to-water heat pumps (A/W HPs) are better suited to zones with low-heat density. By selecting waste heat sources at temperatures between 30-40°C, the SCOP of the NT-DHC solution can be enhanced compared to reversible A/W HPs. In the case of Ospitaletto, despite having low building heat density compared to larger cities, it is still possible to identify feasible scenarios. This opens the opportunity to many other cases.
This tool has the potential impact in the DHC sector of reducing the energy demand risks, providing more certainty as to which zones a network can expand to be competitive. It is targeted at energy planners, utilities, energy engineers, and DHC specialists since they require decision-making support and recommendations for replicating a new type of DHC system. This tool will enable pre-feasibility studies and preliminary designs to determine the opportunities and limitations of a system of this kind from an economic and technological perspective.

EXPERIMENTAL CHARACTERIZATION OF AIR-WATER FOAMY FLOWS

Igor Matteo Carraretto – Supervisor: Prof. Luigi Pietro Maria Colombo

General Overview

This work deals with the characterization of air-water foamy flow in horizontal pipelines. The literature lacks in treating this subject, which is of significant relevance in the field of multiphase flow. Moreover, foams have been used in the latest years as pipeline deliquification method, paying little attention to the fluid-dynamics within the pipeline. Hence, to improve deliquification procedures, it is important to characterize the flow that sets within the pipelines.

Objectives and Scope

This work aims at providing an initial overview of foamy flows (i.e., flow patterns, pressure drop and void fraction), comparing the results with both a reference (air-water) case and with computer simulations.

Methods, Procedure, Process

First, air-water tests were performed, in the experimental facility of the Multiphase Laboratory at the Department of Energy and retained as reference case. Two inner pipeline diameters were chosen ID = 30 mm and ID = 60 mm, having superficial gas velocities ranging from 2.67 to 8.17 m/s and 0.41 to 2.31 m/s respectively. Then, a static characterization of a selected surfactant was performed at the Non-Newtonian Fluid Laboratory at the Mechanical Engineering Department of the Massachusetts Institute of Technology. Eventually, both experimental dynamic tests and computer simulations were performed at the same conditions as the reference case, the results were then compared.

Results, Observations and Conclusions

Besides the general characterization, specifically to the oil and gas industry, it can be said that surfactants injection to reduce liquid loading within natural gas pipelines is a promising technique and a quantitative understanding of the liquid loading reduction has been assessed.

Air-water campaign

The results of the air-water campaign were compared with models reported in the open literature. Specifically, to the stratified/stratified-wavy flow pattern it resulted that the existing correlations for predicting wall and interfacial shear stresses in the two-fluid model are not suitable for the low gas velocity range, leading to overestimation of both liquid holdup and pressure gradient. Hence, a new empirical expression of the interfacial shear stress has been proposed to extend the application range of the two-fluid model.

Foam static characterization

The rheological characterization was performed to understand the time-evolving elasto-visco-plastic rheology of transient aqueous foams. To measure the key rheology of this transient foam as it evolves due to time and applied shear stress, a new experimental setup to generate foam *in situ* was used. The rheometry results show that after an induction period the Sauter mean bubble radius found by direct imaging increases over time scaling as $t^{0.5}$, in accordance with previous measurements (Figure 1). Rheological measurements of the yield stress and full shear flow curve can be described with good accuracy by the well-known Princen and Kiss model, which was enhanced here by applying the measured variation in radius to predict flow curves onto a time-age master curve (Figure 2).

Air-water-foam campaign

After the flow pattern characterization, the pressure drop was measured and compared to the ones obtained for the reference case. The relative pressure-increase lowers as the superficial gas velocity increases (the foam apparently loses effectiveness). However, the surfactants maintain their ability to reduce the liquid loading (with reduced strength) even though the pressure drop decreases (Figure 3). Eventually, referring specifically to the computer simulations, as no dedicated package is present to model the foam in OLGA®, it was decided to simulate the foam as a gas-based drilling fluid, with the rheological properties obtained through the static characterization. As OLGA® models each fluid as a separate equivalent phase, it requires direct specification of mass flow rate of each single phase and, as only total air and total water flow rates data were available, three different foam velocity profiles were implemented: uniform, linear and turbulent. In the 60 mm ID pipeline the uniform profile is the one that shows the best performance (+ 29 %). In the 30 mm ID pipeline, the linear profile, with a foam aged of 2000 s, provides the best performance (+ 5 %).

Future development

This work can be further broadened selecting more experimental conditions, and either modifying the surfactant concentration or type. Experimental activities with other pipeline diameters can be considered as well along with changing the inclination of the plant, as a major role is played by the gravitational force. Eventually, another software could be considered to simulate the flow of foams within pipelines.

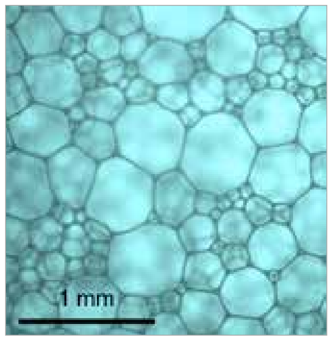

Fig. 1 - Bubble radius evolution.

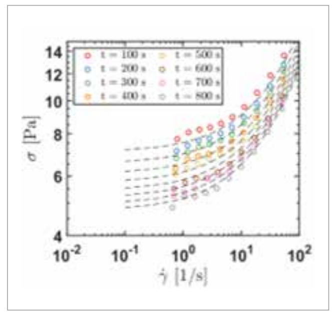

Fig. 2 - Measured flow curves of shear stress vs. shear rate with the overlaid model.

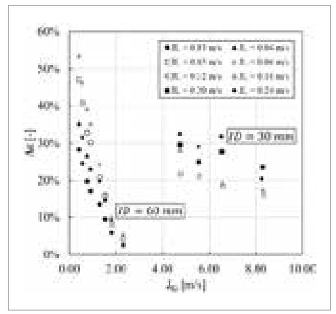

Fig. 3 - Relative void fraction increase as function of superficial gas velocity.

ENERGY COMMUNITY IMPACT: A TECHNO-ECONOMIC APPROACH FOR THE ASSESSMENT OF THEIR FEASIBILITY

Valeria Casalicchio

Supervisors: Prof. Giampaolo Manzolini, Dr. David Moser, Dr. Matteo Giacomo Prina

The European Union has set ambitious targets for the decarbonization of the energy sector, which implies a significant shift towards energy consumption and production based on Renewable Energy Sources.
A crucial role in this pathway can be played by renewable energy communities (RECs). RECs are based on the idea of producing and consuming energy locally and they can take many forms, e.g., cooperatives, associations, and groups of consumers sharing a common interest in renewable energy. The concept of REC was introduced in the 'Clean energy for all Europeans' package and defined in the Directive on common rules for the internal electricity market (2019/944/EU) (EMDII) and in the revised Renewable Energy Directive (2018/2001/EU) (REDII). With the REC development, end-users become active agents in the energy market; this poses multiple challenges such as the planning of the REC configuration, the coordination of the stakeholders, the development of appropriate technologies, and a suitable regulatory framework. The Italian incentive regulation has still to be implemented, but a tariff incentive will be granted for the energy shared within a REC.
This thesis investigates the potential role and feasibility of RECs in achieving a sustainable and decentralized energy transition. To this end, an innovative techno-economic model of RECs is designed, which allows for a comprehensive perspective of the economic, environmental, and social outputs of RECs, while ensuring a fair benefit distribution among the participants.
The methodology adopted is based on oemof (Open Energy Modelling Framework), a tool for the optimization of energy system models which allows to freely select the temporal and spatial resolution of the analysis. The model has been tailored to simulate any REC and perform its dispatch and operational optimization to reduce economic expenditures by choosing the best utilization of sources to meet demand with photovoltaic generation and storage systems. It is also possible to set constraints on emissions. The model is highly customizable and allows for any configuration of RECs with an unlimited number of nodes, enabling variable spatial resolution based on specific application requirements.
The REC configuration of the model is defined mainly through the following inputs: the load profiles of the participants and production profiles of photovoltaic systems with hourly resolution, the system technical constraints and all the economic and investment parameters.
It is possible to investigate several features, including flexibility options that allow for the optimization of various configurations, such as demand response and energy storage and it to assess the impact of REC member organization and design features Additionally, the model enables the assessment of potential synergies among the electric, thermal, and transportation sectors of the energy system, by including various electric fixed and flexible loads, domestic hot water loads, space heating and cooling loads, and electric vehicles loads and the evaluation of the equity in benefit allocation among stakeholders.
A heuristic allocation metric is proposed based on the marginal contribution of each participant to the overall system, optimizing the global satisfaction and maximizing the social welfare, while ensuring a fair distribution of benefits among participants. This approach helps prevent disproportionate benefit distribution and addresses computational costs, ensuring fairness in a REC system where members have varying demands for resources and provide different services and productions.
The model is validated on the Italian case study with the aim of demonstrating the feasibility and profitability of RECs. However, the model can be applied to cities in different climate zones, to examine the effects of various REC configurations through multiple scenarios, encompassing different techno-economic factors, such as energy prices, types of users and loads, sector coupling, demand-side management strategies, economies of scale, centralized and distributed photovoltaic and storage systems, and benefit distribution mechanisms.

