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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
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SPATIAL HETEROGENEITY EFFECT ON FORCES DRIVING TWO-PHASE FLOW AND RECOVERY OF OIL RESERVOIRS

Payam Alikhani - Supervisors: Prof. Fabio Inzoli, Prof. Alberto Guadagnini

Data on hydrocarbon reservoir attributes (i.e., permeability, porosity) are only available at a set of sparse locations, resulting an incomplete knowledge of properties distributions. There has been considerable research devoted to simulating fluid flow but mostly failed to match predicted behavior to what is measured. The subject is riddled with the incomplete knowledge of properties distributions, which propagates to uncertainty in evaluations of reservoir performance and the resulting oil recovery.
Stochastic models were developed to determine the uncertainty resulting from incomplete knowledge of properties' spatial distributions. Regardless of whether the interest lies in simulating the spreading of a contaminant in aquifers or predicting recovery in a hydrocarbon reservoir, a variety of studies framed in the context of a stochastic approach. Monte Carlo (MC) simulation is the most popular and reliable method in uncertainty analyses but requires many high-resolution realizations. Improving computer performance-to-cost ratio during the last years made MC applications more convenient; thanks to technology developments. On the other hand, the ability to simulate the multiphase flow of fluids in porous media is crucial in developing an understanding of flow in the presence of heterogeneity. Cumbersome black-box commercial codes that are mainly stuck in a 70s time-warp make simulation predictions doubtful. In oil fields with orders of magnitude variation in permeability over several spatial scales, an accurate numerical solution with an adequate description of properties' stochastic nature is essential to simulate oil reservoirs.
We developed a numerical solution via a Finite Difference approach.
We start by assessing the accuracy of the numerical scheme employed through a comparison against the classical Buckley-Leverett analytical solution. The Enhanced Oil Recovery (EOR) central object is to improve ability in at least one of (a) viscous (b) gravity (c) capillary and (d) wetting forces to drive oil towards production. Therefore, we generalized the numerical solution by adding gravity and capillary forces and considering the wetting effect in both relative permeabilities (Kr) and capillary pressure (Pc) curves. In the numerical solution, Taylor series expansion is used to approximate the derivatives. High order terms in the expansion are considered for approximations of state variable derivatives to improve the accuracy of the solution. Later, grid convergence analysis utilized to increase the accuracy of our numerical base model. We then focus on the numerical solution of the system within randomly heterogeneous permeability fields using a typical MC framework. The latter enables us to quantitatively assess the relative strength of the differing forces acting on the system in the presence of uncertain spatial distribution of permeability.
Results highlight that (1) the uncertainty in spatial permeability distribution propagates to final oil recovery in a way that depends on the joint effects of forces, (2) increasing the spatial variability of permeability yields an enhanced uncertainty in oil recovery, (3) increasing viscous and/or gravity force, decrease the uncertainty associated with final oil recovery predictions, continuously, in a way that at very high viscous and/or gravity forces, the effect of permeability spatial heterogeneity on final oil recovery would be masked, (4) in the presence of both gravity and viscous forces, the largest uncertainty value is when viscous and gravity forces are counterpoise, (5) capillary pressure is effective on final oil recovery uncertainty only in case of high permeability contrast and may cause an increase or decrease in the uncertainty associated with final oil recovery prediction, (6) Spontaneous imbibition (controlled by capillary forces) is less effective recovery process in comparison to direct displacement (due to gravity and viscous forces), even in highly heterogeneous reservoirs and finally, (7) oil wettability tendency resulted in a drastic reduction in oil recovery with much higher uncertainty in comparison to the water-wet case.

In the next part of our work, the spatial heterogeneity effect is investigated on a carbonate oil reservoir in Oman. Carbonate reservoirs are characterized by extremely heterogeneous permeability. We start a stepwise procedure by conducting different laboratory experiments to measure properties of rock and fluid samples sourced from the referenced reservoir. Later, we perform core flood experiments using reservoir rock and fluids samples to monitor oil productions. We then focus on Pc and Kr functions that need to be back calculated by inverse model calibration, which is conditional to the generated experimental data. Calibrated numerical models are representative of the Omani oil reservoir. Finally, we implement different level of permeability spatial variations on a calibrated model within a MC framework. The latter enables us to quantitatively assess uncertainty, which is propagated to oil recovery evaluation of the calibrated model representing the referenced reservoir.
Rock, reservoir brine and oil samples were supplied from the referenced reservoir. We measured the viscosities of the brine and oil samples using Bohlin Rheometer Gemini at the reservoir temperature. Later, we evaluated the wettability of the sample rock by contact angle measurements using the reservoir sample rock and fluids. The result shows that oil drop dispersed on the rock surface in the way that we can consider the sample rock in the preferentially oil-wet category.
We also measured the porosity and permeability of the rock. Finally, the core sample is aged in the oil sample, and later a core flood test is performed in a rig facility designed explicitly in the oven for working at high temperatures. Core flood tests have been carried out, and oil production is monitored.
There are several input parameters in the reservoir models, but hydrocarbon's recovery is substantially controlled by both Kr and Pc functions. Different methods have been proposed to measure, estimate, or model Kr and Pc curves, but all are associated with a level of uncertainty. We used an inverse calibration method to back-calculate a set of Kr and Pc parameters conditional to the experimental data. Unknown parameters of Kr and Pc correlations are selected and a range of variability considering the oil wettability tendency of the sample rock chosen. Acceptance-rejection sampling is used, which is proved to produce reliable outputs even though it is a computationally demanding method. In this strategy, random sets of model parameters are independently sampled within the specified ranges, and then, candidate parameters set is accepted or rejected by considering threshold criteria based on the likelihood function. Results highlight that there is a good match between experimental data and the calibrated model results.
In the next step, MC approach used to perform random heterogeneous permeability fields on the calibrated model representing the referenced Omani oil reservoir. The uncertainty propagated to oil recovery evaluation was not negligible because 1% over or under estimation of recovery translates to huge profit or loss, especially for the referenced Omani oil reservoir with high oil reserves.
A comparison of the oil recovery predicted in homogenous and heterogeneous cases reveal the interesting result that homogenous assumption leads to an off-range prediction of oil recovery. In other words, results highlight the importance of considering properties spatial heterogeneity in reservoir models, including for the referenced Omani oil reservoir.

MEASUREMENT TECHNIQUES FOR NON-IDEAL COMPRESSIBLE FLUID FLOWS: APPLICATIONS TO ORGANIC FLUIDS

Giorgia Cammi - Supervisor: Prof. Andrea Spinelli

Co-supervisor: Prof. Alberto Guardone

Organic Rankine Cycle (ORC) power systems are a convenient option for power production in the 0.1 to 100 MW range when low/medium source temperatures are involved, thanks to their relatively high efficiency, low cost and plant simplicity with respect to traditional steam Rankine cycles.
Such temperatures and power ranges are often found in the case of renewable energy sources, such as geothermal reservoirs, biomass combustion and waste heat recovery from several industrial processes (power plants, cement and glass factories).
ORCs involve flows of heavy and complex organic compounds in thermodynamic regions close to the liquid-vapor saturation curve and to the critical point, where intermolecular forces are not negligible. As a result, ORC turbine flows differ from standard turbomachinery ones because they are highly supersonic and show significant non-ideal gas effects, such as flow field dependence on stagnation conditions. Given this, the design of such machines is particularly critical, also considering that turbine efficiency impacts the economic competitiveness of the ORC technology.
Several computational fluid dynamics tools embedding complex thermodynamic models suitable to simulate such flows are currently available. However, detailed experimental data characterizing non-ideal compressible flows, which are needed to validate these tools, are unavailable in the open literature up to date. These data can be obtained in dedicated wind tunnel facilities. However, running these facilities presents many technical challenges due to the high temperature, high pressure and thermodynamic conditions close to the fluid thermal stability limit.
This thesis presents three successful experimental campaigns conducted on a wind tunnel operated with organic vapors. Several experiments were conducted on the TROVA (Test Rig for Organic VApours) at the CREA (Compressible fluid dynamics for Renewable Energy Applications) laboratory.
The TROVA facility is a blow-down wind tunnel specifically designed to reproduce supersonic flows of organic vapors in conditions representative of ORC turbine expansions. The TROVA test section can be equipped with planar nozzles, designed for different fluids and/or operating conditions, and it can also accommodate linear blade cascades.
In the presented experimental campaigns, four different planar nozzle was tested with three different fluids, nitrogen, silixane fluid MDM (octamethyltrisiloxane) and siloxane fluid MM (hexamethyldisiloxane).
Nozzle expansions were characterized by total temperature and total pressure measures, by static pressure measurements along the axis and by the Schlieren technique to visualize the two-dimensional density gradient field along the axis direction. A wide range of inlet conditions was explored in order to systematically span the thermodynamic region of superheated vapor for the organic fluids. Conditions varied from highly non-ideal to almost ideal gas conditions.
This thesis focuses on measurement techniques, with particular reference to the effect of the peculiar thermodynamic conditions in which measurements are carried out.
The thesis provides an extensive assessment of the measurement techniques suitable to perform experiments in non-ideal compressible fluid flows. An ad-hoc calibration technique for piezo-resistive pressure transducer is presented together with technical details regarding pressure tap and test section design. A novel technique capable of automatically detecting in schlieren images flow structures locally approximable with straight lines was presented. The method permits to obtain local Mach number measurements on the axis of the supersonic region of nozzle flows.
The measurement techniques adopted proved to be suitable to detect non-ideal behaviors in compressible non-ideal flows.
Experimental results allowed to verify that nozzle expansion is influenced by total inlet conditions because of the non-ideal nature of the flow. Both MDM and MM nozzle flows proven to be non-ideal, since the inlet thermodynamic conditions significantly affect both the pressure ratio and the Mach number distribution along the nozzle axis, contrarily to the well know behavior of perfect gases. Indeed, the very same nozzles operated with nitrogen showed no such dependence on total conditions. Total inlet conditions are identified measuring total temperature T_T and total pressure P_T. These two parameters univocally identify a supersonic non-ideal expansion inside a nozzle with a given geometry.
However, it was investigated whether a single parameter can be used to assess the level of non-ideality of a MM nozzle flow and thus, to characterize the expansion and predict pressure ratio profiles with acceptable accuracy. Analyzed parameters were the compressibility factor Z_T and the fundamental derivative of gas-dynamics Γ_T, both evaluated at total conditions (subscript T).
Z_T is defined as

$$Z_T = \frac{P_T}{\rho_T(T_T, P_T) R T_T}$$

where R is the gas constant and is the stagnation density:
The compressibility factor Z identifies how much the volumetric behavior of a fluid differs from that of an ideal gas. Thus, it can be used to quantify the level of flow non-ideality.
The fundamental derivative of gas-dynamics instead provides information about admissible nozzle flow behaviors since it represents the non-dimensional variation of the speed of sound with pressure along an isentropic process. At total conditions, it is defined as where c is the speed of sound, v is the specific volume, s is the entropy. A Helmoltz energy based fundamental relation of Span-Wagner type was used to calculate all derived thermodynamic quantities.
It was concluded that, in the thermodynamic region explored for MM with experiments between Z_T = 0.60 and Z_T = 0.98, parameter Z_T can be used as univocal identifier of non-dimensional MM nozzle expansions in a given geometry. Contrarily, in the region where Z_T < 0.60 another parameter is needed to univocally characterize a non-dimensional nozzle flow and a possible parameter can be

$$\Gamma_T = 1 + \frac{\partial c}{v_T}\left[\left(\frac{\partial c}{\partial \rho}\right)_s\right]_T$$

It was proven that alone cannot be used to identify the level of non-ideality of a nozzle flow of siloxane MM. Indeed, the same values of are found in thermodynamic regions featuring rarefied conditions, where non-ideal compressible effects are negligible, and also in regions close to the critical point where non-ideal effects play a major role.
A comparison between MM and MDM nozzle flows at the same total reduced conditions was performed. It was concluded that, in the thermodynamic region explored pressure ratio profile of MM and MDM flows differ less than 1.5 % for all axial coordinate up to x/H= 12.3 and less than 5 % in x/H = 14.33.
The present thesis provides significant validation data for the improvement of state-of-the-art thermodynamic models and of design tools for siloxane fluids. The comparisons between CFD simulated and measurements data presented confirmed that still some work is required in order to achieve a better agreement between simulations and experiments in non-ideal compressible flows.
Hence, the present study confirms the need of accounting for non ideal effects in the design and analysis of component operating in the non-ideal compressible regime of molecularly complex vapor. Also, the measurement techniques selected proven their suitability in detecting non-ideal behaviors in compressible flows. A reliable methodology is therefore reported, which is applicable to perform experiments on high temperature and potentially condensing vapor flows in highly non-ideal thermodynamic conditions. This allows to provide the demanded experimental data and to establish reference test cases for non-ideal compressible flows.
Future works will focus on broaden the measurement techniques applicable to non-ideal compressible flows. In particular, on-going studies on the insemination process of organic vapors will probably lead to the possibility of performing LDV measurements, which would permit the direct acquisition of local velocity data. Moreover, the TROVA facility is being used to study non-ideal compressible flows around diamond-shaped airfoils, this will lead to a better understanding of the losses introduced by shock waves. Finally, the opportunity of using the TROVA as a wind tunnel for calibrating directional pressure probes for organic fluids is being analyzed. This would lead to the possibility of performing detailed measurements in actual turbines. These huge experimental efforts run in parallel with the creation of improved numerical tools, better tuned with the peculiar features of non-ideal compressible flows.