This thesis highlights the importance of renewable energy power plants and heterogeneous community structures in creating profitable and feasible RECs, provided they are properly configured and optimized.
This model highlights the attractiveness, but also the complexity, of RECs. The DSM, the sector coupling, or increased attention to the heterogeneous household composition can help make the most of the REC potential, however, the level of profitability still depends on many parameters and constraints and must be evaluated case by case.
Results have shown that the profitability and feasibility of RECs is assured, provided that it is possible to install a renewable energy power plant and the community is not completely homogeneous, thus allowing energy sharing.
For instance, in a six-residential household REC, it was assessed that a centralised system with a larger capacity is more cost-effective when energy prices are in line with pre-Covid prices, due to economies of scale and the incentives of energy sharing. The flexibility provided by the DSM has been shown to be important in contributing to the reduction of storage capacity, resulting in a 2-year reduction of the payback period. The heterogeneity of the REC or the inclusion of an industry profile further improves the profitability of the REC: increases the self-sufficiency (+20%) and significantly reduces payback period (-5 years) and emissions (-25%).
Finally, this model can support investment planning, benefit distribution, and community composition. It allows for the comparison of different REC configurations and identification of optimal scenarios to aid citizens and policymakers.

EXPERIMENTAL AND MODEL-BASED STUDY OF CROSS-OVER PHENOMENA AIMED AT THE DESIGN AND DEVELOPMENT OF AN INNOVATIVE SELECTIVE LAYER FOR VANADIUM REDOX FLOW BATTERY

Marco Cecchetti - Supervisor: Prof. Matteo Zago

The increasing penetration of energy from non-programmable renewable sources in the energy market and the future evolution of the load profiles due to the diffusion of electric mobility require reliable and efficient energy storage systems.
Vanadium Redox Flow Batter (VRFB) is a very promising technology for stationary energy storage due to high efficiency, decoupled energy and power, high flexibility and low response time. However, some technological limitations, such as vanadium crossover, prevent an extensive commercialization by limiting the operating current density and increasing the costs. Vanadium cross-over, i.e. the undesired permeation of vanadium ions through the non-ideally selective membrane, leads to battery self-discharge, capacity depletion and imbalanced operation. Battery manufacturers employ thick or low conductive membranes to tackle this phenomenon, leading thus to large ohmic losses and high capital costs (20%-40% of stack capital costs).
In this PhD thesis the issue of vanadium cross-over was addressed, investigating firstly vanadium cross-over in ad-hoc defined experimental methodology to enhance the understating of the influence of cross-over phenomena on battery self-discharge and electrolyte imbalance, with the support of a modelling activity for the evaluation of the cross-over fluxes. In particular, charge-discharge cycles with fixed exchanged capacity allowed to isolate cross-over losses during the operation of the battery. Moreover, an innovative system of through-plate reference hydrogen electrode was applied to the battery to directly measure in-operando the Open Circuit Potentials (OCP) of the electrodes, providing further insights on the electrolytes self-discharge and imbalance. The defined ad-hoc experimental methodology was coupled with a physical-based model of the operation of the battery, allowing a more accurate calibration of the model parameters than the classic approaches of the literature. The model was then employed to investigate how operating conditions influence cross-over fluxes and which are the main transport mechanisms.
The results of the modelling analysis were propaedeutic to the design of an innovative selective layer for enhancing the selectivity of thin membranes for VRFB. The goal of the selective layer, named "barrier" and described in the patent WO 2019/197917, is to enable the use of thin membranes in the technology to reduce costs and efficiency losses due to ohmic losses. The barrier was initially manufactured through Reactive Spray Deposition Technology (RSDT) by University of Connecticut and it was composed by a mixture of Vulcan XC-72R nanoparticles, carbon-rich particles generated by the RSDT flame and Nafion ionomer as binder. The barrier layer had a thickness of 2 µm and it was directly deposited on Nafion N212, a 50 µm commercial membrane. The barrier was then tested in a battery and its performance were compared to a reference battery employing Nafion N115, a 127 µm membrane.
The barrier allowed to reduce the self-discharge of the battery to a third with respect to the reference battery with N115 during charge-discharge cycles with fixed exchanged capacity and to reduce the capacity depletion due to cross-over to a fifth in classic cycles with cut-off voltages without hindering the efficiency of the battery. Considering that N115 is a membrane more than two times thicker than N212, the results proved that the barrier can significantly improve the efficiency of thin membrane.
The composition of the barrier layer was then further investigated in order to improve selectivity of the barrier and enhance the efficiency of the battery. After identifying the optimal composition, the barrier was also deposited on a thinner membrane of 25 µm (Nafion N211), which cannot be employed in commercial applications due to high cross-over fluxes. The barrier proved to be able to enhance the selectivity of such thin membrane, enabling its use in commercial applications. Moreover, it was demonstrated that the barrier layer can operate with optimal stability for 1200 hours of cycling operation with results highly competitive with the best alternative solutions proposed in literature.
The barrier on a thin membrane such as Nafion N211 offers not only advantages in terms of cross-over loss reduction and efficiency improvement, but also a 33% reduction of the stack cost with respect to a VRFB employing Nafion N115.
In the last part of the thesis, an alternative manufacturing process was investigated to empower the scale-up of the barrier at commercial scale. The investigated process was the Ultrasonic Spray Coating (USC), a spray-based technique that exploits ultrasonic vibrations of the nozzle tip to obtain a better coating with respect to air-based spray coating techniques. USC is an already commercial technique and its scalability is widely demonstrated, therefore it was a strong candidate for the scale-up of the barrier layer. The influence of machine process parameters and ink composition on the quality of the coating, barrier selectivity and battery efficiency were investigated by both morphological and electrochemical characterization. This analysis allowed the author to manufacture a barrier layer with the USC able to effectively mitigate cross-over losses with comparable performance both in terms of battery efficiency and cross-over mitigation with respect to the layer manufactured with the RSDT in the first part of thesis, successfully demonstrating the possibility of manufacturing the barrier via USC.
The development of the barrier through Ultrasonic Spray Coating continued during the Post-Doc activities of the author. The ink composition was further investigated and optimized, allowing an improvement in the barrier layer selectivity. Moreover, the barrier layer was also deposited with an active area of 100 cm^2, a size representative of the real applications, to evaluate the scalability of the barrier layer. The barrier proved to mitigate cross-over losses also at large scale, demonstrating thus that the barrier can be successfully manufactured at commercial scales.

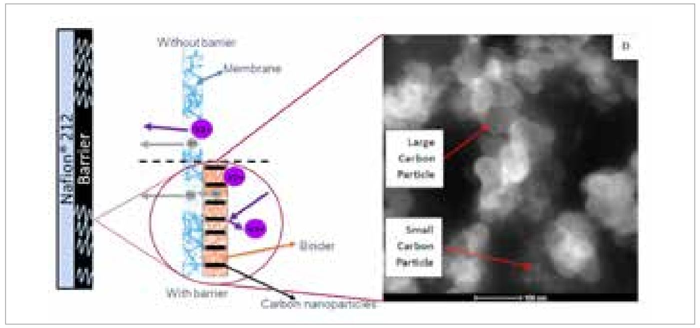

Fig. 1 - Schematic representation of the barrier layer (left) and HAADF TEM image of the barrier cross-section (right).

ELECTRICAL GRID BALANCING WITH FAST-RAMPING FUEL CELL AND ELECTROLYSIS SYSTEMS: ANALYSIS, MODELLING AND OPTIMIZATION

Elena Crespi

Supervisors: Prof. Stefano Campanari, Prof. Giulio Guandalini

Objective and Scope

This work investigates the use of hydrogen-based Power-to-Power (P2P) systems, adopting industrial-scale fast ramping electrolysis systems and Fuel Cell (FC) power plants based on low temperature Polymer Electrolyte Membrane (PEM) cells, to help increasing the reliability of the power grid. These systems are identified either as a promising option for medium- and long-term energy storage, that can improve local electricity exploitation, and as sources of flexibility that can be used for grid balancing purposes. In this framework, the objectives of this thesis are to: i) preliminary assess P2P systems as locally energy storage, ii) assess flexible operation of FC Power Plants and electrolysis systems and optimize their performance, iii) assess hydrogen-based P2P systems for the provision of ancillary services to the grid.

Methods and procedure

To preliminary assess P2P systems as locally energy storage, a techno-economic optimization of a hybrid P2P system - including both a P2P system and a battery energy storage system - connected to a renewable generator (Fig. 1) is implemented in Matlab, following a mixed-integer linear programming (MILP) approach. The model simulates the behavior of the system and finds the optimal size of the components and the optimal operation schedule. The model is applied to a case study where a constant load is supplied with different share of electricity locally generated by a PV field. Then, numerical modelling and simulation of PEM FC power plants and PEM electrolysis systems are carried out to evaluate their flexibility and optimize their performance. A stationary model of the FC system is developed with the simulation tools Aspen Plus®, and used to optimize the system design and operating point. Dynamic models of the FC and the electrolysis systems are realized with the simulation tool Matlab Simulink, and applied to the optimization of systems variable load operation and start-up. While most of the models available in literatures focus mainly on the stack, the models here developed includes all the main balance of plant components, to study the performance of the entire system. The models of the FC and the electrolysis stacks, based on a lumped-parameter approach, reproduces the real cells performances through semi-empirical polarization curves, regressed on experimental current-voltage data. The balance of plant component sub-models mainly solve mass and energy balances. In the dynamic models, dynamic effects related to mass accumulations, thermal inertia and mechanical inertia are included. Additionally, PI-type and on/off type controllers are implemented for the control of the system operation. The numerical simulation models are validated on the base of experimental data collected on the 100-kW FC pilot plant developed in the EU project H2020 Grasshopper (Fig. 2), and on a 60-kW commercial electrolyzer (Proton Onside Model C10) in collaboration with the University of California, Irvine's National Fuel Cell Research Center.
Finally, participation to the Ancillary Service Market (ASM) is included in the techno-economic optimization model previously introduced, to identify the ancillary services that P2P systems can provide to the grid with reference to the Italian electricity market.

Results and discussion

The application of the FC and electrolysis system models to compare different plant layouts and operation strategies has allowed optimizing design and operation of these systems. The simulations confirm the system ability to rapidly ramp-up and -down between the minimum and the maximum load, without negative effects on the net efficiency. The system flexibility makes them suitable for the provision of ancillary services to the grid.
The economic analysis shows that hydrogen-based storage systems

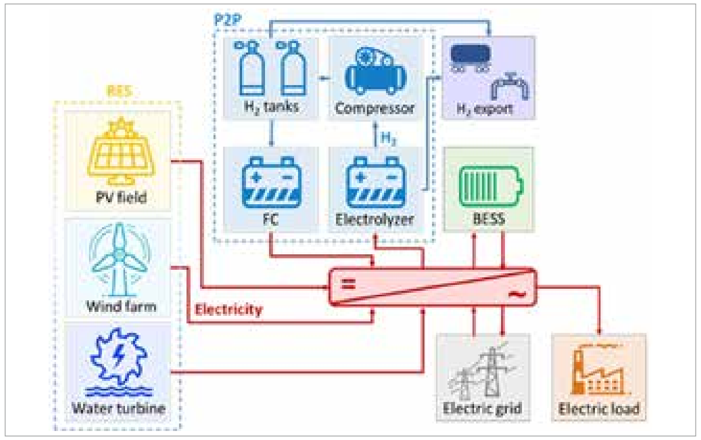

Fig. 1 - Schematic of system components and energy flows in the proposed hybrid storage system

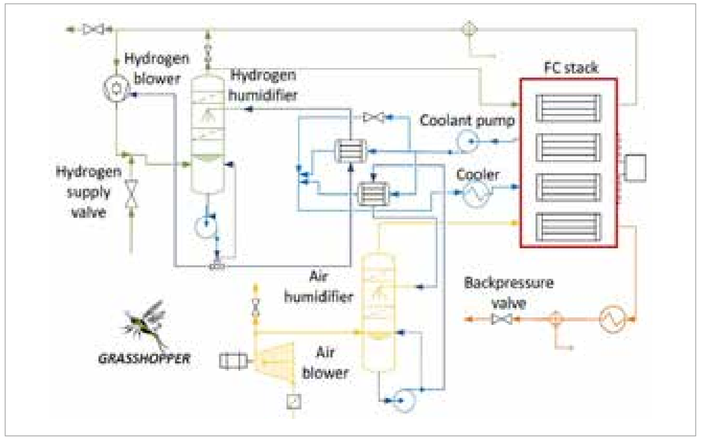

Fig. 2 - Layout of Grasshopper 100-kW PEM Fuel Cell pilot plant

can be economically favorable when medium- and long-term energy shifts are needed or in scenarios where the renewable energy is curtailed or sold at very low prices. However, with the present cost of the technology, high costs of the electricity are obtained. Thanks to the flexibility of low-temperature PEM FC and electrolyzers, additional incomes can derive from the provision of grid ancillary services, whose importance will increase with the higher penetration of renewable energy sources in the power grid. However, the economic profitability of the provision of grid services depends on the electricity market structure. The possibility of presenting asymmetric bids is advantageous and the presence of a capacity payment can promote the system participation to the ASM. The development of a smart bidding strategy to optimize the offers results, after all, the most important aspect. In this framework, the next step of this work can include the development of a smart bidding strategy and the simulations of different market regulations. This activity would allow to give suggestions on how to modify the present market rule to favor the participation of P2P system to the ASM.

SETTING AND TUNING OF BUILDING STOCK ARCHETYPES FOR URBAN BUILDING ENERGY MODELLING (UBEM)

Martina Ferrando - Supervisor: Prof. Francesco Causone

In Urban Building Energy Modelling (UBEM), one of the main challenges is the characterization of the buildings' geometry with the features necessary to run an energy simulation (e.g., building fabric, systems, schedules, etc.). Usually, this phase is resolved by using archetypes. Archetypes are a full set of characteristics applicable to a building geometry based on basic characteristics such as building use, construction years, etc. Nevertheless, particularly in the Italian context, archetypes are currently not available, and they must be derived from existing databases or available data by modellers. Since organized databases are not common practice in cities, this hinders the use of UBEMs.
The presented methodology involves four different types of data analyses based on databases that may be available to modellers in UBEM contexts to set archetypes for the Italian climatic zone E and tune them in a data-driven way for the specific case study. The starting point is a small model counting 110 buildings characterized by the default archetypes provided by CityBES (one of the main available UBEMs tools). A primary check between the registered and modelled energy results is performed by exploiting the smart meter readings on an hourly base and other temporal scales but also at different spatial scales. Then, with Goal 1, the Italian archetypes related to Climatic Zone E are developed and used in the same model. Goal 2 and Goal 3 regard the creation of a rule-based HVAC deduction scheme and an occupants' model based on the smart meter readings. In Goal 4, these two goals are combined with the archetypes developed in Goal 1 to create customized archetypes specific for the case study. Finally, Goal 5 is a scale-up of these archetypes to a larger model comprehending 855 buildings, the whole Milan Public Residential Housing Stock.
The main results reached during the process are: archetypes valid for the Italian climatic zone E (generally North of Italy counting for 50% of the Italian Municipalities), a rule-based deduction scheme for HVAC systems, an occupants-related schedules model, and customized archetypes for the specific case study. An additional result is the scale-up of these customized archetypes to a model of the Public Housing Stock owned by the Municipality of Milan.
The customized archetypes reduce the difference between the registered (hourly and daily smart meter readings of electricity and gas use) and the simulated data. The Normalized Mean Bias Error (NMBE) for hourly electricity values and monthly electricity values were respectively -152.28% and -167.48% at the beginning of the process, and they were brought to 12.32 % and 7.6% at the end. For the daily and monthly gas use, the NMBEs were 13.93% and 15.15% respectively at the beginning, -7.43% and -8.09% at the end. The Coefficient of Variation of the Root Means Square Error (CVRMSE) is investigated through a heat map with different spatial and temporal aggregations. The final CVRSME values for the whole model are 40% for the hourly electricity use and 22% for the daily gas use. Also, the scale-up of these customized archetypes to the large model of all public housing stock in Milan shows an error of 9.9% for annual gas use and -8.3 % for annual electricity use.
The initial climatic zone E archetypes and the customized archetypes can be directly used as a baseline to develop Italian case studies with various UBEM tools since they provide reference information when specific data are not available. Overall, the project workflow can be followed by other researchers to develop archetypes for other case studies and locations. Moreover, the methodologies used for the rule-based HVAC deduction scheme and the occupants' model can be helpful and set examples for other researchers. Particularly, the schedules resulting from the occupants' model can be used in case studies of multi-family residential housing in large cities with similar climates to Milan.

INDUSTRIAL ECOLOGY FOR SUSTAINABLE ENERGY TRANSITION: THE ROLE OF CARBON EMISSION REDUCTION MECHANISM

Nicolò Golinucci - Supervisor: Prof. Emanuela Colombo

We live in an increasingly interconnected society, in which the role of energy has always played and will continue to play a fundamental role being one of the main drivers of economic growth and have enabled past industrial revolutions. The use of natural resources is largely represented by the exploitation of fossil energy resources, which over the last century has allowed economic development in many areas of the world, but at the same time has increased emissions of greenhouse gases and polluting gases.

Today, a growing number of countries, predominantly those with high per capita income, are making efforts to significantly reduce CO2 emissions into the atmosphere. The general objective of this research is to investigate the role of carbon emission reduction mechanisms (CERMs) in the energy transition. In particular, the focus is on the role that carbon pricing policies can play in changing consumption, production, and investment choices within the sustainable energy transition.

An informed decision-making process, supported by multiple modelling approaches, is essential and may be pivotal to supporting the guidance for the needed decarbonisation pathway. Few models explicitly consider the sector-by-sector representation of the meso-economic relations that are physically constraining the dynamic evolution of global economic activities by a clear representation of supply chains. Therefore, as highlighted in the literature, the need for a proper modelling framework arises. The identification of a suite of models aimed at properly assessing the role of carbon emission reduction policies represents the **first specific objective** of this work.

Input-Output (IO) analysis, currently experiencing a renaissance driven by increasing improvement in accounting, represents one of the most appropriate methods to capture the complex interconnections within and among economy and ecology. Nevertheless, the applicability and reproducibility of studies may be hampered by data handling, also driven by improvements in databases' detail. Therefore, the **second specific objective** of this thesis is the development of a data management tool to perform transparent and reproducible IO studies. Finally, on the path towards achieving the first two specific objectives, several findings on different CERMs have been collected. The definition and the testing of an innovative and efficient carbon emission reduction mechanism identify the **third** and last **specific objective**.

The IO framework has been proved scientifically robust in providing useful insights on how different carbon emission strategies can impact global emission reduction and on other environmental and socio-economic dimensions.

Different research questions raise the need for the proper set of the proper IO model. Developing a tool capable of easily setting the scope and the detail of an IO model (called MARIO) and extending the classic Supply and Use framework – introducing the accounting of *needs* and *technologies* – simplified enormously the rigorous application of these methodologies.

Applying multiple policy approaches within diverse socio-economic contexts shaped the proposal of innovative CERM called BitCO2. Having an individual (vs. national), consumption-based (vs. production-based), and incentivizing (vs. coercive) CERMs offer multiple advantages that can justify its practical implementation. This has been tested for a specific carbon-intensive and hard-to-abate sector (i.e. Italian private transportation) adopting a life-cycle methodology and a system dynamics model developed for the purpose.