MODELLING AND EXPERIMENTAL INVESTIGATION OF NATURAL CIRCULATION IN PRESENCE OF DISTRIBUTED HEATING

Marco Tudor Cauzzi - Supervisors: Prof. Lelio Luzzi, Prof. Antonio Cammi

This thesis deals with the set-up of an experimental facility to study Natural Circulation (NC) in presence of Distributed Heating (DH). The framework of the work is the Molten Salt Fast Reactor (MSFR) research, in particular in the context of the Horizon 2020 SAMOFAR Project. This Project deals with the safety assessment of the MSFR, an innovative liquid-fuelled nuclear reactor characterised by a molten salt thermal carrier, which contains also fissile material. After irradiation the fluid is subject to decay power production. This unique characteristic must be considered when evaluating the safety of the MSFR, as the presence of a volumetrically DH source alters the concept of the Decay Heat Removal System (DHRS), a key component of a nuclear reactor safety system, for the MSFR. It is common practice in nuclear applications to use NC in DHRS, due to its potential higher reliability with respect to using active components. NC takes place in a fluid subject to differential heating due to buoyancy forces caused by density gradients. The presence of a heat source and heat sink drives a flow that transfers power from the source to the sink. However, NC is subject to dynamics instabilities that can cause insufficient or irregular flow, hence an accurate design of NC systems is required to prevent instabilities. One possible cause of instability of NC is the way the power is provided to the system, and previous studies showed that DH can have a great influence on NC equilibrium stability. The presence of DH in a NC system is an issue that has been little studied before. Recently, some studies have been performed from a computational point of view, approaching the problem by considering a simpler geometry, i.e., in the so-called NC Loops (NCLs). Studying NC on a simple geometry allows focusing on the physics of the problem, giving a ground base on which to develop more complex models. A NCL is a closed pipe loop containing a fluid and provided of heat sources and heat sinks. In the context of the SAMOFAR Project, ten experimental cases have been selected to be performed and predictions of the system behaviour have been made both with models developed previously and with models developed by partners of the SAMOFAR Project. Each of the models makes different assumptions and shows the difficulty of treating the problem of NC in presence of DH, as the results of the predictions made with state-of-the-art models are mostly disagreeing. This shows the need of an experimental facility to obtain data to assess the models in specific DH conditions and to verify their ability to predict the behaviour of a system. To obtain such experimental data a facility able to operate in DH conditions is needed, since NCLs currently available are unable to perform experiments with DH. The DYNASTY (*DYnamics of NAtural circulation for molten SalT internallY heated*) NCL, that can be operated with either water or a molten salt as thermal carrier, is presented. In the context of the presented activities, DYNASTY has been set up, brought to full functioning, and first sets of data have been collected. Fig. 1 presents a picture of the facility, along to a schematic view of its structure. DYNASTY can operate in DH conditions and will be used to assess the models previously developed to study NC with DH. Such models have been used in the context of this thesis to perform the facility design from scratch. In addition, DYNASTY was developed to be operated even in more 'conventional' working conditions, heating only some sections of its length. An additional NC issue is considered, namely the presence of a secondary NC system acting as heat sink of a NC system working with DH. An instance of such system is represented by the intermediate circuit in the DHRS of the MSFR. To have experimental data for assessing models developed to study such type of system, the DYNASTY facility has been extended, to include a secondary loop (eDYNASTY) to act as coupled NC cooler to DYNASTY. Fig. 2 shows a schematic view of DYNASTY and eDYNASTY together. In the context of this work, the eDYNASTY facility has been designed, built and brought to functioning. In this thesis, the modelling work performed to study previously developed models and to improve their ability to describe DYNASTY is presented. In addition, the extensive technical and multidisciplinary work related to designing, developing and building all the accessory systems of the DYNASTY facility (such as the data acquisition and control system) is also presented. During the set-up, many challenges were faced to identify and reduce most of the source of data acquisition uncertainty. Preliminary experiments have been performed operating DYNASTY with water to test the facility operability. In addition, the salt to perform the experiments has been prepared and its melting point has been tested to verify the eutectic composition. The preliminary experiments using DYNASTY showed interesting characteristics and behaviours of the facility. First, transient experiments have been performed, verifying that the reached condition after initial transient are independent of the state before the transient. Second, when the boundary conditions applied to DYNASTY pipes (in terms of provided power) are symmetric to the facility mid-plane, the mass flow is subject to oscillations and no steady state is reached, which is the type of behaviour found by some of the developed models. The construction of the DYNASTY facility paved the road to lots of future developments of research in the field of NC with DH. The DYNASTY facility will provide a benchmark for models developed to study NC with DH, as well as in conventional conditions.

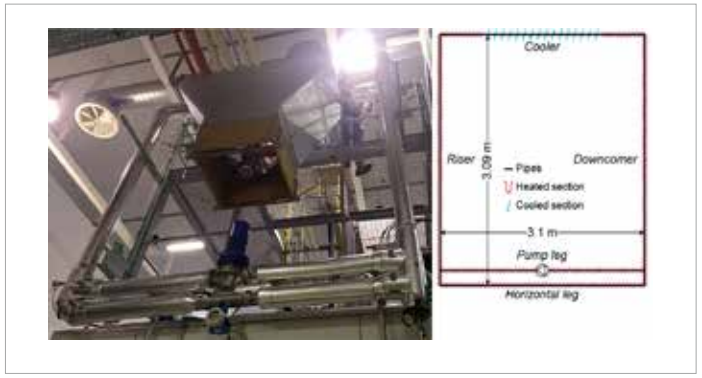

Fig. 1 - DYNASTY facility: actual picture and schematic view.

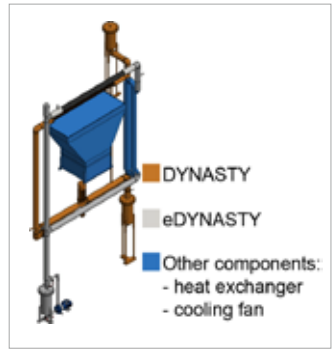

Fig. 2 -The coupled DYNASTY-eDYNASTY system.

POWER-TO-HYDROGEN FOR LONG-TERM POWER AND TRANSPORT SECTOR INTEGRATION

Paolo Colbertaldo - Supervisor: Prof. Stefano Campanari

The energy transition is an ongoing process worldwide and most countries have set ambitious targets to attain low-carbon energy systems by mid-century. Given the amplitude of the challenge, actions must involve all sectors and all actors. Shifting to renewable energy sources (RES) plays a key role in decarbonisation, together with strong energy efficiency measures. Electrification of loads can provide efficiency enhancement in some uses, whereas diversification of energy forms improves flexibility. The main drawbacks of RES are intermittency and seasonality, which are inherent to major alternatives (solar, wind, hydro). Their fluctuating output poses issues of stability and curtailment, which occur already at present installation levels. To overcome the uneven distribution and dynamic availability, large-scale energy storage and electric grid reinforcements will be required to manage overgeneration and supply shortages. Sector coupling and integration will be crucial to provide further flexibility to the overall system while supporting decarbonisation in hard-to-electrify sectors, like transport, farming, aviation.
This research work explored the integration of the power and transport sectors at nation scale, studying the role of energy storage in general and focusing on Power-to-Hydrogen (P2H) as key interweaving component of future energy systems, which couples the expected surplus electricity (due to massive increase in intermittent RES installed capacity) with the production of a multi-purpose energy vector (hydrogen). Looking at the long term, the projected co-presence of plug-in electric vehicles (PEVs) and fuel cell electric vehicles (FCEVs) is essential in supporting the sector coupling advantage.
The study developed a multi-node multi-sector model, building on the electric grid zonal structure to provide an adequate representation of power transfer constraints that affect the instantaneous supply-demand equilibrium. For each energy vector (electricity and hydrogen), the model includes spatially-resolved balances with demand terms from both sectors. Any number of energy storage technologies can be considered, each represented by balance equations that account for conversion losses, input-output flows, and self-discharge if applicable. For energy vectors that also have a non-electric destination, an output term is specified to account for direct use (most important for hydrogen). The model considers active-energy flows on 15-min or 1-hour time steps, so that generation fluctuations and load dynamics are taken into account, assessing demand mismatches and peak shaving needs, whereas short-term dispatch and management aspects are out of the scope.
The first model application looked at Italy with a 'given scenario' approach. A moderate and an aggressive evolution of clean power generation were matched with limited or dramatic changes in passenger car stock and shares, obtaining four scenarios that were compared to assess the interaction of energy flows over time and the overall system performance in terms of RES shares and GHG emissions. Results show that even the projected massive increase in clean generation only approaches the EU decarbonisation targets in the power sector (63% RES and -46% GHG from 1990). A large replacement of conventional vehicles is crucial to obtain a positive outlook in the transport sector (-59% GHG from 1990 with 34% PEVs and 30% FCEVs). The role of electric energy storage was evaluated, considering existing pumped-hydro plants and assessing the installation of battery energy storage systems (BESS) under operational constraints. However, location and operational constraints limit their impact on the system (1-2% of total demand). P2H is an optimal solution to treat the inevitable surplus, providing 80% of H_2 demand from FCEVs.
The use of hydrogen requires an adequate distribution infrastructure. Refining the model spatial resolution from electric market zones to provinces, a delivery network was designed under a techno-economic assessment. The investment cost is significant but in line with infrastructural investments on energy networks, e.g., electric grid or natural gas pipelines. Moreover, proper planning allows to distribute it along 20-30 years, thus spreading the effort over time while the market strengthen. The final cost of hydrogen appears limitedly impacted by distribution, even with the costly option of liquid storage, whereas hydrogen production from surplus electricity is a large cost item (~50%) due to low operating hours. This could change by valuing the role of electrolysis to flexibility, e.g., low pricing of electricity or shifting to a business case of grid service provision (upward and downward flexibility).
The second model application looked at California. Its electric sector is comparable to Italy (similar annual consumption and peak load, as well as expected solar-based future capacity), whereas its passenger car sector shows higher consumption despite a smaller stock. This assessment exploited a 'given target' approach, estimating the installed capacities of generation and storage required for 80-100% RES share. The presence of large shares of battery electric vehicles (BEVs) and/or FCEVs increases the annual electric demand by about 33% (slightly more in a FCEV-only case, slightly less in a BEV-only scenario). At the same time, the RES installed capacity needed to attain 100% RES supply on both sectors is nearly 50% more than that required for full-RES supply of the power demand without mobility. The different flexibility of hydrogen production for FCEVs vs. electricity provision to BEVs leads to smaller storage capacities in high-FCEV cases. Interestingly, results indicate that, despite most installed capacity is made of solar PV plants, the main seasonal effect is played by wind generation. The alternative of BESS as exclusive storage option for the power sector leads to massive capacities (~30 TWh_{el}) and extreme rise in total investment costs (in the range of $ trillion), confirming the prospective advantages of P2H and P2P.
Overall, the work shows that in future energy system architectures, where installed capacity of RES for power generation increases dramatically, sector integration via P2H is not only beneficial for the system but also essential for an effective multi-sector decarbonisation.

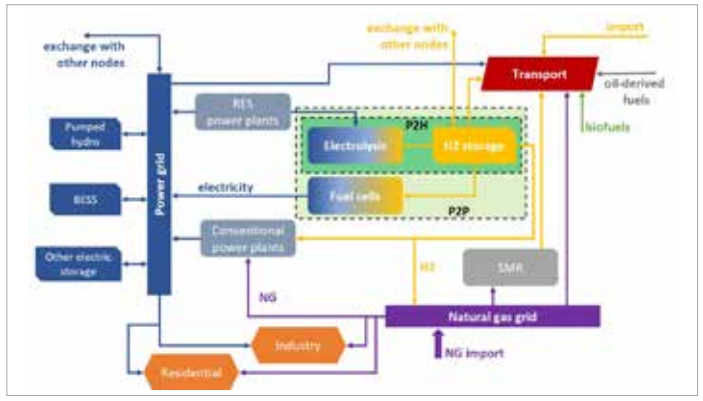

Fig. 1 - Scheme of energy flows and their interaction in future interwoven energy systems.

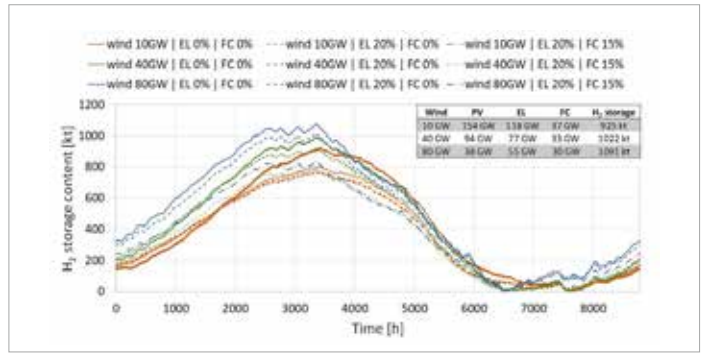

Fig. 2 - Year-long hydrogen storage profile in 9 simulated cases of California 100% RES energy systems, at 3 values of wind installed capacity and different assigned minimum capacity factors for electrolysis (EL) and fuel cell (FC). Time axis starts on June 1st.

NUMERICAL MODEL FOR NEW GENERATION DISTRICT HEATING SYSTEMS WITH DISTRIBUTED RENEWABLE HEAT SOURCES

Alice Dénarié - Supervisor: Prof. Mario Motta

The aim of this PhD thesis is to build fast and accurate district heating simulation tools to enhance the integration of renewable energy sources in district heating systems to increase their sustainability.
New generation district heating systems are going to face new challenges related to new heat sources and new customers: the increase of renewable energies integrations, especially in a distributed form, and the connection of energy performing buildings will lead to a different operational behaviour.
Overall district heating network will be characterized by a great variety of low temperature highly variables energy profiles in the network.
Therefore, traditional modelling tools are no more suitable to analyse these systems: these reasons lead to the need of building new tools.
A specific thermo-hydraulic simulation model has been built to simulate the entire network and its components.
The model aims at being fast and accurate in predicting temperature propagation, heat losses and pressure drops over the entire network. A model for every element composing the network, namely pipes, pumps, substations and generation systems, has been built. Hourly monitoring data of heat demand at users' substations and of heat production at generation plant are the inputs of the simulation of the DH network. The model combines accuracy and rapidity.

Concerning the problem of heat transmission in pipes, the modelling approach is an updated version of the node method and it includes the turbulent flow characteristics.
The proposed method of heat transmission over long pipes shows advantages over other methods, making it a suitable alternative for the simulation of complex DH network dynamics. The improved plug-flow model considers the temperature difference between the fluid core and the viscous sublayer in a turbulent flow, while it reduces the error propagation in long pipes.
The mathematical approach used to solve the thermal transmission problem—the splitting approach—yields accurate results with low computational effort.
The model results are comparable to those of the high-discretisation FVM, but the proposed model is faster and does not include artificial diffusion.
Compared with the node method, it retains the simulation speed, avoiding sharp temperature variation smoothing.
The model accuracy is investigated by applying it to a real DH network, located in the municipality of Lodi (Italy). The model of the entire network is validated with one-year monitoring data.
The same network has been used also as a case study to analyse the feasibility of distributed solar thermal plants.
A methodology to choose the best location for solar thermal plants and to assess their environmental and economic benefits has been elaborated and applied to the case study network. The thermo-hydraulic model has been finally used to verify the performances of the distributed solar thermal plants and their impact on the network.
As a result, the detailed simulation confirmed the result of the presizing methodology, validating it. On the other side the dynamic simulations showed some detailed aspects of the network management such as flowrate peaks and heat losses.
The thermodynamic simulation model confirms being an important tool to investigate operational and management aspects of renewables integration in DH.
Results shows that, even if the solar plants have a better performance if integrated in a centralized plant and without storages, the distributed integration allows a further primary energy savings by reducing heat losses and electrical consumptions due to pumping work. Finally, this application has shown that solar energy can definitely represent a good opportunity of primary energy savings even in the retrofitting of existing district heating system with relatively high distribution temperatures
The model results' comparison with monitoring data revealed very good correspondence making it usable for the foreseen purpose. The application of both the planning methodology and of the simulation model have shown that distributed renewable energies integration can have important benefits on the existing network from both environmental and economic points of view. The analysis of the case study with the thermohydraulic model allows the identification of detailed control strategy improvements and optimisation opportunities.
From the results of this research it clearly stands out how these phenomena related to the increasing dynamics of future district heating systems with a high share of distributed renewable energies need to be identified and analysed with robust thermohydraulic simulation models.

In conclusion, new generations district heating systems with low energy demand buildings and a share of aleatory renewable energy sources are characterized by much more fluctuating and unpredictable energy profiles, in particular if the generation systems are distributed along the networks.
For this reasons, new decision support tools need to be developed and applied to district heating systems integrated with several renewable energy sources.

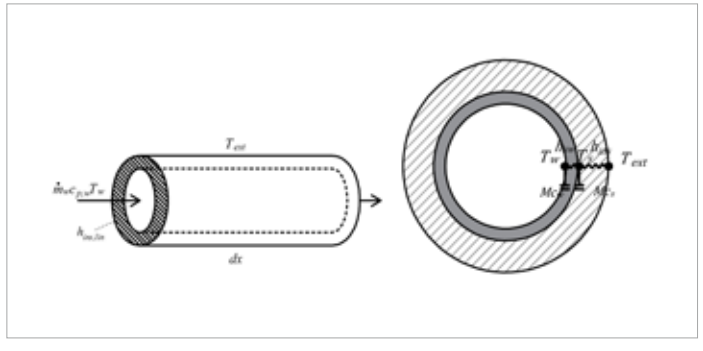

Fig. 1 - 1Longitudinal and transversal DH pipe section modelling scheme

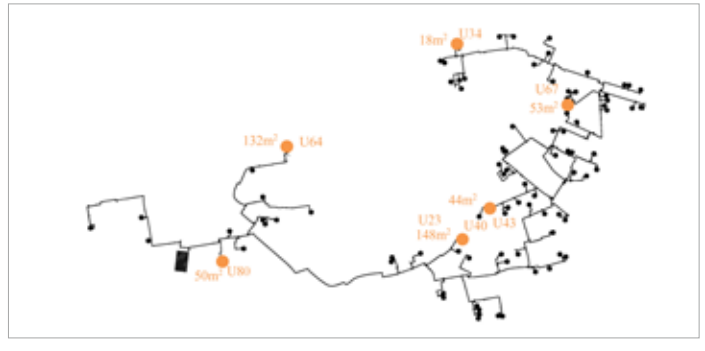

Fig. 2 - DH network case study: users selected for solar thermal integrations

SYSTEMATIC OPTIMIZATION OF HEAT EXCHANGER NETWORKS WITH INTEGRATED THERMODYNAMIC CYCLES

Cristina Elsido - Supervisor: Prof. Emanuele Martelli

The techno-economic optimization of integrated utility systems, Rankine cycles and Heat exchanger Networks (HEN) is a challenging problem that has a great relevance in industrial practice, in the first place because it involves a considerable part of the capital and operational costs of a power or poly-generation plant. Moreover, the large penetration of intermittent renewable energy sources requires that novel power or poly-generation plants are operated in a flexible way, and there are no methods available in literature that can consider also expected operating conditions during the plant lifetime.
The majority of works over the past decades has dealt with the optimal synthesis of HENs and utility or energy system design as separate problems with limited integration options between the HEN and the thermodynamic cycles or utility streams. In this work, a general and systematic synthesis methodology has been developed to optimize simultaneously the utility systems, Rankine cycles and HENs at the nominal condition ("single-period") or considering different off-design operating conditions ("multi-period"). The great advantage of the simultaneous optimization model is that it allows to generate several options for Rankine cycle designs (i.e., selection of number of pressure levels, components and mass flow rates, with fixed pressure and temperatures) and for heat integration with the process heat sources/sinks, while considering the techno-economic constraints (and the off-design efficiency, in the multi-period optimization) at the same time.
From a modelling and mathematical programming point of view, the major contributions of this work are:

- The development of a general superstructure for complex utility systems and Rankine cycles, and its integration in a model for the simultaneous optimization of the design of utility systems, Rankine cycles and HEN. The model can accommodate a variety of constraints and specifications, including technical design constraints, such as forced/forbidden matches and the "no stream splitting" constraint on the HEN layout, and detailed costs models. In Fig. 1 a schematic representation of the integrated problem with a Rankine cycle superstructure.
- The ad-hoc bilevel decomposition method that combines three state-of-the-art relaxation techniques (outer-approximation linearization, McCormick relaxation, and adaptive piecewise linearization of the cost functions) with two original additions: the inclusion of heat cascade constraints to tighten the problem relaxations and the use of nested integer cuts to speed up the convergence. In general the ideas of combining different linearization techniques, including redundant heat cascade constraints and using "nested" integer cuts may be useful for other synthesis problems and other classes of Mixed-Integer NonLinear Programming problems (MINLP).
- The model and algorithm have been implemented in GAMS. For the considered class of problems, the ad hoc methodology performs way better than general-purpose solvers (such as BARON) and a proposed heuristic algorithm. The results over a set of test cases show that the computational time of the bilevel decomposition method is up to 2 orders of magnitude shorter than the heuristic approach. The method is effective in solving extremely challenging problems, as it has been successfully applied to problems with up to 35 streams, 11,755 variables (2,843 binaries) and 17,040 equations. In addition, the convergence of the algorithm is not affected by the choice of the initial point and it is very effective in finding potentially good feasible solutions in all the search space.
- The extension to the multi-period optimization problem: ad-hoc "uncontrolled HX constraints" have been implemented to ensure feasibility of the solutions in part-load operation, due to the necessity to model uncontrolled heat exchanges. The standard hypothesis of heat exchangers with bypass or recycles, typical of chemical process applications, is not suitable for power plants and HRSGs.

From an application perspective, the proposed methodology has been successfully applied to several case studies such as NGCC, waste heat recovery ORCs, CBTLE demonstration and full-scale plants, IGCC and ISCC plants. Among these applications, the method has been used for the optimization of the heat recovery cycles and heat integration in two international projects involving the Department of Energy of Politecnico di Milano:

- NETL project (funded by the US DOE), in cooperation with Princeton University, to optimize the heat integration and the heat recovery steam cycle for a CBTLE plant to co-process lignite and woody biomass into jet fuel (using gasification and Fischer-Tropsch synthesis) with CO_2 capture and storage.
- EU Horizon 2020 project FLEDGED, "FLExible Dimethyl ether production from biomass Gasification with sorption-enhancED processes". The method has been used for the optimization of the heat recovery system for different sizes of the plant, considering steam cycles and ORCs, both in a single- and multi-period framework.

The general and systematic methodology can be used to explore the design criteria of novel utility systems and Rankine cycles (unconventional steam cycles and ORCs) that are highly integrated with a process. The approach is particularly interesting for heat integration problems in which the process features multiple hot and cold streams at different temperatures making it necessary to optimize not only the Rankine cycle configuration but also the HEN. Compared to current design criteria, the proposed methodology allows to obtain more efficient and cost-effective solutions for waste heat recovery.
The extension to the multi-period optimization allows to find the optimal trade-off between efficiency and costs while guaranteeing the operational flexibility, for plants that are expected to operate in different modes. The presented models and algorithms allow to deal with a class of problems that cannot be solved with any other available approach, and this is particularly useful in the design of novel flexible plants, such as IGCC and ISCC plants.
In summary, the proposed methodology is an effective design tool that allows to save a large amount of engineering time and to explore a much larger number of solutions compared to conventional design methodologies.

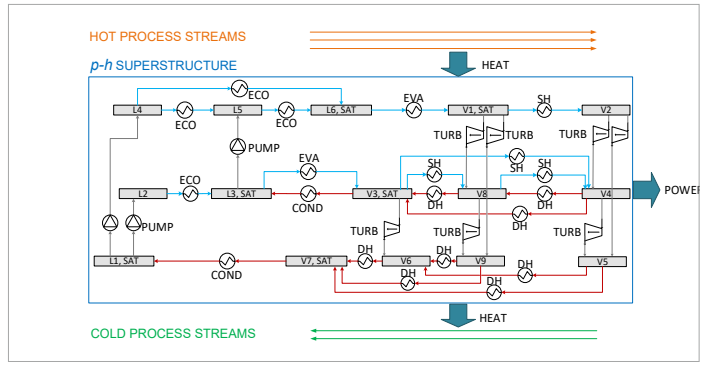

Fig. 1 - Schematic representation of the integrated heat recovery Rankine cycle and HEN design optimization.

MULTI-DIMENSIONAL CFD SIMULATION OF INTERNAL NOZZLE FLOWS IN HIGH PRESSURE FUEL INJECTORS

Filippo Giussani - Supervisor: Prof. Federico Piscaglia

The present work focuses on the modelization of in-nozzle flow and primary break-up of high pressure fuel injector for Gasoline Direct Injection (GDI) engines. Experimental high-speed camera visualizations on transparent glass-nozzle replica of gasoline fuel injectors have been used in combination of a novel in-house developed high-fidelity LES-VOF multiphase solver in OpenFOAM to study the evolution of vortex flow and cavitation in GDI injection, and the extent primary jet atomization. The development of a single-fluid solver supporting phase-change and able to capture the evolution of three fluids, two of which are miscible into the sharp interface capturing Volume of Fluid (VOF) approximation, is presented. The transport of each phase-fraction is solved independently by a flux-corrected transport method to ensure the boundedness of the void fractions over the domain. The closure of the system of equations is achieved by a cavitation model that handles the phase change between the liquid and the fuel vapor, and it also accounts for the interaction with the non-condensable gases. Verification of the solver has been performed on two numerical benchmarks: a two-dimensional bubble rising in a liquid column and a cavitating/condensing liquid column. Afterwards, a first validation of the solver has been performed using a test case at low injection pressure (2.2 bar): numerical predictions from large-eddy simulations have been compared against experimental results available from literature for that operative pressure condition; in particular, validation against high-speed camera visualizations (Fig. 1) and Laser Doppler Velocimetry (LDV) measurements of cavitating in-nozzle flows in a fuel injector is reported.