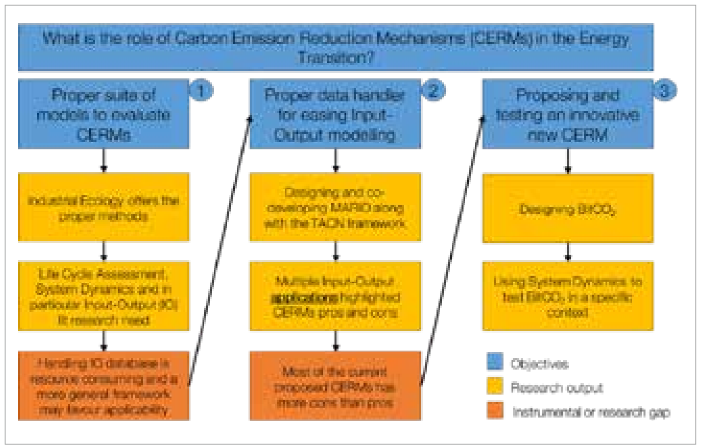

Fig. 1 - Graphical abstract

ADVANCEMENTS IN MODELLING THE THERMAL-MECHANICAL BEHAVIOUR OF MOX-FUELLED PINS AND APPLICATION TO LIQUID-METAL FAST REACTOR CONDITIONS

Alessio Magni
Supervisors: Prof. Lelio Luzzi, Dr. Alessandro Del Nevo, Dr. Paul Van Uffelen

The future of nuclear energy foresees the development of innovative Generation IV (Gen-IV) fast reactors, i.e., ASTRID and ESFR, sodium-cooled; ALFRED, lead-cooled; MYRRHA, an Accelerator-Driven System cooled by lead-bismuth eutectic. The current fuel pin design for all these Gen-IV demonstrators and prototypes features U-Pu mixed-oxide fuel (MOX) and cladding materials belonging to the family of 15-15Ti austenitic stainless-steels. The corresponding fast reactor (FR) irradiation conditions are more demanding than the ones typical of commercial Light Water Reactors (LWRs), i.e., fast neutron fluxes, higher pin temperature regimes and target fuel burn-up, liquid metal-cooling environment harsh from the thermal and chemical points of view. Moreover, a strategic option under investigation consists in the potentiality of Gen-IV concepts to burn and transmute minor actinides (MAs, e.g., Am, Np, currently long-lived high-level wastes), to demonstrate the long-term sustainability of fission technologies by reducing the radiotoxicity of spent nuclear fuel. In support of the optimized utilization of MOX and MA-MOX fuels in Gen-IV future systems, a fundamental research activity is represented by the accurate description of the thermo-physical properties of such fuels under fast neutron spectrum, and the improvement and assessment of engineering-scale simulation tools targeting the performance of pins fuelled with FR-type fuels. his is the target of the PhD research presented in this thesis, developed in the framework of a POLIMI-ENEA-JRC international collaboration, grafted onto the INSPYRE H2020 European Project and with follow-ups in the framework of the PATRICIA and PuMMA H2020 Projects.

The FR irradiation conditions, that fuel pins in Gen-IV reactor cores will face, call for a dedicated and advanced modelling of material properties and behaviour under irradiation with respect to the current state of the art. This is pivotal in particular for fuel performance codes (FPCs), simulation tools able to provide engineering estimations of the thermal-mechanical response of fuel, cladding and external coolant in the reactor core.

The TRANSURANUS FPC, the European reference code focus of this work, is widely assessed and validated for LWR conditions and applications. Hence, code upgrades and a dedicated assessment must be achieved before the FPC application to safety evaluations on fuel pins designed for future Generation IV fast reactors, consisting in reliably verifying the compliance with pin safety requirements (margin to fuel melting, allowed cladding plastic strain, maximum cladding temperature due to corrosion issues under liquid-metal cooling environments).

Among the main properties and phenomena governing the pin performance under irradiation, the fuel thermal properties and the fission gas behaviour are crucial. The fuel thermal conductivity is the main responsible for the pellet central temperature, and coupled to the melting (solidus) temperature it allows to evaluate the safety margin to melting. The fission gas behaviour is driven by the fuel temperature and determines the fuel swelling and coupled fission gas release (FGR) in the fuel-cladding gap. It impacts on one side on the gap conductance by polluting the initial inert composition of the gap (hence producing a feedback on the fuel temperature itself), while inducing the gap pressurization on the other side, potentially leading to critical situations for the cladding mechanical integrity in terms of stress levels under internal pressure. The modelling approach followed in this work is physically-grounded and multi-scale at the same time, since it accounts for data and information pertaining to the lower-length (atomistic) scale and hence allows FPCs to provide engineering outcomes on a physical basis. This represents a significant step forward with respect to the available modelling in simulation tools currently applied to nuclear analyses.

The novel models for FR MOX fuel properties developed and validated in this thesis account for relevant dependencies (Pu and MA contents, high off-stoichiometry, high burnup) in wide ranges targeted by applications in future Gen-IV systems. Hence, they extend the FPC suitability to properly simulate the fuel performance under fast neutron spectra. The modelling activity performed in this PhD work encompasses also the verification and evaluation of the predictions provided on FR fuels by the SCIANTIX grain-scale code that the thesis' author contributes to develop within the Nuclear Reactors Group at Politecnico di Milano. SCIANTIX allows the coherent and mechanistic calculation of oxide fuel swelling and FGR as resulting from the description of the intra- and inter-granular gas dynamics.

The model verification, separate-effect validation and implementation are followed by the integral FPC assessment and application in support of FR fuel characterization, design and licensing, as a fundamental complement to experiments in nuclear reactors. To this end, the extended predictive capabilities of TRANSURANUS, benefiting from the novel models for MOX thermal properties and from the coupling with the SCIANTIX fission gas behaviour module, are herein assessed against available experimental data from FR irradiation experiments. Both the standard code version (prior to the developments performed in this work) and the upgraded one are employed and compared in terms of engineering-level outcomes, in the framework of model sensitivity analyses and of a code benchmark involving the GERMINAL and MACROS FPCs. Lastly, the end-point of the improvement process of any FPCs consists in their application to design indications on fuel pins for irradiation in future reactors (in terms of material compatibility, as-fabricated characteristics and geometry specifications), verifying the compliance with safety requirements (e.g., margin to fuel melting, allowable cladding plastic strain) and supporting the path towards the reactor deployment.

TRANSURANUS simulation of the pin materials and operating conditions envisaged for the ASTRID and MYRRHA Gen-IV FRs are performed. Case studies related to these Gen-IV reactor concepts have been selected since currently targeted by major interests and efforts of the European nuclear community: the MYRRHA system is under construction in Belgium, while the sodium-cooled technology is under consideration also as scalable and modular, targeting future advanced nuclear energy systems.

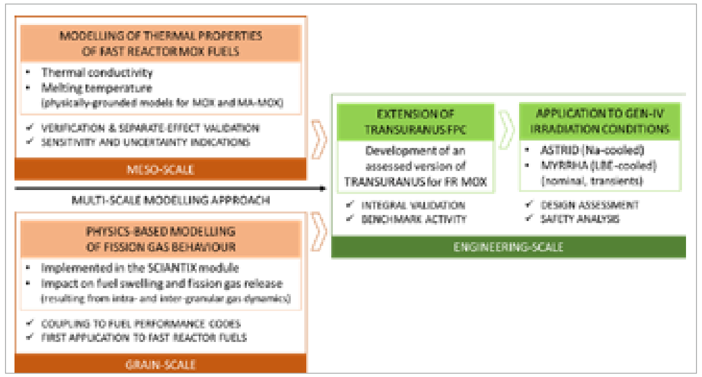

Fig. 1 - Schematic map representing the development strategy adopted in the thesis work.