Finally, the solver has been validated on two configurations of a glass nozzle injector, provided by Continental. These two geometries have been chosen among ten glass-nozzle injectors, which can be easily mounted on the same feeding system, since they have shown opposite behavior in terms of Jet Wise Penetration (JWP). In particular, they have been analyzed under a working pressure condition of 100 bar. Due to high pressure condition and reduced size of the nozzle orifice, only high-speed camera visualizations were available as experimental measurements. The simulated domain has been reconstructed from X-ray Computed Tomography (XCT) performed on the real nozzle replica. Fig. 2 shows the process followed for the geometry reconstruction proposed in the present work: from the nominal CAD project to the transparent glass nozzle replica has been built up. XCT and microscope measurements have been used to reconstruct an estimate of the real surface in stereolitography format (STL).

Both experiments and simulations capture the formation of unsteady vapor structures inside the nozzle volume. The first type, which is referred to as “shear-cavitation’’, is found at the core of the recirculations zone and originates at the sharp corners at the nozzle entrance. This is also called geometry-induced cavitation. The second type, which is referred to as “string-cavitation’’, is found at the core of high vorticity area along nozzle axis. It is shown that the numerical solver provides an accurate capture of the interface among the different phases within the nozzle hole and a very detailed description of the vortex generation in the injector nozzle; strings appear within the time scales that are relevant for a typical gasoline injection event and, for the specific case and operating condition studied, their generation seems mostly related to the flow pattern of the upstream region of the nozzle. Vorticity and surface dynamics have been then used to identify the main factors for the formation of the surface instabilities, that lead to the so called “primary atomization’’. Additionally, an interface resolution analysis has been performed in the spray domain to investigate the limits of the Algebraic VOF (AVOF) employed for the simulation. Predictions of the primary atomization of jets on real nozzle geometries have been finally validated against the experimental visualization taken with high-speed camera visualization (Fig. 3).

Fig. 1 - Internal nozzle flow test case . Left) developed LES-VOF solver; right) visualizations from experiments.

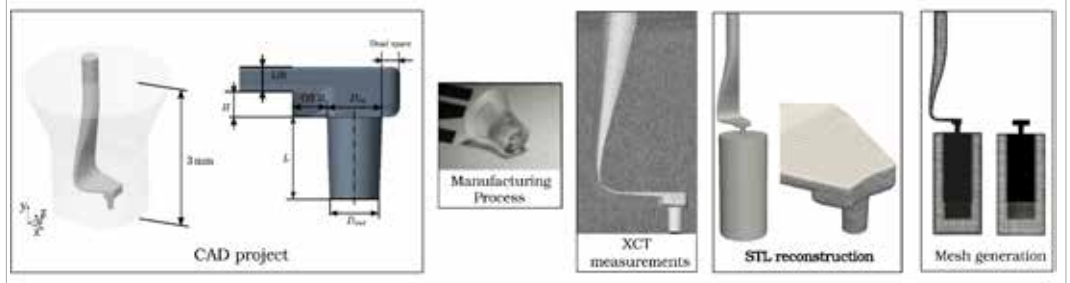

Fig. 3 - Sketch of the process from CAD project to mesh generation

Fig.3 - Primary atomization: qualitative comparison of the front view for config. ID-3 (left box) and ID-10 (right box). For each box, left picture denotes experimental view, while right picture denotes numerical view.

DESIGN AND MODELING OF A MICRO GAS TURBINE WITH A BOTTOMING ORGANIC RANKINE CYCLE: STEADY-STATE AND DYNAMIC APPROACH

Sonia Laura Gómez Aláez - Supervisor: Prof. Paolo Silva

Co-supervisor: Prof. Andrea Giostri

This PhD dissertation deals with the integration of a bottoming Organic Rankine Cycle (ORC) cycle to recover heat from the flue gases of a commercial micro gas turbine (mGT) for the production of electricity. The off-design behavior is modelled with a steady-state approach and, in addition, the transient response is analyzed.
The research project aims to develop simulation models to evaluate the performance of the overall system. The application of this system aims to instantaneously satisfy the electricity demand of a set of 150 houses in Cologne (Germany).
The first part of the research aims to study how the system behaves in nominal conditions. A commercial mGT (on-design electric power output equal to about 100 kWe) is selected for this application and a thermodynamic optimization of the design of the bottoming ORC is performed aiming to maximize the electric power output. To study how the system behaves in nominal conditions, two main models are developed in Matlab®: one to evaluate the performance of a commercial mGT and another one to optimize the design of the bottoming ORC module in terms of electric power output. As regards the ORC, different working fluids are investigated and the most promising one in terms of electric power output and environmental impact is the R1233zd. This fluid seems the perfect alternative to R245fa in terms of environmental impact and cost (20-25€/kg for the R1233zd vs 30-35€/kg for the R245fa). Introducing the bottoming ORC results in an increment of the electricity production from 100 kWe to almost 120 kWe at ambient temperature of 15°C (split in 93.9 kW from the mGT and 25.8 kW from the ORC), increasing the efficiency of the overall system from 29.5% to 36%. In order to complete the design, the geometries of the heat exchangers are determined. The ORC equipment is sized subsequently after the complete design. The determination of the geometries is mandatory to evaluate the mass and volume of each heat exchanger, which rule the dynamic behavior of them. Two different procedures are used here according to the heat exchanger that has to be simulated. For the regenerator of the mGT, a 3D model is developed in Matlab® to recreate the existing heat exchanger with the dimensions available in the literature.

The heat exchangers of the ORC are designed by using the commercial software Aspen Exchanger Design & Rating®. Plate-fin heat exchangers are the most optimal ones in terms of compactness.
The second part of the research aims to study the part-load performance of the designed energy system. This is a mandatory part for the transition in the study of the system behavior from nominal conditions to dynamic conditions. The off-design study aims to analyze how the system behaves when the operating conditions (i.e ambient temperature, power demand) differ from the nominal ones. The off-design conditions obtained from the steady-state models in Matlab® are then used for the study of the dynamic behavior in different ways. These results are the basis to validate the performance of the dynamic model developed with Dymola by imposing different operating conditions and checking the final steady-state results from the dynamic model. Moreover, for control purposes, the off-design steady-state conditions are used in two different ways. The first one consists in imposing a physical limit to the required electric power (i.e. the controller cannot ask to the system more than what is physically possible even if the electric demand is higher) and imposing the set point of the ORC turbine inlet temperature (TIT), aiming to maximize the ORC power output. The second one consists in detecting different off-design equilibrium points in which the system will be linearized to proceed with the design of the control system.
Once the steady-state models, simulations and results are concluded, the third part of the research aims to move forward the steady-state conditions and analyze the dynamic response. For this purpose, dynamic models are developed in Modelica (in Dymola environment). As mentioned before, the steady-state results obtained with the dynamic models are validated with the off-design steady-state results. After that validation, open loop (i.e. without a control system) simulations are performed. These simulations bring to the conclusion that a control system is needed for studying the dynamic response.
If there is no control system, the operational conditions can be harmful for the equipment and for the stability of the system (e.g. reaching too high metal temperatures, obtaining undesirable performance electric output). Therefore, a simple control system is designed using the most common controllers in the market, PI controllers. The control system consists of three controllers guaranteeing the behavior of the electric output, the turbine outlet temperature (TOT) of the mGT and the TIT of the ORC. The controllers are designed using the PID Tuner tool of Matlab®, looking for a compromise in the response in terms of fast response and overshoot. The dynamic behavior is then analyzed by studying the electricity demand profiles of the two most critical days of the year: the one with the highest and the lowest load profile. The simulations are performed considering a time step of one second, however, two type of profiles are imposed: real demand conditions and one-minute-averaged demand conditions. Those profiles are imposed as set points in the electric power controller. After analyzing the transient response, it is concluded that the proposed system formed by the mGT and ORC cannot work in stand-alone conditions to satisfy the demand instantaneously, as there is a difference in the demanded electricity and the given electricity. As the system is not able to fulfill the demand by its own instantaneously, and a parallel system should be needed, the results show that taking an averaged profile helps to get considerably smoother results, therefore, the equipment would suffer less as the temperature gradients are lower. Taking an averaged profile is unrealistic if the proposed system formed by mGT and ORC has to work on its own, but it could be very efficient when working with a parallel system consisting of a battery or the electric grid itself, which allows peaks to be satisfied.

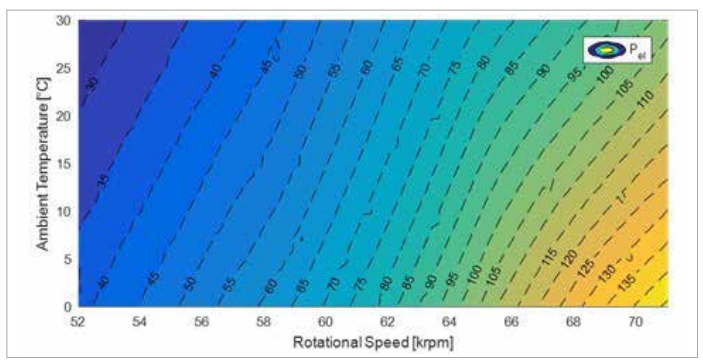

Fig. 1 - Variation of the power produced by the overall system mGT+ORC in part load conditions.

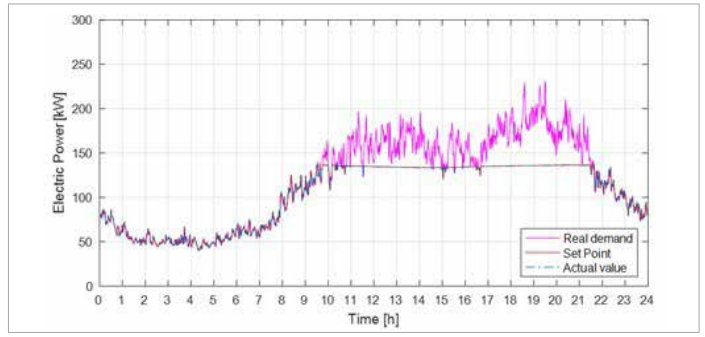

Fig. 2 - Electric power request and response of the system for the day with the highest electricity demand

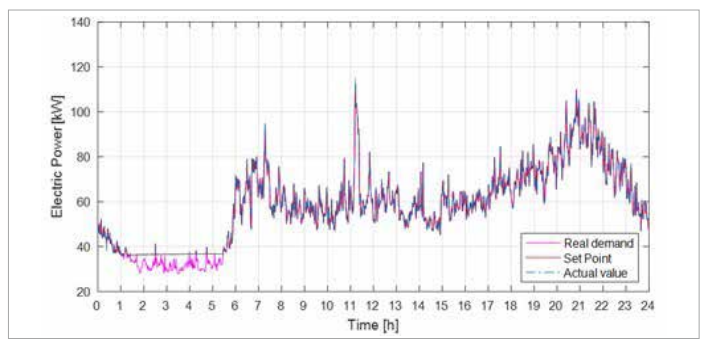

Fig. 3 - Electric power request and response of the system for the day with the lowest electricity demand

TECHNO-ECONOMIC ANALYSIS OF AQUEOUS AMMONIA BASED ABSORPTION PLANT FOR CO_2 CAPTURE SUPPORTED BY EXPERIMENTAL DATA

Stefano Lillia - Supervisor: Prof. Gianluca Valenti

The aim of the thesis is the study of two different post-combustion carbon capture technologies by chemisorption applied to coal fired power plants. The analyzed technologies are the Aqueous ammonia and the Mixed-Salt Technology.
The Aqueous ammonia absorbs CO_2 from the flue gasses with aqueous ammonia solvent. This technology is based on the Chilled Ammonia Process patent by General Electric which exploits aqueous ammonia solvent as well to capture CO_2. The difference between the two technology is the absorption temperature. The Aqueous Ammonia absorbs the CO_2 at environmental temperature (20°C) while the Chilled Ammonia Process absorbs at chilled conditions (7°C). The process simulations of the two different technologies returns benefit in terms of performance and plant operation for the Aqueous Ammonia despite a higher temperature rises the ammonia slip and penalizes the thermodynamic of the absorption reactions. Indeed, the higher temperature of absorption avoids the electric consumptions of the chilled needed for the gas and the solvent cooling with a reduction of the Specific Primary Energy Consumption for the CO_2 Avoided (SPECCA). Moreover, at 20°C the salt precipitation in the absorber does not occur avoiding problems of corrosion and pipe clogging which are one of the main operative issues of the Chilled Ammonia Process. The two processes are simulated in Aspen Plus® with an equilibrium-based approach with the Extended-UNIQUAC thermodynamic model and the results return a SPECCA of 2.58 MJ/kg_{CO2} for the Aqueous Ammonia and a 2.86 MJ/kg_{CO2} for the Chilled Ammonia Process.
Selected the best process, the kinetic of absorption is characterized experimentally. The experimental set-up used is the Wetted Wall Column which measures the overall mass transfer coefficient and permits the measurements of the Arrhenius parameters of kinetic of the reaction between NH_3 and CO_2 with the following result:

Afterwards, a rate-based model is developed in Aspen Plus® in order to simulate the absorber considering the effect of the heat and mass transfer and the kinetic of reactions. The model is calibrated with the data of the Munmorah pilot plant available in literature with an error lower than 20% and an average error lower than 5%.
After the calibration, the rate-based model is exploited for the component design and overall plant simulation. The capture plant has been integrated with the coal fired power plant and simulated with a “retrofit” and a “green-field” approach. The retrofitted approach follows the EBTF (European Benchmark Task Force) guidelines where the steam for the solvent regeneration is extracted from the IP/LP crossover at a fixed pressure determined by the power plant. Found the performance of the integrated plant a techno-economic analysis is assessed and the results compared with the reference case reported in the EBTF report. The results return a lower SPECCA for the Aqueous Ammonia (3.21 MJ/kg_{CO2} vs. 4.35 MJ/kg_{CO2}) and consequently lower a Levelized Cost Of Electricity (LCOE) (87.66 €/MWh_{el} vs. 92.27 €/MWh_{el}) and a lower cost of CO_2 avoided (47.03 €/t_{CO2} vs. 51.62 €/t_{CO2}) mainly due to the higher net electric efficiency of the overall retrofitted power plant (36.32 $\%_{LHV}$ vs. 33.40 $\%_{LHV}$).
On the other hand, the green-field approach follows the NETL (National Energy Technology Laboratory) guidelines where the steam for the solvent regeneration is extracted at as low pressure as possible since the power plant is designed maximizing the steam expansion in the power plant and consequently to maximize the gross power output of the power plant. The performance of the integrated plant a techno-economic analysis is assessed and the results compared with the reference case reported in the NETL report. The results return a lower SPECCA for the Aqueous Ammonia compared to the Cansolv technology (3.23 MJ/kg_{CO2} vs. 3.30 MJ/kg_{CO2}) and consequently lower a Cost Of Electricity (COE) (124.3 $/$MWh_{el}$ vs. 133.2 $/$MWh_{el}$) and a lower cost of CO_2 avoided (66.50 $/$t_{CO2}$ vs. 75.25 $/$t_{CO2}$) due to the higher electric efficiency (33.06 $\%_{HHV}$ vs. 32.50 $\%_{HHV}$) and the lower investment cost caused by the necessity of less quality materials since the less corrosive solvent with respect to amines.

The Mixed-Salt Technology patented by SRI-International exploits an aqueous mixture of ammonia and potassium carbonate as a solvent. The aim of the potassium carbonate addition aims to reduce the ammonia slip and the specific heat duty for the solvent regeneration without reducing too much the kinetic of absorption and without reducing the regeneration pressure under the atmospheric pressure like what happens in the technologies with aqueous potassium carbonate solvents.
The thermodynamic of this system is modelled with the Extended-UNIQUAC model after a further recalibration with 8000 experimental data from the literature in order to increase the accuracy of the CO_2-NH_3-KOH-H_2O system modelling. After the calibration, the model is used for the thermodynamic characterization of the solvent. The results show a reduction of the specific heat duty of regeneration and a reduction of the ammonia slip without scarifying the CO_2 capture capacity of the solvent.
After, the kinetic of the CO_2 absorption is studied experimentally with the Wetted Wall Column maintaining constant the CO_2 capacity of the solvent. The results show a reduction of the kinetic of the absorption reducing the temperature and rising the CO_2 loading of the solvent. Moreover, rising the K_2CO_3 in the solvent, the kinetic of absorption decreases because the reduction of the free ammonia in liquid phase reduces the rate of the reaction between the NH_3 and the CO_2 which is the faster reaction and the more influent on the rate of the overall process.
The process in then simulated in Aspen Plus® with an equilibrium-based approach in order to evaluate the thermodynamic performance. A sensitivity analysis optimizes the design parameters to have the lower consumptions. The best case selected is integrated and simulated with the coal fired plant used in the NETL report following a greenfield approach. Here, the steam is extracted at the lower pressure as possible since the power plant is designed maximizing the steam expansion in the power plant. The performance of the integrated plant a techno-economic analysis is assessed and the results compared with the reference case reported in the NETL report. The results return a lower SPECCA for the Mixed-Salt Technology compared to the Cansolv technology (2.19 MJ/kg_{CO2} vs. 3.30 MJ/kg_{CO2}) and consequently lower a Cost Of Electricity (COE) (117.55 $/$MWh_{el}$ vs. 133.2 $/$MWh_{el}$) and a lower cost of CO_2 avoided (51.58 $/$t_{CO2}$ vs. 75.25 $/$t_{CO2}$) due to the higher electric efficiency (35.00 % vs. 32.50 %) and the lower investment cost caused by the necessity of less quality materials since the less corrosive solvent with respect to amines.
Finally, the Life Cycle Assessment (LCA) compares the environmental impact of the amines technologies such as MEA and MDEA with respect to inorganic solvents such as ammonia and potassium carbonate. The results show a lower environmental impact of the inorganic solvent with respect to amines mainly caused by less impact of the chemical processes used for the solvent production which exploits reagent with high toxicity.

TISSUE-EQUIVALENT PROPORTIONAL COUNTERS AS CONNECTING BRIDGE FROM MICRODOSIMETRY TO NANODOSIMETRY

Davide Mazzucconi - Supervisor: Prof. Andrea Pola

In the last decades, radiation therapy with ion beams has been spreading worldwide for the treatment of cancer. With respect to conventional photon radiation therapy, better dose conformation to the target and increased sparing of the healthy tissue surrounding the tumor can be achieved with ion beams, due to the different physics of interaction of charged particles into matter.
The biological effectiveness of this treatment is nowadays based on the absorbed dose, a macroscopic and averaged quantity, which is inadequate in describing the energy deposition at micrometric level, since it does not take into account neither the stochastic of particle interaction in the target volume, nor the track structure of ionizing charge carriers.
Microdosimetry and track-nanodosimetry are two branches of radiation physics which develop theoretical and experimental methodologies for the description of the radiation interactions with cellular and sub-cellular biological structures. Microdosimetry provides a characterization of the statistical fluctuations of the energy locally imparted to a micrometric site, while track-nanodosimetry is focused on the description of the ionizing particle track structure.
The Tissue Equivalent Proportional Counter (TEPC) is the most accurate device assessing the properties of a particle beam in its interactions at micrometric level. It is actually well known that the biological damage of the radiation starts with interactions at a lower level, the nanometric one, involving the chromatin fibres and the DNA segments. Therefore, the track structure of the ionizing particle becomes fundamental, and track-nanodosimetry is the only way to investigate it. Nanodosimetric quantities, that derive the single-event distribution of ionization cluster size, demonstrated to be strongly correlated to the biological damages at the DNA level.
Present nanodosimeters show significant limitations, due to their complexity and dimensions. On the other hand, common TEPCs are able to provide microdosimetric spectra resulting from interactions in sites of dimensions down to 300 nm. With respect to nanodosimeters, TEPCs are transportable and easier to be used: they could be used for characterizing therapeutic hadron beams.
This thesis aims at finding a connecting bridge between microdosimetry and track-nanodosimetry. This goal is pursued through a systematic characterization of two conceptually new Tissue Equivalent Proportional Counters (TEPCs). These novel devices are capable of measuring microdosimetric distributions from 500 nm down to 25 nm in simulated site size.
The main feature of the nano-microdosimetric TEPCs is the presence of a third electrode, a helix, surrounding the anode wire. The first TEPC is called sealed and can be easily transported between different therapeutic and research irradiation facilities. The second TEPC, instead, is defined wall-less since it is installed inside the STARTRACK nanodosimetrer (INFN-LNL) gas chamber. The wall-less TEPC can allow the systematic comparison between microdosimetry and track-nanodosimetry.
The sealed TEPC has been irradiated with several hadron beams. The behavior of the microdosimetric distribution against the simulated site size (in the range 500 - 25 nm) has been studied for neutron, proton, helium, carbon and oxygen beams. The obtained spectra show that the nanometric domain distributions are highly influenced by the features of the track-structure of the impinging ions. Moreover, the nano-microdosimetric characterization of the CATANA (protons) and CNAO (carbon ions) therapeutic beam lines was performed. The systematic study of nanometric scale distributions compared to biological data suggested that the proton RBE could be assessed just using experimental physical results coupled with a simple model. The comparison between the RBE assessed by the TEPC and a radiobiology experiment on a cell-line is shown in Figure 1. Several Monte Carlo simulations were carried out with the FLUKA code showing an overall good agreement with experimental data.
The wall-less TEPC has been constructed and assembled in the STARTRACK gas chamber (Figure 2). A first phase was devoted to the characterization of the novel device. This procedure was carried out by employing two different gases (propane and DME) and by exploiting an isotopic alpha source. The gas gain was computed for different pressures and several track-structure simulations were carried out by exploiting an ad hoc code.
The wall-less TEPC was irradiated at different impact parameters showing that, once calibrated, it is capable of assessing a nanodosimetric cluster size distribution for some tenths of nanometers in simulated size. This latter result is an indication that the gap between microdosimetry and track nanodosimetry can be partially filled with avalanche-confinement TEPCs.
A Monte Carlo code was developed from scratch for studying the gas gain of the TEPC. The code considers different models for evaluating the electron cross sections from thermal energies up to some eVs. The complex TEPC electric field is also considered by exploiting the finite elements analysis application COMSOL. The code was compared to experimental results showing a remarkably good agreement in terms of both gas gain and shape of the working windows of the wall-less TEPC. Then, the code was adopted for studying the feasibility of further improving the gas performances of an avalanche-confinement TEPC.
On the basis of the obtained results, a low-cost novel TEPC prototype was designed and built. This prototype is characterized with alpha and neutron sources showing a remarkably higher gas gain with respect to the former ones (sealed and wall-less) without a noticeable loss of resolution. The further improvement of the TEPC gas gain will be matter of future work.

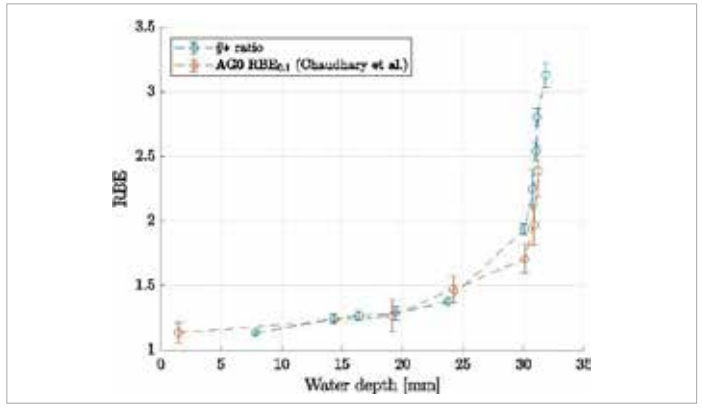

Fig. 1 - Comparison between biological RBE (AG0 cell-line in the legend) and the physical quantity derived with the sealed TEPC measurements.

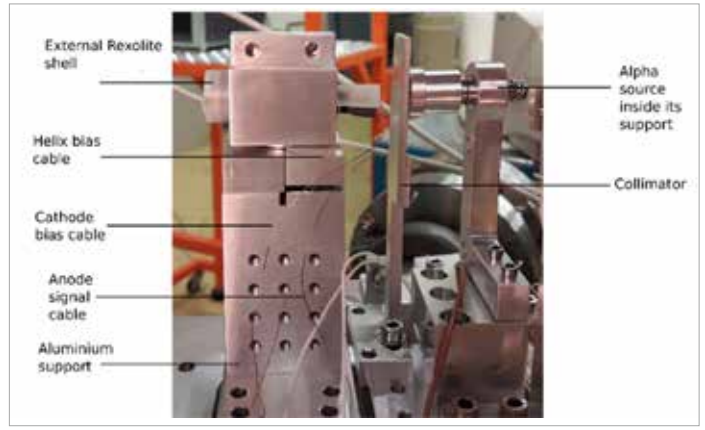

Fig. 2 - Wall-less TEPC assembled in the STARTRACK vacuum chamber.

DESIGN AND OPTIMIZATION OF A CROSS-FLOW INDIRECT EVAPORATIVE COOLING SYSTEM FOR DATA CENTER APPLICATIONS

Samanta Milani - Supervisor: Prof. Stefano De Antonellis

The PhD thesis focuses on an Indirect Evaporative Cooling (IEC) system as innovative solution to be used in confined environments as data centers. The objective of the study is the design and the optimization of a cross flow air to air heat exchanger in which one of the two airflows is constantly wetted during the heat exchange process. Thus, one of the two airflows (named secondary airflow) is first cooled through an adiabatic humidifier, and then it is used to cool a working airflow (named primary airflow). The secondary airflow is kept close to the saturated conditions throughout the process itself in order to increase the temperature difference between the two airflows and increase the heat transfer from the non-wetted primary airflow.
The research theme is investigated with both experimental and numerical approaches. The experimental part concerns the analysis of the performance of IEC systems in typical data centers operating conditions, to characterize and optimize the performance of the components, acting on the constructive parameters. The numerical part focuses on the development and the implementation of a model of the cooling system, starting from simplified models based on available data from existing literature. Adding information from the experimental part on two-phase heat transfer phenomenon for different geometries, materials and humidification configurations, the model becomes a tool to predict the system performance.