DOSIMETRIC CHALLENGES IN RADIOTHERAPY: RADIOCHEMICAL AND COMPUTATIONAL APPROACHES

Gabriele Magugliani - Supervisors: Dr. Eros Mossini, Dr. Elena Macerata

This work aimed at obtaining insights and developing new methodologies useful for the dosimetry of challenging radiotherapy techniques, namely in the field of quality assurance of stereotactic treatments and in the in- and off-target dosimetric characterization of intraoperative electron RT (IOERT) procedures. Gel dosimetry for PSQA The complexity of modern RT techniques is at the basis of their efficacy. This however also corresponds to an equivalent difficulty in the planning of treatment sessions, which is performed via dedicated optimization software known as treatment planning systems (TPS). From a quality assurance (QA) perspective, an experimental verification of dose delivery must be implemented. This process of treatment plan validation is also known as patient-specific QA (PSQA), or pre-treatment dosimetry. These QA aspects are even more critical in the case of stereotactic treatments (stereotactic radiosurgery – SRS and stereotactic body radiation therapy – SBRT), which represent one of the most recent RT approaches. The goal of this work in the field of PSQA consisted in the development of a dosimetric system capable of volumetric dose mapping for SRS/SBRT treatments. This challenge was tackled via the use of an innovative formulation of a polymer gel dosimeter. Thanks to intrinsic characteristics of tissue equivalence and volumetric response, these devices are promising candidates in fulfilling the complex requirements of PSQA.
An innovative formulation of the PAGAT polymer gel dosimeter was developed. Addition of polymerization inhibitors to the reference gel composition was tested to find a compound capable of quantitatively controlling the sensitivity of the dosimeter. Following preliminary studies, the best performing inhibitor, p-nitrophenol, was selected and dosimeters doped with this compound were further studied in terms of ideal inhibitor concentration. As gels are passive devices, the overall dosimetric system must also be constituted by a complimentary analysis technique. Nowadays, the gold standard approach for the 3D analysis of polymer gel dosimeters is magnetic resonance imaging (MRI). Characterization of dose response was therefore performed via this technique on samples uniformly irradiated with a RT linac. Collected data indicate that the optimized inhibited PAGAT gel maintains a similar precision, accuracy and relative resolution to those of the literature composition.
Most notably, regulation of inhibitor concentration allows for a quantitative control of the dose range of response and sensitivity of the gel.
The other fundamental constituent of the dosimetric system other than the gel itself is the MRI protocol adopted for its post-irradiation 3D analysis. This therefore also requires optimization to fully exploit the potentiality of the gel. The optimal MRI pulse sequence identified for the scanner in use (Philips Achieva 1.5 T) was a Gradient Spin Echo. As a final step in the characterization of this innovative gel formulation, a protocol based on an internal calibration approach was developed to allow for the determination of phantom-specific dose response curves and conversion to absolute dose. After optimization of both composition and analysis protocol, the gel dosimeter managed to resolve with excellent accuracy dose gradients in excess of 25 Gy/mm with an isotropic 3D spatial resolution of 1 mm3 and spatial stability > 3 months after irradiation.
The performance and reliability of the developed gel dosimetry system was determined by performing PSQA evaluations on 60 actual SRS/SBRT treatment plans. The agreement between TPS-planned and gel-measured dose distributions was quantified by employing the gamma index criterion. The performance of the developed gel dosimetry system was therefore evaluated in terms of discrepancies from equivalent measurements of the same plan, i.e. gamma evaluations, obtained with the Delta4 (ScandiDos AB), a state-of-the-art commercial dosimetric phantom for patient-specific QA.
Collected data suggest that volumetric dose data obtained via gels can reliably employed in PSQA evaluations according to the comparison criteria of most common clinical use, down to 2%/2 mm.
Most notably, such results were obtained from >10'000 measurement points (voxels) under 1 mm3 isotropic resolution from the gel system, to be compared to only ≈200 of the Delta4 for the same plan, thus supporting the superior spatial resolution of the former.
Intraoperative radiation therapy: Monte Carlo approach In contrast to the nowadays common TPS-based approach, some RT techniques may not exploit software-based planning due to some of their peculiarities. A typical example is IOERT which in Italy is primarily employed for the treatment of breast cancers. In these situations, optimization of patient exposure dictates the use of radiation shielding disks. These devices are temporarily implanted below the lesion to be treated and serve the role of attenuating the primary beam downstream of the target.
Notably, electron backscattering induced by disks may result in non-negligible in-target dosimetric alterations. Since the experimental characterization of these effects is very cumbersome, the Monte Carlo (MC) method was employed to study two aspects of IOERT treatments, namely concerning the alteration of volumetric isodose geometry in presence of shielding disks and the evaluation of typical relative skin dose values. To this last point, the effectiveness of shielding materials to be positioned on top of the patient during irradiation was also evaluated, with the goal of assessing their efficacy in optimizing radiation exposure.
The dedicated IOERT accelerator NOVAC7 was implemented in the FLUKA simulation package.
The highest acceleration energy available to the linac was considered (9 MeV nominal).
Cylindrical applicators of 100 down to 40 mm were considered, with target thicknesses ranging from 1 up to 3 cm, representative of typical clinical treatment conditions. The MC implementation was validated by comparing dose profiles scored in reference conditions with corresponding experimental measurements.
The evaluation of in-target dose geometry perturbation induced by shielding disks was studied by considering several disk materials representative of common clinical choices. Obtained result indicate that the volumetric dose effect of shielding disks can range from negligible to very significant, depending on disk material, with fully metallic disks being the most caution worthy. These in some instances may in fact induce severe hot spots in thin targets.
With regard to context of target coverage, the dosimetric effect of applicator boli was also studied with the goal of determining their optimal thickness to be employed according to irradiation geometry Collected data indicate that the use of these boli results in very favorable in-target dosimetry, with significant improvements in target coverage and dose uniformity.
Dose scoring in the superficial region of a phantom was also performed in order to evaluate relative skin dose values to be expected during typical IOERT treatments. Both straight and 45° beveled applicators were considered, with diameters ranging from 40 up to 100 mm.
In general, beveled applicators resulted in locally higher skin exposure in proximal off-target regions due to the in-target asymmetry caused by the applicator shape itself. On the contrary, by considering dose volume histograms, straight applicators resulted in higher average exposure. Finally, the effectiveness of adhoc shielding was also investigated, with results indicating that the use of water-equivalent 1 cm boli can result in a relative skin dose attenuation of at least 50% in most critical conditions.

A DEEP REINFORCEMENT LEARNING-BASED FRAMEWORK FOR OPTIMAL OPERATION AND MAINTENANCE OF COMPLEX ASSETS OF THE ENERGY INDUSTRY

Luca Pinciroli - Supervisors: Prof. Piero Baraldi, Prof. Enrico Zio

The optimization of Operation and Maintenance (O&M) in complex energy systems has become a great issue of concern since O&M accounts for a large percentage of the assets life cycle costs. Nowadays, with the rapid advancement of sensoring and monitoring systems and the integration of advanced analytics into industry, new sources of information have become available and new powerful algorithms have been developed to detect anomalies, diagnose their causes and predict failure times. This is leading the interest of researchers towards prescriptive maintenance, which is a maintenance strategy in which O&M action are recommended by the algorithm, allowing the automatization of the maintenance decision-making process, making it less dependent on the subjective experts' knowledge. In this context, the present PhD thesis proposes a machine learning – based methodological framework for the optimization of O&M in complex energy systems. The proposed framework aims at: i) exploiting all the available sources of information related to the system and its environment; ii) being suitable for dealing with different complex systems; iii) being robust with respect to the uncertainties of the system and its environment. The main novelties are the use of deep reinforcement learning for the definition of the optimal O&M strategy and the achievement of prescriptive maintenance for different complex energy systems. The effectiveness of the proposed framework is shown by means of its application to artificial case studies related to the optimization of the O&M strategy of a wind farm and a microgrid. The robustness of the framework is also tested by means of ad-hoc experiments.

DEMAND-NEEDS NEXUS IN OFF-GRID ENERGY PLANNING: THE UNDERVALUED DRIVER OF DEVELOPMENT

Nicolò Stevanato - Supervisor: Prof. Emanuela Colombo

In order to meet the first target of SDG7, and guarantee access to sustainable and affordable electric energy to more than 700 million people and to modern cooking services to roughly 2.5 billion people worldwide, is crucial to design appropriate and effective technical solutions tailored to the specific but diversified contexts. To this purpose, effective and efficient energy planning and strategies are, more than ever, pivotal. The use of Energy Modelling over the last decades has proved to be a key support tool in defining such strategies and solutions design. The existing literature on the subject of energy modelling for supporting access to energy has so far mainly focused on the characterisation of the supply side of energy systems, improving technological detail and geospatial resolution. The demand that such systems are meant to satisfy is generally provided as an exogenous parameter, but its role is crucial since it constitutes one side of the most important governing equation of the model: the energy balance. Despite this relevance, the demand side has not received much attention from the scientific community until the binary conception of access to energy was superseded by international organisations promoting a multi-tier framework for energy access, for the first time ever associating energy to the real need of the people at household level, community services and productive uses.

In line with this rising awareness, key to this dissertation is the concept of access to energy as an instrumental right which is essential to assure people needs at household level, community service and productive uses that will determine development opportunities for local populations. On these premises the *Demand-Needs Nexus* is conceptualized in this work with a focus on electricity, showing the relevance of accurate demand modelling for energy solution sizing and optimisation. Alongside, a set of novel methodologies and tools are developed to allow the integration of the *Nexus* into energy modelling. A set of case studies is used to analyse the effects of the load demand definition tailored on the needs of a specific community or area, in terms of more efficient resource allocation, techno-economic benefits in the optimization and more effective prioritization of strategies compared to the base cases. While developing tools and methodologies the data quality and availability problem emerged as a limiting factor and therefore, the second part of the work deals with the scarcity of data availability for demand characterization in the context of rural areas of developing countries, where traditional methodologies for demand forecasting may not be applied, given the fact that electricity has never been experiences before. Two methodologies are hence proposed to deal with the issue. First, a top-down approach based on three macro parameters is presented, the methodology makes use of archetypical load demands, better linking the energy use to the categories of users, including household uses and community service like education and health services. The archetypes are adaptable to the Sub-Saharan region thanks to geographical and economical parameter variations, and the replicability of the methodology is assessed. The second approach is meant to generate input data for bottom-up load estimation methods and contribute to close the data availability gap. A database is constructed to correlate socio-economic and geographical drivers with appliance adoption and use trends in recently electrified communities. The database, which contains more than 16 thousand entries, can be used for investigating similarities across different contexts and for load demand estimation. Finally, the database is used to train a machine learning algorithm to estimate future appliance presence in perspective users of off-grid communities, with results reporting an accuracy of the model in predicting appliance presence in new users of more than 70%. The main conclusion of the work lies in having confirmed the need for more attention to be drawn to the *Demand-Needs Nexus*, it is highlighted how linking the definition of load demand for modelling energy system returns lower economic costs, more effective strategies and increases possibility for sustainability of the system under analysis. This main conclusion is complemented with tailored methods and models to allow modellers to fully consider the *Nexus*, in both system sizing and strategy definition modelling. Ultimately two different methodologies and, respective tools are developed for ensuring more precise and tailored load estimation in future energy modelling works.

Once having understood and assessed the impact under the techno-economic and strategy development point of view of better modelling the load demand around the specific needs of communities, two methodologies are proposed: a set of archetypes for rural energy users and an open-access database correlating drivers of appliance adoption, with patterns of appliance adoption and use in recently electrified communities. The database is used to train a machine learning algorithm for estimating potential load demand of non-served communities.