The study of innovative techniques for cooling systems characterized by a lower consumption of primary energy and greater efficiency is a hot topic for confined spaces such as data centers, which release a massive amount of heat through their continuous operation. The increasing number of data centers, which spread during the last decades, and the improvement of IT hardware components led to a significant increase in the power of cooling systems required to ensure equipment reliability. The electricity consumption for cooling is up to the 50% of the total energy consumption of data centers. To guarantee computers' highest performance, the indoor air should be maintained within strict ranges of temperature and humidity throughout the year independently of weather conditions and seasonal changes in temperature. Recently, guidelines for data centers widened the suggested temperature ranges according to IT equipment and achievable performance. As a consequence, the use of free-cooling extends, and indirect evaporative cooling systems become relevant to reduce the indoor temperature since they can be used in a greater number of hours during the year.

Experimental study
The experimental part provides a detailed experimental analysis of the indirect evaporative cooling system in typical working conditions of data centers. Performance of the IEC system are evaluated through a test rig designed to provide airflows at controlled conditions (temperature, humidity ratio, and mass flow rate). Primary air conditions are kept constant in representative conditions for data center applications. Secondary air conditions are set in order to compare directly the experimental results, evaluating effects of inlet air dry bulb temperature, wet bulb temperature and humidity ratio on system performance.
To minimize the water consumption and to increase the system performance, the following parameters are evaluated:

- Water distribution arrangement (nozzle number, type, and flow direction);
- Plenum structure and dimensions;
- Water supply positioning (i.e. from the top, from the bottom, etc);
- Plate dimension and plate spacing;
- Surface coating material.

Tests show a significant effect of water flow rate on system performance. In particular, a greater cooling effect is observed as the water flow rate increases, with little influence given by the number and type of nozzles used for the distribution of water inside the plenum. A significant influence on the overall performance is given by the water inlet positioning, since it defines the water distribution on the plates. The best configuration to foster water evaporation all over the plate is the one that allows inserting the water from the top of the heat exchanger, in the same direction of the secondary airflow, due to the drag force of the liquid film acting in the same direction of the gravity force. The comparison of an aluminum heat exchanger with a hydrophobic coating and one with hydrophilic coating shows the importance of surface coating material on distribution of water on the heat exchanger plate. Surfaces treated with hydrophilic coating get a more uniform water film especially at low water flow rate.

Numerical modelling
The numerical part focuses on developing, calibrating and validating a novel heat exchanger model using a finite volume approach. A simplified model based on literature is enhanced to account for the effects and characteristics of the system observed during the experimental campaign. A correlation to predict the saturation efficiency through the secondary air inlet plenum is obtained, in order to calculate the secondary air inlet conditions in the heat exchanger and the water flow rate entering the plates.
Then a correlation to describe the surface wettability factor (σ) is developed to link the actual system operating conditions and the non-uniform distribution of water on the heat exchanger plates (σ≠1). A correlation is decisive because the primary airflow outlet temperature calculated with σ=1 greatly overestimates the experimental results. The wettability on the heat exchanger plates is considered as decreasing linearly in the secondary flow direction. Part of the work concerned the optimization of the wettability factor, in order to correctly describe the heat and mass transfer phenomenon that occurs in the heat exchanger for each configuration, size of heat exchanger, and surface coating material. The data collected during experimental tests are used to calibrate the model. The model is then widely validated in different operating conditions, within and outside the calibration range, with further tests. Numerical results show very good agreement with experimental data.

Conclusion
In the thesis work, a solution to the cooling of controlled environments such as data centers is proposed. IEC technology, which recently sees a renewed interest in scientific literature, is studied.
The optimization of the IEC system has been developed using an experimental and numerical approach. Through an experimental test campaign the influence of construction parameters (both of the heat exchanger and of the water misting system) and of operational parameters (e.g. air and water flow rate and thermo-hygrometric conditions) was analyzed and optimized. The system allows to achieve high performance and cooling of the primary air when the humidification upstream of the heat exchanger is in counter-current with respect to the secondary airflow and occurs in a plenum that allows a good mixing between air and water supplied. Furthermore, the plates of the heat exchanger must have a dimple pattern as to spread the water film uniformly, also using hydrophilic coating materials to foster the wettability of the plate.
A numerical model has been developed to predict the heat exchanger performance with a change in the parameters analyzed in the experimental campaign. The results of the model follow the experimental data with good accuracy, due to the introduction of an experimental correlation for the adiabatic humidification (that occurs upstream of the heat exchanger inlet section), and one for the distribution of the water film on the plate inside the heat exchanger.
The numerical simulation of operation in different climate zones (in combination with indirect free cooling) shows that the system has the potential to eliminate compressor-based cooling in most climates. IEC system operation can be extended by running the data center within the allowed envelope.

OPTIMAL OPERATION OF MICROGRIDS AND MULTI-ENERGY SYSTEMS ACCOUNTING FOR FORECAST UNCERTAINTY

Luca Moretti - Supervisor: Prof. Giampaolo Manzolini

Co-supervisor: Prof. Emanuele Martelli

A microgrid is a local electrical network of Distributed Energy Resources (DERs) (generators, storage systems, and energy users), controlled in a coordinated fashion by a central Energy Management System (EMS). The microgrid can be islanded or connected to other networks. Multi-energy microgrids, or more in general Multi-Energy Systems (MES), represent an extension of the electric microgrid concept, integrating the supply of additional energy-related services such as heating, cooling, and/or the production of ancillary goods (e.g. purified water, ice, etc.). Their field of application ranges from off-grid systems for the electrification of rural communities to energy efficient and cost-effective urban energy districts.
A key feature of MEMGs is to facilitate the penetration of non-dispatchable Renewable Energy Sources (RES), relying on demand-side management, storage systems and distributed dispatchable generators to cope with fluctuations in RES generation, as well as with the intrinsic demand variability. To this end, predictive optimal planning of the strategic decisions related to MES operation is essential to achieve optimal performances. This thesis deals with the development of advanced formulations, based on Mixed Integer Linear Programming (MILP) techniques, of the optimal operation problem for MES (day-ahead and intra-day Unit Commitment, UC, and Economic Dispatch, ED): a deterministic formulation, protected against uncertainty by enforcing spinning reserve constraints, and an Affinely Adjustable Robust formulation. The effectiveness of the proposed formulations is assessed by simulating the operation of real-life systems, proposing multi-layer EMS architectures that can cope with forecast errors by implementing real-time dispatch adjustments. Given the potential severe consequences of unbalances between demand and generation, especially in electric off-grid systems, the PhD research has focused on ensuring the resilience of the optimal dispatch solution with respect to forecast uncertainty, while analyzing the impact that enforcing conservativeness has on the system performance.
The proposed deterministic formulation aims at defining a flexible approach to model complex Multi-Energy Systems, by discussing alternative modeling techniques for the components compatible with the MILP framework, but characterized by different levels of representativeness and computational cost. The Affinely Adjustable Robust formulation proposed features an advanced definition of the uncertainty set, the accounting of multiple internal uncertainty factors, and several ad hoc adjustments that can be implemented to reduce computational time, one of the main drawbacks of adopting the robust formulation. Furthermore, an expedient to account for the recursive contribution of quick-start units without introducing binary recursive variables is proposed and discussed. Finally, a thorough critical examination of the limitations and intrinsic misrepresentations associated to the Affinely Adjustable Robust formulation of the scheduling problem is discussed, by identifying synthetic case studies to highlight limitations in the effectiveness of the recursive robust scheduling solution.
The adoption of the two MILP formulations within two-layers EMSs overseeing nominal operation scheduling and real-time dispatch is assessed by means of numerical simulations, in the case of systems operating according to a day-ahead scheduling planning. Different second layer dispatch algorithms are proposed and tested. Three case studies are defined: an off-grid electric microgrid, and two grid-connected CHP systems, a Hospital a University Campus. Multiple system architectures are considered for the CHP systems, exploring various combination of flexible and non-flexible units, and thermal storage sizes.
The analysis indicates that resorting to the robust formulation for nominal day-ahead scheduling allows to effectively plan the commitment of the units, eliminating the need for real-time modifications to the commitment plan during the rest of the day. This is essential in situations where real-time adjustments to the commitment plan are unpractical or unfeasible. Furthermore, the recursive decision rules yield by the robust formulation provide a useful reference for the real-time management of dynamic components, defining a conservative trajectory that can serve as a useful reference to real-time dispatch algorithms in order to ensure system reliability. Conversely, in systems where the commitment status of units can be easily and rapidly changed and the nominal scheduling solution can be readily adjusted to account for the actual system evolution, the deterministic approach proves to be effective in identifying a less conservative and better performing operating schedule, while effectively coping with forecast uncertainty by means of adequately tuned reserve constraints. This is also true for systems featuring large storage units with high charge/discharge efficiency, that can limit the impact of incorrect nominal scheduling decisions and provide a redundant buffer that reduces the importance of correct unit commitment planning.
A more challenging case study for the off-grid electric microgrid was then analyzed, introducing the more uncertain RES generation contribution of a wind farm, and envisioning the installment of a large size non-flexible biomass-fueled ORC power plant for base-load supply. The management problem was tackled according to a Rolling Horizon approach, ensuring the possibility of updating every three hours the nominal scheduling plan, but introducing a delay in the actuation of start-up commands which depends on the generator technology. The analysis confirms that when the capacity of the system to respond to forecast errors is reduced, even more so as the forecasts accuracy worsens, the deterministic formulation is not effective in identifying cost-effective and reliable scheduling solutions, while the robust formulation, in virtue of the explicit accounting of recursive dispatch corrections and of the feasibility guarantee over the uncertainty space, manages to combine adequate solution conservativeness while limiting the impact on the operating costs.
The deterministic formulation was used to propose a two-layers predictive EMS (P-EMS) for practical implementation in the control system of sub-Saharan off-grid hybrid microgrids, in virtue of its higher modeling flexibility (that allows to account for non-linearities) and very good performance when forecast uncertainty is limited. Results confirm how adopting MILP-based formal scheduling optimization can have a significant impact in reducing costs and increasing penetration from renewable sources, allowing for an effective commitment of generation resources and for the strategic management of batteries to anticipate the availability of RES generation, limiting RES curtailment and maximizing the added value of storage systems.
Finally, an innovative MILP-based design algorithm based on an adaptation of the deterministic formulation of the scheduling problem has been proposed and compared with a heuristic algorithm developed at MIT, for application to the optimal regional electrification planning of sub-Saharan areas. With respect to the heuristic approach, the MILP-based algorithm proves to be effective both in reducing costs, particularly in larger systems that feature a dispatchable generator, associated with more complex and flexible scheduling. Once again, in addition to remarkable cost reductions, resorting to MILP optimization also allows to attain higher penetration from RES, as well as increasing service reliability for off-grid customers.

DEVELOPMENT OF NOVEL EXTRACTING SYSTEMS FOR SAFE TRANSURANIUM ELEMENTS SEPARATION FROM SPENT NUCLEAR FUEL

Annalisa Ossola - Supervisor: Prof. Mario Mariani

Co-supervisors: Dr. Elena Macerata, Dr. Eros Mossini

Over the XXI century, nuclear energy can play a central role to face with increasing energy demand while mitigating climate changes and preserving the environment. However, its development is hindered by public opinion due to problems related to nuclear waste management. Up to now, solely uranium and plutonium are industrially reprocessed. However, this process itself produces a High Active Raffinate (HAR), currently vitrified and properly stored for at least 3000 years, since it still contains long-term radiotoxic Minor Actinides - MA (Am, Cm) and Fission Products.
A further stage of MA recycling by the so-called Partitioning & Transmutation (P&T) strategy could significantly contribute to reduce the volume and the long-term radiotoxicity of the final high-level waste. In this perspective, multistage hydrometallurgical partitioning processes are constantly under development for efficient MA partitioning from lanthanides (Ln). In fact, Ln, being characterized by high neutron capture cross section, would scavenge neutrons, thus hindering successful MA transmutation. Besides selectivity, the extractants employed in MA partitioning must satisfy several others criteria:

- good solubility and proper fluid-dynamic properties to minimize the eventuality of third-phase formation/precipitation and maintain constant phase separation;
- fast complexation kinetics to allow counter-current applications in short residence time contactors;
- high metal loading capability to allow successful reprocessing of fuel with high metal ions concentration;
- reversibility of cations retention to enable phase recycling and successive processing;
- stability towards hydrolysis and radiolysis to guarantee stable performance in the HAR high radiation field;
- easy synthesis for large scale production.

In addition, ligands should be constituted only by C, H, O and N atoms to be completely incinerable without producing secondary solid waste. The achievement of these conditions is a challenging but key issue to demonstrate the technical feasibility and success of the P&T strategy.
Since none of the so far developed extraction systems has fully matched the above-mentioned requirements, this Ph.D. research project was focused on the investigation of novel solvent formulations for MA and Ln co-extraction or separation. The experimental activity was mainly carried out at Radiochemistry and Radiation Chemistry Laboratory (Department of Energy) and at L.G.S (*Laboratorio Grandi Strumenti*) Facilities (Department of Chemistry, Materials and Chemical Engineering) of Politecnico di Milano, with the support of University of Parma that supplied the ligands. Moreover, due to particular technical requirement, an abroad research period at CEA (*Commissariat à l'Énergie Atomique et aux énergies alternatives*) was essential for the development of a part of the research activity. Most of the results obtained have already been presented and published in important international conferences/journals.

Methods

The research activity mainly focused on *1-cycle*-SANEX (Selective ActiNide EXtraction) and *innovative*-SANEX (*i*-SANEX) processes. In the former, MA selective extraction is carried out directly from HAR thanks to a lipophilic ligand selective for MA. Conversely, in the latter, firstly MA and Ln are co-extracted from HAR thanks to an unselective lipophilic ligand and afterwards MA are back-extracted exploiting a MA hydrophilic selective ligand. Experimentally, after solubility and fluid-dynamics verification, batch liquid-liquid extraction tests were performed to assess extracting system performances (e.g. MA efficiency and selectivity) and reversibility of cations retention for phases recyclability. They were performed by mixing and then separating two immiscible phases. After phase separation, an aliquot of each phase was sampled for subsequent analyses. Metal ions concentration measurements were carried out by mass, alpha and gamma spectrometries. The hydrolytic and radiolytic damage experienced by the ligand solutions during reprocessing was simulated by gamma irradiation (^{60}Co source) with different dose rates. Analytical techniques (HPLC-MS and ESI-MS) were exploited on degraded ligands solutions to quantify and identify degradation by-products.

Results

The first ligand investigated belongs to the diglycolamides (DGA) family. It is an O_3-type ligand conceived for MA-Ln co-extraction (according to *hard soft acids and bases* Pearson's theory) and envisaged as an alternative to TODGA (European reference ligand). However, even if preliminary studies suggested an improvement with respect to TODGA ligand, deepened studies of its extracting behavior allowed to ascertain that the chelating unit is more affected by protonation than other DGA, thus resulting in a decreasing efficiency at process conditions ($[HNO_3]$ = 3÷4 M). Moreover, a comprehensive experimental campaign revealed a high ligand instability both towards hydrolysis and radiolysis, thus making the proposed ligand unsuitable for industrial application.
Contrarily, promising results were collected for the ligands belonging to the PyTri-family. They are conceived for selective MA separation (according to Pearson's theory) and characterized by the same N_3-donor set of PyTri-Diol, European reference ligand for the *i*-SANEX process.
In detail, solubility constraint strongly limited a proper evaluation of the extracting properties of the newly developed lipophilic PyTri ligands. Just one of them manifested suitable solubility in all the diluents tested, thus a comprehensive study of its extracting properties was performed. Nevertheless, the solubility data acquired will be useful for the future design of new lipophilic ligands. The best lipophilic PyTri ligand manifested satisfactory MA selectivity, fast extraction kinetics, easy cations back-extraction, suitable performances even at process temperatures and promising radiochemical stability. Representing a valuable alternative to the reference ligand, it was introduced in the European GENIORS Horizon 2020 project by its scientists committee. This will allow to perform further and deepened studies in collaboration with other European laboratories, exploiting their expertise and resources.
Moreover, a modification of the hydrophilic PyTri-Diol structure was studied as an attempt to further improve its efficiency and overcome the competitor sulphonated-BisTriazinePyridine (BTP), former *i*-SANEX reference ligand. In the light of the results obtained, it is possible to assert that an opposite effect was achieved. In fact, the modified PyTri-Diol demonstrated to be less efficient than original one. A well-established collaboration with KIT (*Karlsruhe Institute of Technology*) was exploited to confirm this result by spectroscopic investigations. Anyway, since the data collected enabled to understand the effect of such kind of addition on ligand basicity, these could be exploited to differently modify the PyTri ligand structure in order to further enhance its performance. Finally, deepened studies were performed with the already established PyTri-Diol ligand.
Firstly, its applicability at process temperatures was verified. Moreover, thanks to an abroad research period at CEA funded by European GENIORS project, it was successfully tested towards organic phases loaded with macro-concentration of ^{241}Am(III), ^{239}Pu(IV), Y, and Ln (La-Gd).

Conclusions

In conclusion, the information collected in this doctoral research will be helpful in the future design of new extractants as well as in the comprehension of extraction behavior and degradation mechanism of other ligands. Moreover, the results collected could significantly contribute to the development of advanced separation processes towards the closure of the nuclear fuel cycle.

RENEWABLE ENERGY HIGH PENETRATION SCENARIOS USING BOTTOM-UP MODELLING

Matteo Giacomo Prina

Supervisors: Prof. Giampaolo Manzolini, Dr. David Moser (EURAC research)

One of the greatest challenges of the international community to mitigate climate change is to lower anthropogenic greenhouse gas emissions. The heat, electricity, transport and industry sectors account for almost 75% of the total amount. To address this challenge and improve the security of the energy system, an increasing number of countries have set strict energy targets and expanded their share of renewables. The European Union adopted the "2020 climate and energy package" in 2007 and the "2030 climate and energy framework" in 2014.
Energy planning is therefore taking a central role in assessing the future energy system and helping policy makers to set targets and subsidizing mechanisms.
The increase of installation of variable renewable energy affects the stability of the grid and has an impact on the existing power plants portfolio and on the electricity price dynamics.
In particular, Combined Cycle Gas Turbine (CCGT) are the most flexible capable of working at partial load and supporting several rump-up/down cycles in a day. These bring about lower efficiency, higher specific emission of carbon dioxide and therefore higher consumption of fuel compared to full load operation. The role of the power modulation source, its capacity and management is a first challenge towards the integration of renewable energy sources. The optimal integration of distributed energy systems in the traditional context is essential to guarantee the maximization of the renewable energy benefits, such as reduction of carbon emissions and of grid energy losses as well as the minimizations of investments and operation costs.
The main purpose of this thesis is the improvement of existing energy planning model techniques realizing a method with the following characteristics: i) it should take into account the three sectors of the energy system: electric, heat, transport, ii) it should follow a multi-node approach to consider the interactions between the different market zones divided by transmission constraints. This fact highlights the possibility to compare costs and benefits caused by storage systems implementation, "averaging in time", to those from grid extensions, "averaging in space", iii) it should be coupled to a multi-objective optimization algorithm to find the best configuration of the energy system and iv) it should integrate transient analysis considering in this way all flexibility options.
Three different models have been developed and the final results have been compared to highlight the limits and advantages of the different modelling techniques. The first developed model, EPLANopt, is a bottom-up short-term model that couples the deterministic simulation model EnergyPLAN, developed by Aalborg University, to a Multi-Objective Evolutionary Algorithm. The simulation model performs the hourly dispatch while the evolutionary algorithm solves the investment or expansion capacity optimization. In EnergyPLAN, conventional power plants are modelled as fully flexible power plants that can reduce or increase their production without limitations and ramp rates. Thus, the production can move from 0 to 100% in one single hour if needed. Hence it is possible to conclude that EnergyPLAN has a low resolution in techno-economic detail. In order to overcome that, a specific external code to model combined cycle gas turbine (CCGT) systems has been developed to account for current technological constraints and additional costs of CCGT flexible operation.
EPLANopt is a single-node model and can be classified to have a low resolution in space. In order to overcome this limitation, another model in the field of bottom-up short-term energy system model have been developed. This model, named Oemof-moea, is based on the Oemof framework which is a free, open source toolbox to assess energy supply systems, and a Multi-Objective evolutionary algorithm. Oemof covers all sectors of the energy system. It is multi-node. It utilizes a medium or high time resolution. It performs the dispatch optimization based on a linear programming or mixed integer linear programming technique while the evolutionary algorithm takes care of the investment optimization with a multi-objective approach.
Short-term energy system models evaluate the best energy mix in a future year while long-term models considers a wider horizon focusing on the whole transition between the current state of the energy system and a future year.
In the field of bottom-up long-term energy system models the literature review has highlighted an issue related to the not detailed time representation when evaluating the behavior of the energy system during each period of the transition, performed in a limited number of aggregate time-slices. This choice is justified by the reduction of computational burden, but introduces a questionable approximation when applied to energy systems characterized by high penetration of intermittent RES, storage, flexibility options and other technologies or demands. Hence a new model has been implemented, leading to the development of a long-term variant of the EPLANopt model, called EnergyPLAN optimization for Transition Pathways (EPLANoptTP). EPLANoptTP is the first long-term model to combine the high time resolution of static models with a conventional long-term perfect foresight structure, as well as to use a Multi Objective evolutionary algorithm.
The three methods have been applied to the Italian energy system considering the horizon from 2015 to 2050. The results show the strong difference between a modelling technique characterized by high resolution in space and in techno-economic details and a modelling with lower resolution. Moreover, available bottom-up energy system models models make use of single-objective optimization solvers in order to minimize the costs of the system.
When CO_2 emissions reduction in such models is considered, this is done either through the inclusion of annual emission targets that have to be respected by each evaluated solution, or by assigning a monetary cost to the emissions through carbon taxation. Both these approaches, however, only provide the user with one solution, without the possibility of assessing in a single run the impact of carbon abatement on the costs of the energy system. Using a multi-objective optimization instead provides the user with a Pareto front of optimal solutions. The solution is a curve describing the minimum increase of costs related to the reduction of CO_2 emissions that can be achieved acting on the selected decision variables.

VERTICAL INTEGRATED METHOD FOR THE DEVELOPMENT OF CARBON NANO-STRUCTURED ELECTRODES FOR VANADIUM REDOX FLOW BATTERY

Eugenio Rovera - Supervisors: Prof. Andrea Casalegno, Dr. Fabio Di Fonzo (IIT)

Vanadium Redox Flow Battery (VRFB) is an electrochemical storage system considered as one of the most promising technologies to be coupled with renewable sources. VRFB peculiar features allow to perfectly match the requirements of stationary storage: reduced capacity decay and long durability, low cost, and high versatility due to the capability of decoupling installed energy and power. Alongside all the advantages, the main drawback of VRFB is the low power density, caused among other phenomena mainly by the carbon electrodes, still not optimized for the specific VRFB application. In fact, commercial VRFB electrodes are carbon gas diffusion layers coming from the fuel cell technology suffering low surface area and thus poor electrochemical performances towards vanadium. To go beyond the current state of art is necessary to develop innovative electrodes with increased surface area and enhanced kinetics in order to accelerate the sluggish vanadium reaction rates, increasing power density and then reducing the battery cost. This PhD work treats the development of a vertical integrated method for the fabrication of optimized carbon nano-structured electrodes for VRFB application. The project has been carried out across two laboratories: the N2E lab at the Center of Nano Science and Technology of the Italian Institute of Technology and the MRT Fuel Cell Lab of the Energy Department of Politecnico di Milano.
The fabrication consists in the deposition process of an optimized carbon meso-porous film on top of commercial GDL carbon fibers, where the vertical integration goes from carbon meso-porous film synthesis from the gas phase in a prototypal plasma source (fig.1) and, through out various steps, reaches the electrochemical testing of such electrodes in real working conditions in a lab scale device.
The vertical integration allows to decouple the contribution given by the various components of the treatment, providing a mastery of all the steps of the process and to perform an iterative optimization.
The first step of the method consists in depositing the film on a flat substrate, to be characterized without the contribution of the commercial electrode. Meso-porous films deposited on glassy carbon substrate (fig.2) have been characterized from a physical, morphological and chemical point of view in order to understand how various process' steps determine properties. Films have been also used as electrodes in a three-electrode cell set-up to perform electrochemical characterization and to provide a fast screening of materials before the device fabrication. This approach highlighted the effect of carbon structure and of meso-porous film properties on electrochemical activity: in particular, graphite edge's content and carbon sp^2 hybridization are the nano-particle's properties directly related to single activity, together with with film thickness and relative density. Deposition parameters of the source revealed to be determine film's structure, and the synthesis process proved to be able to provide fine tuning on all the electrochemically relevant quantities.
Transient and steady state models have been developed, providing tools for the quantitative interpretation of electrochemical performances. Modelling activity of the three-electrode cell system lead to the correlation of film's properties to electrochemical response, providing a deep understanding of kinetic and mass transport coupling used to highlight governing phenomena in the meso-porous films. Modelling highlighted how kinetic rate is the limiting phenomenon inside the porous media, while mass transport is governing outside the electrode.
Some predictions were made for the behaviour of the film once deposited on a GDL, stating how film thickness is the crucial parameter to be optimized: on one hand increasing the thickness determines higher active area without limiting the transport inside the film's pores, on the other hand it leads to GDL's pore clogging. Depending on GDL fluid dynamics, given by different flow field distributors employed, the optimum thickness has to be found experimentally. Modelling predictions has been verified in real working condition, testing the treated and untreated electrodes in the symmetric cell set-up, a configuration able to study separately the contribution of positive and negative electrodes.
For the positive half-cell of the battery, the deposition of meso-porous film did not show significant gain in performances, while in the negative electrode the effect was dramatic, leading to a remarkable boost in kinetics especially with the interdigitated flow field, where the current density was almost doubled. Negative electrode's symmetric cell campaign identified the optimum film thickness for the interdigitated flow field distributor and for the serpentine. Moreover, the interdigitated resulted to be the more performing flow field distributor, and it has been chosen for full cell characterization. Treated electrodes have been finally tested in a real VRFB device (fig.3), showing excellent results in terms of overall performance and stability, exhibiting an efficiency decay from 78% to 76% after 125 cycles, at a current density of 200 mA/cm^2. Furthermore, this work solved the coupling of kinetics and mass transport in a VRFB, suggesting that the optimization of a nano-structured coating has to be done considering cell's features: the optimization on VRFB's components (such as electrode's morphology and thickness, molarity, flow distributors, redox couple,etc.) will reflect in a different match with film's properties. The proposed method overcomes state of art issues of nano-particle coatings, such as the poor control on nano-structure's properties and its coupling with fluid dynamics, offering the possibility of a wide range of further optimization. Future works will mainly focus on the chemical doping of nano-particles to further increase the kinetic rate.