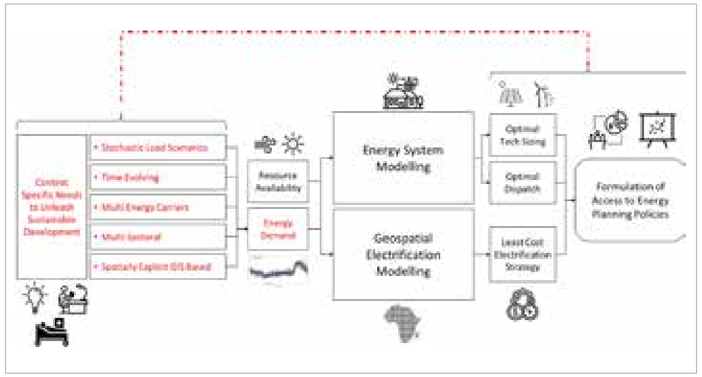

Fig. 1 - Relevance of Need-Demand Nexus

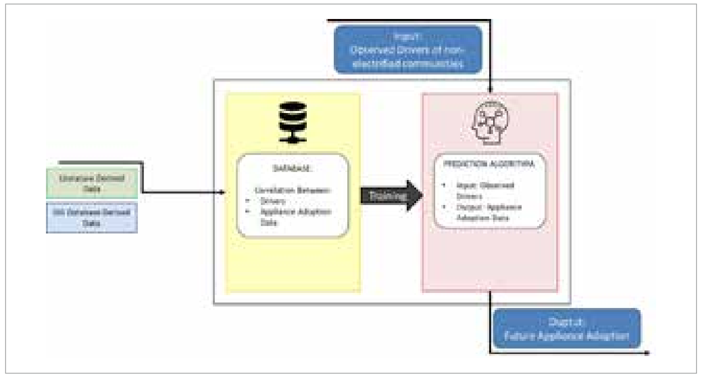

Fig. 2 - Estimating the Load Demand of non-electrified Areas

PHYSICAL/DATA-DRIVEN DYNAMIC MODELLING OF FIRE-TUBE BOILERS AND DEMAND PREDICTION AIMING AT ADAPTIVE OPTIMIZATION OF THE SUPPLY SET-POINT CONDITION

Marco Tognoli - Supervisor: Dr. Behzad Najafi

This project aims to optimize the supply conditions of fire-tube steam/hot-water boilers for industrial and residential applications in near real-time. The project is divided into three activities as described in the attached Figure.

In the first activity, physical heat transfer correlation in smooth horizontal fire-tubes is optimized using a one-dimensional reduced Finite Volume Method (FVM). The FVM model takes into account convective and radiative terms and is validated over a wide range of operating conditions. The optimized physical models are calibrated using experimental data obtained through temperature and pressure profiling of the flue gases. The calibrated FVM model is in good agreement with the CFD model but at a reduced computational cost. The results indicate a reduction of 42.4% in the error for the estimation of tubes outlet temperature.
In the second activity, the investigation objectives of the first activity are extended to horizontal fire-gas tubes equipped with inner helical-coil inserts. A CFD model is first developed and validated using experimental data and literature. Next, an FVM model is developed using state-of-the-art physical correlations for simulating the flue-gases behavior. The convective heat transfer and friction factor correlations are calibrated using a multi-objective genetic algorithm-based optimization procedure, which results in a reduction of 11.00% for the temperature estimation and 22.07% for the pressure drop estimation.
In the third activity, a detailed dynamic model of fire-tube boilers equipped with stagnation point reverse flow (SPRF) combustor is implemented. Experimental data are used to validate the developed model, and a PID controller is tuned for each boiler model. The dynamic behavior of the considered boilers is simulated while addressing different steam demand profiles, and the corresponding overall efficiency is determined. The results show that boiler No. 2 is the most economically promising choice beyond a certain size. Similarly, a dynamic physical modeling procedure is implemented for simulating the thermal dynamic behavior of a fire-tube boiler that addresses hot-water. A PID controller is tuned for the considered boiler's configuration, and a validation procedure is implemented, which demonstrates that the developed model provides accurate estimations, resulting in a limited boiler thermal efficiency bias of 1.2% compared to the historical data.
In the second activity, data-driven models are developed to simulate the dynamic behavior of a boiler, with separate pipelines for estimating the supply hot water temperature at different prediction horizons.
The performance of several machine learning models is compared, and the results demonstrate that even the model with the longest prediction horizon provides an acceptable accuracy, with a mean absolute relative difference error lower than 6%. The developed data-driven model can be used in combination with an advanced operation management system to improve the boiler's operating conditions and potentially reduce energy consumption. The developed physical model can be utilized in the sizing procedure of the unit, considering the customer's demand profile.
In the third activity, a multi-setpoint control strategy is implemented to address the steam demand with a notable (daily) variation in the requested pressure level. A dynamic PID controller is developed and tuned to enhance the boiler's controllability at partial load conditions, and a multi-setpoint strategy is implemented, in which the pressure setpoint is dynamically modified following the desired pressure profile.
The proposed strategy results in reducing the yearly fuel consumption by 4.5%, compared to the currently utilized constant-setpoint approach. The approach can be employed by many steam end-users in the food and beverage industry, specifically in Italy, whose needed pressure level is highly variable.
In the fourth activity, an hourly supply temperature optimization strategy is simulated for a district heating system equipped with fire-tube hot water boilers. A detailed physically inspired methodological approach is proposed for hourly predicting the thermal energy demand of a district heating network based on data-driven modeling of the generation, the distribution side, and the demand side separately. A set of machine-learning models is introduced, and results of the models' estimation performances are compared within the separate prediction horizons.
An optimization procedure is implemented through the formulation of an objective function, utilizing the above-mentioned hot-water distribution system's losses model, the buildings' side heat exchanger thermal load forecasting models, and the predicted thermal output of the generation side.
The adaptive optimization procedure aims to minimize the system's energy consumption by determining the optimal hot-water supply conditions at the primary circuit, thus minimizing the thermal losses along the distribution network.
The simulations conducted on the set of buildings in the system have demonstrated a fuel saving potential, compared to the conventional controller, of nearly 4% of fuel required to address the requested thermal demand, which is equivalent to a yearly fuel cost saving of 64436 €. A notable reduction in thermal demand peaks has also been observed, allowing a potential reduction in the power plant thermal installed capacity or a more efficient energy production mix when reducing the number of active thermal supplying boilers.

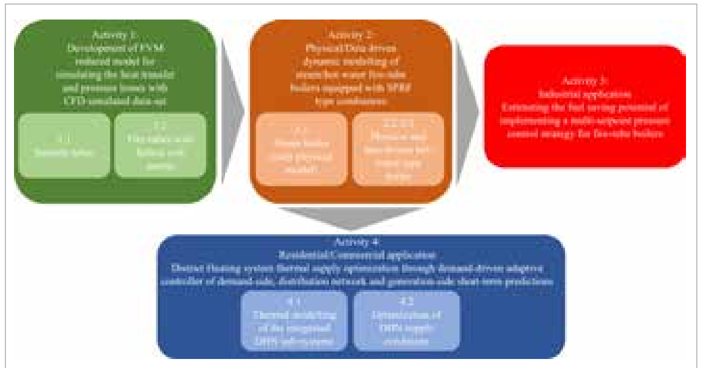

Fig. 1 - Schematic map representing the development strategy adopted in the thesis work.

MODELLING OF BOUNDARY PLASMAS IN LINEAR DEVICES AND TOKAMAKS

Elena Tonello - Supervisors: Prof. Matteo Passoni, Dr. Andrea Uccello

Thermonuclear fusion is one of the key technology that could play a role in sustaining an energy system with net-zero emissions in the next centuries. This process is based on the fusion of two light nuclei to form a heavier, more stable product, releasing energy. Among the various nuclear fusion reactions, the one between deuterium and tritium nuclei, yielding helium and a fast neutron, has the highest reaction probability at the lower energy and it is thus considered the most feasible. Fusing together two nuclei, however, requires overcoming the Coulomb barrier. Nuclei have to be supplied with tens of keV of thermal energy, corresponding brings the system to hundreds of millions of degrees Celsius. At these temperatures, the atoms dissociate in electrons and ions, forming the so-called plasma state. Today most of the fusion power-plant-oriented research is based on the tokamak concept, which exploits a magnetic field to confine the plasma in a toroidal chamber. The ITER tokamak, under construction in France, is the most ambitious international project on fusion and aims at operating the first experimental fusion reactor capable of producing a 10-fold fusion energy gain.

Among the various challenges that the design and operation of a magnetic nuclear fusion power plant face, this thesis focuses on power exhaust and plasma-wall interaction (PWI). Indeed, plasma confinement by the magnetic field is imperfect. Particles diffuse radially across the magnetic flux surfaces ultimately reaching the wall of the torus. The mitigation of the particles and power loads onto the plasma-facing components (PFCs) is crucial to operating a tokamak ensuring steady-state output power while avoiding excessive degradation of the first wall material and impurity contamination of the main plasma.

Presently, there are several tokamaks in operation worldwide which have many relevant plasma parameters close to reactor conditions. However, concerning the PWI properties, there are still significant gaps in some crucial parameters, like ion fluxes and fluences at the strike point and temperature of the PFCs. Linear plasma devices (LPDs) offer the possibility of closing these research gaps by emulating the conditions of plasma-material interaction (PMI) in fusion plasmas which can not be reached in today's tokamaks. LPDs are thus ideal to test material erosion and other plasma-wall interaction processes under well-defined and controlled conditions.

A relevant concern of PMI is dealing with helium plasma in a tungsten environment. Under specific conditions of material temperatures, fluxes and fluences, He ions lead to the formation of nanostructures on the surface of tungsten. This phenomenon is known as tungsten fuzz. The nanostructures modify the erosion properties of tungsten PFCs, thus being of particular concern for the working condition of the ITER W-divertor. In ITER, indeed, helium ash will be present in the plasma mixture during the D-T active phase and, more importantly, He will be used as the main plasma species during the Pre-Fusion Operation Phases. Controlled experiments investigating the formation conditions for W-fuzz are performed in linear plasma devices. Moreover, very recently experimental campaigns with helium plasmas were performed in ASDEX-Upgrade and JET tokamaks to answer whether W-fuzz can be observed in present-day experiments, if it is expected under ITER operational conditions and how its presence affects the plasma operation.

Finally, alternative magnetic configurations for tokamak scenarios with improved confinement and reduced PWI impact are of great interest for the design of next-generation fusion reactors. Among these, negative triangularity (NT) is considered very promising, besides only a few tokamaks can operate with NT equilibria. Experimental observations on TCV and DIII-D tokamaks showed that this configuration may exhibit increased plasma confinement with respect to analogous positive triangularity (PT) discharges. Concerning the edge plasma behaviour and the PWI properties, however, NT configurations are still understudied if compared to standard PT scenarios.

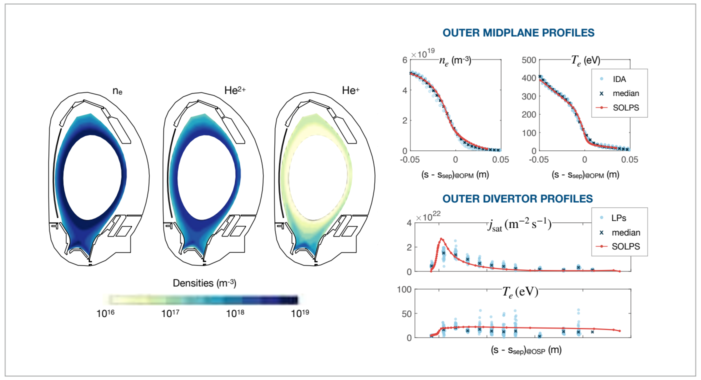

Fig. 1 -2D density distributions of different plasma populations reproducing a helium discharge in ASDEX-Upgrade tokamak (left) and the relative profiles at the outer midplane (right-top) and outer strike-point (right-bottom). Simulation results (red lines) are benchmarked against experimental data.

In the context described above, understanding, predicting and mitigating plasma-wall interaction and the resulting particle and heat loads on the divertor and first wall is a crucial requirement for a fusion reactor. To investigate a complex system such as the edge plasma of a magnetically confined plasma numerical tools are also essential. Sophisticated numerical codes describing plasma transport within the boundary region of a tokamak are indeed needed for interpreting experimental results and for making predictions in the design phase of new machines. To further the understanding of the theoretical framework of boundary plasma and plasma-material interaction modelling, this thesis work aims to extend the applicability of standard boundary plasma codes to non-standard conditions. In particular, the work focused on improving the available modelling tools to describe linear plasma devices, which constitute an asset for the research on material for the PFCs of future fusion reactors. In light of the ITER Pre-Fusion Operation Phases, the investigation of helium plasma properties is crucial, especially concerning the behaviour of the edge plasma and its interaction with PFC materials, tungsten in particular. In this thesis, these aspects are investigated through modelling both in linear device and tokamak geometries. Results of ASDEX-Upgrade modelling are shown in figure 1. Moreover, following the recent interest in negative triangularity as a promising configuration for the development of reactor-relevant scenarios, this thesis presents a study of plasma detachment in negative triangularity, in comparison with standard positive triangularity scenarios.

METHODS FOR ASSESSING ENERGY-ECONOMIC IMPACTS OF LOW CARBON ENERGY TRANSITIONS IN REGIONAL ECONOMIES

Roberto Vaccaro - Supervisor: Dr. Matteo Vincenzo Rocco

The transition towards clean, sustainable, and independent energy systems has become a major objective for scientists and policymakers at various territorial levels. Among them, the regional scale is particularly crucial since it intersects two major levels of governance: local, which is closer to citizens, and national and supranational. Concrete measures to promote the low-carbon transition are developed and promoted in local strategies and action plans, making the regional level critical in achieving this objective.
In literature and practice, the development of governing tools for the low-carbon transition is often supported by bottom-up engineering modelling tools. Although valuable, these cost-technical analyses fail to capture the impacts of low-carbon energy scenarios on the local economy, such as their effects on value added, taxes, imports, and employment. On the other hand, macroeconomic models are unable to capture the complexity of energy systems resulting from the diffusion of intermittent renewable sources and their time-dependent interaction with the economy, making them incomplete. These limitations underscore the need to develop a more comprehensive modelling approach that can combine the benefits of both methods.
This thesis aims to advance research on the linking of bottom-up engineering modelling tools and empirical meso- and macroeconomic models at the regional level. It investigates how such hybrid models can effectively inform local policymakers about the economic impacts of the low-carbon transition on their territory, supporting them in developing sustainable policies and measures.
The literature review identified the characteristics required by the models to be linked and the two modelling approaches used in this study: EPLANopt, developed by Eurac research, and Input-Output Analysis for the energy and macroeconomic parts, respectively. It also revealed inconsistencies regarding definitional aspects related to model linking, leading to the development of a novel classification scheme that enables the unambiguous identification of the developed hybrid models. Additionally, it highlighted the aspects and criticalities incorporated into the different models of this study. Three hybrid models were developed in the Python coding language and tested, with increasing complexity. Applying the first linked model to the South Tyrol case study provided insights into the impact of low-carbon scenarios on different sectors of the local economy, and how this information can support policy development. The further application of the two models allowed for advancements in the understanding of the application of hybrid models in various contexts and the identification of further research avenues.
This thesis investigates the practical aspects of linking these two models. By applying the model in the South Tyrolean context, the thesis identifies the potential relevance of the information obtained for policy makers. However, the results are mainly methodological in nature, and the application to the South Tyrolean context was used to explore the usefulness of the approach rather than to derive detailed information for policy makers.

Main points emerging from the thesis:

An innovative approach was identified for the classification of linked models. That is, those in which the link is not integrated, but consists of sequentially using the results of one model in the other. The classification methodology overcomes the inaccuracies in definition found in the literature, improving the clarity of the analysis.
The analysis of the imprecision in the definitions exposed some issues that stretch beyond simple classification aspects. In particular, the need to achieve convergence is a characteristic of models linked with a CGE, while simple sequential linking avoids the computational problems introduced by the need to reach convergence. Verification of the relevance of this point in the context of a broader literature review has been postponed after this thesis
The thesis made a methodological advancement by improving the method to pre-process the IOA model for transferring data from the energy model to the economic model. Two approaches were identified for the transfer of cost, investment, and energy data, but the thesis applied only one solution for time and resource convenience. Differences in results from the comparison of the two methodologies may be a starting point for future research. The thesis also briefly discussed alternative approaches for allocating installation costs of renewable technologies, which could be a potential line of future research.
The possibility of creating feedback loops was investigated. This step's inherent relevance has several dimensions, such as considering the reciprocal effects of the economy on the energy sector and vice versa. However, one point that emerged is that creating feedback loops may be of less interest on a regional scale. The variables that may be affected by the loop induce limited effects, and the creation of the loop, with all the computational difficulties involved in its implementation, would not substantially alter the level of information attainable.
On the other hand, the thesis emphasizes the importance of analyses with one-way models in which the economic analysis is done downstream of the energy analysis. It also highlights that, to fully appreciate the results of the I/O model, a deeper knowledge of certain characteristics of the economic system is required. These characteristics require in-depth studies not carried out in this thesis.
The soft linked model applied to South Tyrol provided valuable insights. Firstly, the use of IOA at the regional level allows for a more accurate evaluation of the impact of future scenarios on the regional economic system than traditional BU energy models, providing insight into linkages among industries and the contribution of different sectors to regional emissions and GDP. Secondly, the EPLANopt model enables representation of the energy industry with high engineering detail and precise estimation of technology, investment, and operative costs. Thirdly, IOA requires readily available data and uses computationally fast linear algebra equations, making it advantageous compared to other models with limited data availability. However, further research is needed to assess and compare the results of this model with similar approaches, such as a hybrid model built on a CGE model, to provide insights for policy and decision-makers.
In particular, the soft linked model applied in South Tyrol highlights the importance of the service sector in supporting the low-carbon transition, as well as the potential for locally generated value-added in the electronic and construction sectors. However, further analysis is needed to evaluate the growth potential of local firms and tailor policies accordingly. While the model has limitations, such as the constant technological coefficient and unlimited supply inherent in I/O models, it is still a useful tool for exploring the economic impacts of low-carbon scenarios. Future research can address these limitations.
In summary, combining an IO model with a detailed energy model allows for exploration of relationships between economic sectors and quantification of the economic impact of low carbon scenarios. This approach can be easily implemented and can provide valuable insights for policy makers, despite limitations. The steps outlined in this thesis can facilitate the creation of such linkages with other energy models.

BEYOND THE LCOE APPROACH: A NEW METHODOLOGY FOR THE EVALUATION OF COSTS ASSOCIATED TO THE PHOTOVOLTAIC ENERGY

Elisa Veronese - Supervisor: Prof. Giampaolo Manzolini

The photovoltaic (PV) technology will be the main power production technology according to the energy transition that is expected in the next years. It allows to reduce the electricity bills of endusers due to its exploitability directly on site of consumption and promotes the environmental sustainability of the electricity produced by the energy system. However, there are some concerns about the intermittency of the solar resource, so the programmability of PV output must be improved, and the current energy system must make additional efforts to absorb the rising amount of PV energy.
The main aim of this research is to assess the future impacts of the PV penetration in terms of additional costs for the system and to evaluate some mitigation strategies to ensure that the benefits of using this renewable source are not compromised by an unsustainable increase of the energy system costs that are socialized by the entire community. This study focuses on different strategies for a more flexible management of utility-scale PV plants, minimizing the costs for their integration and for the energy system.
Two paths for the future energy transition are identified and both are analyzed to assess their economic and environmental impacts. The first route assigns to battery energy storage systems (BESS) the main role for the management of the PV production variability. The second is more ambitious and introduces additional flexibility at the consumption side. The system costs rise in the first path because more investments are needed to install BESS, the production level of the existing power plants shall be adapted and the grid infrastructure shall be extended to better manage the increased penetration of variable production. In this context, a new parameter is defined to go beyond the common Levelized Cost of Electricity (LCOE) and to apply a more systemic approach in estimating the PV power production costs. This new parameter, called system LCOE, in addition to the power plant costs for PV plants with or without BESS, includes the costs of adapting the existing grid infrastructure to accept a growing share of intermittent electricity without compromising the system reliability as well as the costs associated with changes in the operating conditions of existing fossil fuel power plants. The first are the grid costs and are subdivided into reinforcing distribution and transmission network costs, adequacy costs and curtailment costs. The second are the balancing costs and are classified into decay of efficiency costs and start-up costs. A mathematical definition is provided for each cost component during this study.
The system LCOE is used in the techno-economic evaluation of future utility-scale PV plants to assess how adding the integration costs to the PV generation costs calculation affects their future market parity and profitability analysis. Two different perspectives are adopted: the PV plant investor and the energy system manager perspectives. For the first, the results are discussed in terms of market parity achievement and profitability indexes (net present value, pay-back time, and internal rate of return). For the second, a genetic algorithm is implemented in the energy system modelling tool to perform an expansion capacity optimization aimed to study the effects on utility-scale PV plants dispatchability when the integration costs are added as annual costs.
The second path that the energy transition might follow enables the flexible demand as an alternative to BESS in enhancing the PV production programmability and as a mitigation strategy to lower the PV integration costs. Two opposite strategies for upwards and downwards load shifting are implemented in the energy system modelling tool: an extension of the flexibility interval within the day and an increase of the available flexible demand. Four different scenarios are considered: a baseline scenario that corresponds to the upgrade of the energy system from the rigid to the flexible configuration; a scenario aimed to maximize the use of all the flexibility options to completely avoid PV curtailment; a scenario aimed to avoid PV curtailment without the help of pumped hydro storages; and a scenario in which the utility-scale PV plants installed capacity is doubled.
The impacts of adding the flexible demand to the energy system are studied firstly in terms of avoided BESS installations and are then deepened through some key performance indicators, which are the amount of CO_2 emissions and Renewable Energy Sources (RES) penetration as measure of the environmental sustainability of the energy system configuration according to the targets established by the energy and climate policy taken as reference; the avoided storage and curtailment costs to assess the ability of flexible demand to reduce the PV integration costs and thus the costs for the system; the DSM remuneration to examine the attractiveness of DSM programs.
The innovative contribution of this study is firstly in the approach to the energy transition for which two possible routes are identified and both are studied in terms of costs and benefits thanks to the flexibility options available to improve PV production programmability. Moreover, this study gives not only a generally applicable mathematical definition of the PV integration costs but it also provides a techno-economic estimation on how flexible demand affects the programmability and the integration of a specific power production technology. Finally, it contributes to expand the knowledge of DSM benefits on an energy system at national scale and suggests a simple method for a first evaluation of the possible DSM remuneration.
The Italian energy system and its planned evolution to the year 2030 is taken as reference to validate the methodology. The electricity sector has been modelled with the open-source energy system modelling tool Oemof to apply a multi-node approach to the hourly dispatchability of power production technologies, minimizing the system costs.
The main findings of this analysis suggest that the expected reduction in investment costs of both PV and BESS technologies in the future years is the main driver that allows to easily reach the market parity in the year 2030 even when a more systemic approach in assessing the generation costs is used. However, reaching the market parity does not always guarantee the profitability of the investment. Enabling flexible demand is economically and environmentally beneficial for the energy system because it reduces the need of BESS and the amount of PV production that must be curtailed as well as it increases the RES penetration and lowers the CO_2 emissions. However, the magnitude of these benefits strongly depends on the amount of flexible demand available and how it is managed as well as the energy mix composition and the availability of other flexibility options.
The RES penetration and CO_2 emissions, in particular, are more affected by the amount of RES production available in the energy mix than by the flexibility demand itself. The results are in line with other studies found in the scientific literature that highlight on average a very limited potential of load shifting in promoting RES penetration and reducing the CO_2 emissions of the energy system. The average estimated DSM remuneration is similar in the order of magnitude to the system LCOE of utility-scale PV plants and very near to other research studies based on willingness-to-accept surveys and this opens up to interesting opportunities for applications in the context of energy communities as well as electricity market aggregators in which consumption and production units are managed under the same entity.

MPC COMPARISONS FOR RESIDENTIAL HVACS AND PARAMETRIC OPTIMIZATION OF COMPACT DEC SYSTEM

Ettore Zanetti - Supervisor: Prof. Marcello Aprile

Reducing energy consumption and increasing renewable penetration are necessary to mitigate climate change and achieve sustainability goals. In the building sector, HVAC systems (heating ventilation and air conditioning) account for 20% of the primary energy consumption in developed countries. Furthermore, demand, especially cooling in developing countries, could increase by up to 50% by 2050. Most of the cooling is carried out by electrical chillers further straining the power grid. Thermally activated Desiccant Evaporative Cooling (DEC) systems have become a possible alternative. However, traditional DEC systems are bulky and not suitable for residential applications. Compact DEC systems are being developed, but research is still needed. This thesis aims to study and optimize a compact DEC system named FREESCOO numerically and experimentally.
This specific DEC and in general HVAC systems can benefit from advanced control, since it can help reduce discomfort, running cost and environmental impact. Advanced control, including Model Predictive Controllers (MPC) have a large variety of possible formulations even for the same HVAC system. This left a gap in literature on the influence of each formulation and solver choice. Furthermore, MPC is mainly studied for commercial buildings because in general it is not economically favorable for residential buildings. The aim is to analyze common MPC formulations to find the most suitable methodology and find a way to improve the local controller in a residential scenario using know how coming from an off-line MPC. The case study analyzed is a two-room apartment in Milan that uses floor heating coupled with a heat pump for heating and FREESCOO together with a district heating for cooling. 250 data points were collected for two FREESCOO iterations and a 2D finite volume model was calibrated and validated with less than 6% NRMSE.
Then, optimizing phases times thermal COP was increased by 20% for the cooling season. MPC comparisons lead to the conclusion that nonlinear MPCs do not bring benefit at the cost of longer computational time and more instability in the convergence. Lastly, using the MPC results pre-on and pre-off parameters were found to deal with floor heating high thermal inertia reducing by 90% discomfort in the heating season.

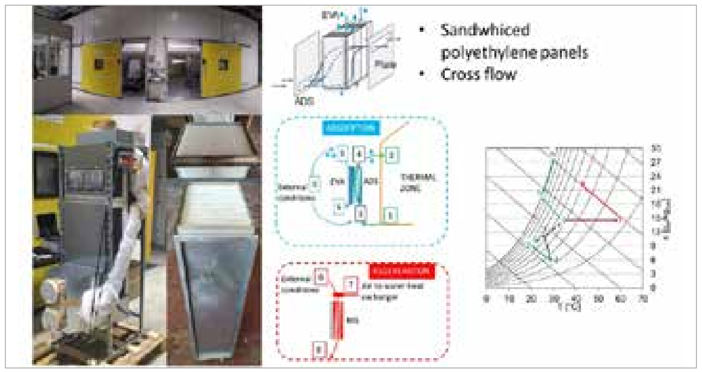

Fig. 1 -Left subfigure: 1) ReLab climatic chambers, 2) Test rig for heat exchanger and 3) Tested heat exchanger. Top rig subfigure: Schematic of the final indirect evaporative heat exchanger concept. Bottom right subfigure: 1) blue quadrant shows the adsorption process 2) red quadrant shows the regenneration process 3) Right diagram shows transformations of the external and process moist air in a Mollier moist arir psychometric chart.

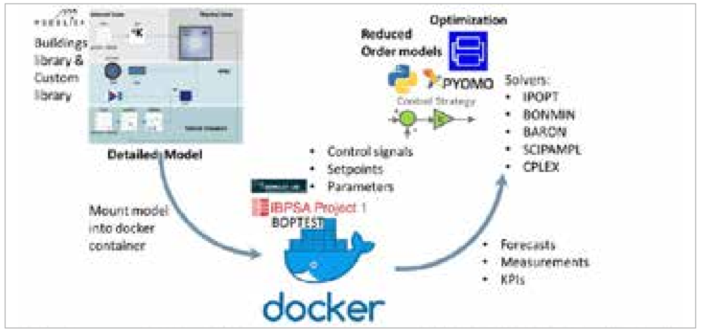

Fig. 2 - Co-simulation setup, on the right the optimization environment in Python Pyomo, on the left the detailed Modeica building and HVAC models and in the middle the software BOPTEST that allows the signal exchange, provides forecasts and KPIs.

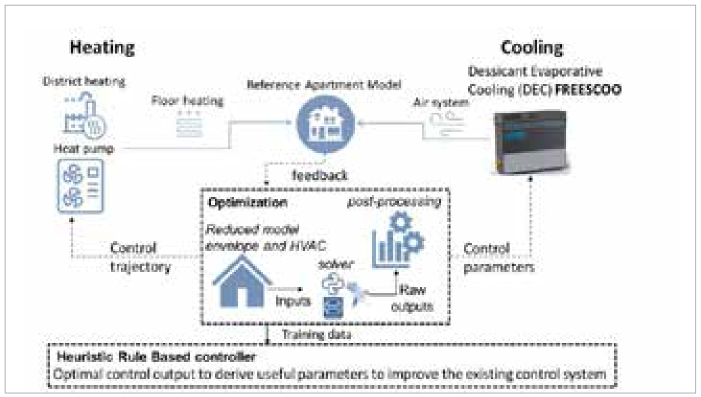

Fig. 3 - General framework of the thesis. Detailed modelling of the building and HVAC components, optimal control and parameter optimization, Heuristic rule based controller definition. Solid lines correspond to physical connection (i.e. HVAC components to building), dashed lines correspond to digital signals exchange.