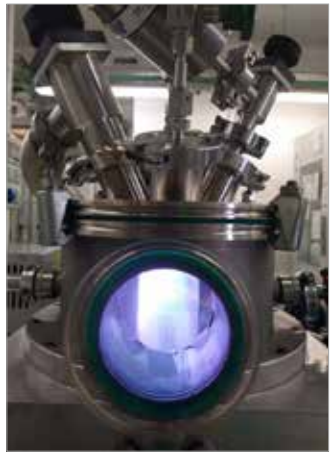

Fig. 1 - Plasma source (called NanoJeD) used for the fabrication

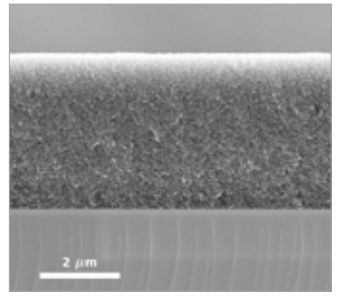

Fig. 2 - SEM image of the carbon meso-porous film

Fig. 3 - Vanadium Flow Battery device

EXPERIMENTAL AND ANALYTICAL STUDY OF SOLAR-ASSISTED HEAT PUMP

Riccardo Simonetti - Supervisor: Prof. Giampaolo Manzolini

Co-supervisor: Prof. Luca Molinaroli

In the last years, it has been registered an increased energy share of renewable energy for heat and electricity production together with an increase of fossil fuels consumptions. In this scenario, Heat Pump (HP) can reduce the primary energy consumptions from fossil fuels for heating and cooling sectors. The integration of solar energy with HP, concept also known as Solar-Assisted Heat Pump (SAHP), could improve the efficiency of this technology, maintain low costs and high installation flexibility and exploit solar radiation more efficiently increasing its penetration in the residential sector. Considering this, the thesis aims to identify the advantages of this system respect to standard technologies and eventual functioning problematics, to compare different typologies of SAHPs and clarify their potentiality in energetic and economic terms.
Firstly, a series of experimental campaigns with different SAHP systems were carried out at SolarTechLab on the roof of the Department of Energy of Politecnico di Milano. In these campaigns an Indirect Solar-Assisted Heat Pump (I-SAHP) system with two different solar fields was studied, as well as a prototype HP in Direct Solar-Assisted Heat Pump (I-SAHP) and Integrated Dual-Source Heat Pump (I-DSHP) assets, the second of these systems was analyzed twice with a reduction of the evaporator capacity in the second campaign. Moreover, two experimentations were done with Photovoltaic/Thermal (PV/T) systems, the first to compared two roll-bond modules with a standard sheet and tube technology, the other to characterize PV/T panels performance.
A program developed with the software LabVIEW™ was used to control the laboratory, monitor the tests, collect the data and save them with a time step of one second. Furthermore, a filtering process was also worked out to remove all the measurements not in steady state conditions. Finally, uncertainty analysis was done to evaluate the goodness of the instruments and the measurement method.
From the comparison of the different PV/T typologies, roll-bond technology was selected, thanks to higher performance and lower costs, to couple with a HP in the I-SAHP asset, outlining the potentiality of the concept, which reaches high values of Coefficient Of Performance (COP), around 5 (Fig. 1), and the importance to a correct sizing of the components. Moreover, from the analysis of the results of the I-DSHP experimental campaign clear advantages respect to a standard Air-Source Heat Pump (ASHP) were observed, but problems were also found in order to obtain high performance due to the prototype nature of the machine. In both the cases, self-consumption conditions were reached in most of the experimental points.
In parallel, analytical models of all the heat pump's components and the solar panels were built using the MATLAB® software. I-SAHP and I-DSHP concepts were mathematically detailed and, after a validation procedure, their behaviors were analyzed as functions of the environmental conditions. Results have confirmed the experimental trends, underlining the problems of I-SAHP functioning in unsuitable conditions (low solar irradiance and ambient temperature) and the benefits of I-DSHP concept in terms of performance, with a gain of 14% respect to a ASHP (Fig. 2).
Considering the annual analysis, the scheduling of the sub-systems was optimized, in a representative winter day, in order to minimize the electricity sold to the national grid and consequently maximize the self-consumption. PV/T panels were used as much as possible to produce the space heating heat as well as preheat the storage, being energetically more convenient respect to the HP. The battery storage accumulated energy in order to minimize the purchasing from the national grid. The comparison between the SAHP studied and a standard ASHP respect to the conventional scenario has shown that, from an energetic point of view, air-based systems had the same PES, varying the number of PV/T modules as well as the battery storage size, reaching a maximum saving of 80% with the biggest battery and 24 panels (Fig. 3). From the economic point of view, ASHP won in all conditions, due to the high cost of the PV/T technology, with a 35% of saving with no battery and 4 PV panels. I-SAHP was resulted the worst system in both energetic and economic terms, because of the strong link between the performance and the presence of the solar irradiance to supply the HP.

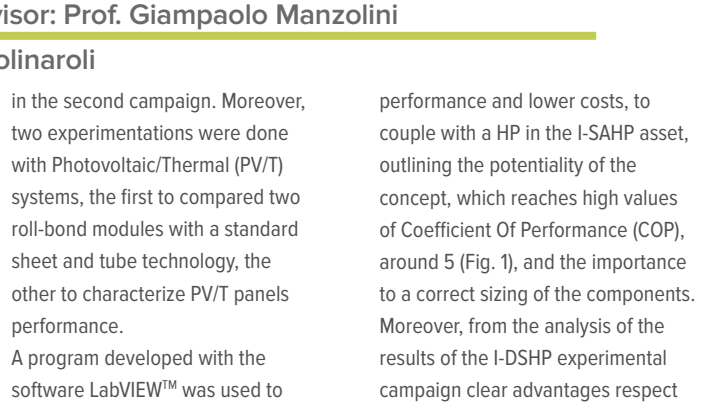

Fig. 1 - Representation of COP as a function of ambient temperature for different condenser inlet temperature for I-SAHP second experimental campaign. Solid lines represent the COP of a standard ASHP

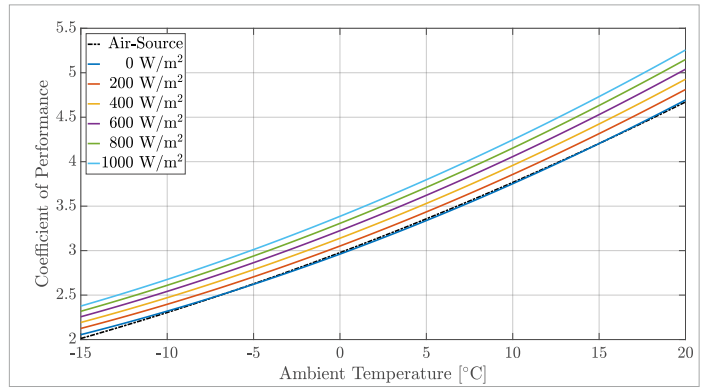

Fig. 2 - Representation of COP for the I-DSHP (solid lines) and for a standard ASHP (dashed line) as a function of ambient temperature and solar irradiance

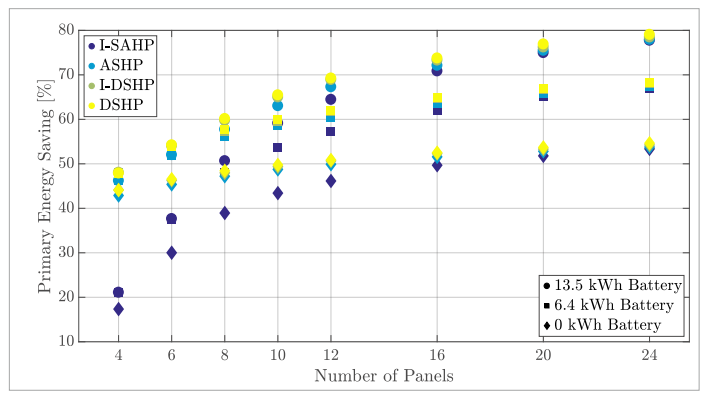

Fig. 3 - Representation of PES as a function of the number of PV/T panels for all the systems analyzed

DEVELOPMENT OF ADVANCED NANO-CERAMIC COATINGS FOR FUTURE GENERATION NUCLEAR REACTORS

Matteo Vanazzi - Supervisors: Prof. Marco Beghi, Dr. Fabio Di Fonzo (IIT)

To regain economical interest and public acceptance, next generation nuclear power plants aim to overcome dated issues connected to traditional systems. Specifically, they are meant to outperform current ones in terms of efficiency, fuel utilization, safety and waste production. Different fission reactor concepts have been proposed as GIV candidates. Lead-cooled Fast Reactors (LFR) are particularly interesting due to the intrinsic safety features brought about by lead. Lead stands above liquid metals because of its chemical inertia, wider operating window and low activation under irradiation. However, the development of LFR is linked to the availability of suitable materials solutions. The greatest challenges in this sense arise from the extremely corrosive environment: at the foreseen temperature (above 500°C) typical corrosion rates produced on bare steels are not acceptable and protective methods are required. In this framework, some of the most interesting solutions are based on the use of smart bulk alloys, surface-alloying techniques or coatings.
While compatibility issues are quite homogeneous in fission systems, in the case of fusion power plants problems are jeopardized and strongly related to the specific parts of the reactor. Among these, the breeding blanket is surely a crucial element in the reactor design. Here, the breeding process on lithium takes place; tritium is formed and then successively used to fuel the fusion reaction. Tritium storage is a major concern due to the high permeability of this gas and its radiotoxicity. In order to face this problem, a gas diffusion barrier is needed. Nevertheless, breeding blanket moduli suffer from the same problems expected for LFR: liquid metal corrosion by the Pb-Li eutectic (in the range of 450-550°C) and radiation-induced phenomena caused by extremely energetic neutrons. Anew, ceramic coatings have been proposed as a valid option, against tritium permeation as well as Pb-Li corrosion.
The deposition of protective coatings on structural materials can provide surface engineering without affecting bulk properties and design requirements. Still, the main problem with ceramic coatings is the lack of self-healing properties, along with their traditional brittleness. Since 2012, an ongoing activity on nuclear-relevant materials has been carried out at the CNST@PoliMi centre of the IIT. An innovative coating of alumina deposited by Pulsed Laser Deposition (PLD) has been proposed as a cross-cutting solution for LFR and breeding blanket components. In the previous works, Al_2O_3 coatings have been characterized with short-term corrosion tests in static lead and Pb-Li, showing chemical stability and protectiveness. The anti-diffusion capability has been verified by permeation tests with H_2 as tritium surrogate. Moreover, the same material has been irradiated with heavy ions to extreme damage levels reporting no delamination, nor degradation. The main feature behind these promising evidences have been identified in the amorphous/nano-crystalline structure of alumina films, which confers a unique assemble of strong adhesion, metal-like mechanical properties and radiation-tolerance. However, since its structural stability and performances depend strictly on the amorphous matrix, further studies are needed to evaluate to amorphous to crystalline transition - especially under irradiation - and how to control this process.
This work represents an important step forward in the development of amorphous/nano-crystalline coatings. Firstly, new tests have been performed on the Al_2O_3 films to assess furtherly the anti-diffusion corrosion-resistant behaviour. Corrosion tests have been performed in static/fluent lead and Pb-Li at 550°C, up to 10000h. Tests have then been repeated on previously ions irradiated films. In both cases, the oxide coating appears able to protect efficiently the underlying steel, even after radiation-induced crystallization. Meantime, new permeation tests have been produced with deuterium, on pristine and previously irradiated samples. Additionally, electron co-irradiation has been used during the permeation tests to simulate the radiation field of a typical breeding blanket system. The performance against H_2 isotopes diffusion remains remarkable, with a permeation reduction factor around 1000 at 450°C, for all the conditions.
In the second part of the present work, an intensive focus has been addressed to the crystallization of amorphous alumina. Different techniques (XRD, XPS, NMR) have been exploited to evaluate the ordering process and the evolution to the crystallinity. The thermal process has been investigated, to define the crystallization threshold of PLD-grown Al_2O_3. Crystallization starts in the 650-750°C range, depending on the annealing parameters. Regarding the main crystalline phases, γ-Al_2O_3, θ-Al_2O_3 and α-Al_2O_3 are successively formed, as usually reported. Later, crystallization under ion irradiation have been studied: Au ions irradiation tests have been performed at different temperatures to decouple the irradiation effects from the purely thermal contribution. Results show a strong dependence of the radiation-induced crystallization on the background temperature: while at 600°C both γ-Al_2O_3 and α-Al_2O_3 are formed, at 500°C only a small fraction of γ-Al_2O_3 - the least energetic metastable phase - is present. Finally, no sign of crystallization appears after the 400°C test. Similar experiments have been repeated, at constant temperature of 600°C. Several dpa levels have been obtained in the low damage regime, from 0.25 to 3.5dpa. The grain size and the mechanical properties of the crystallized films have been evaluated. The structural evolution is characterized by a sublinear grain growth, with the formation of nano-metric grains. Collected data have been used to fit a realistic kinetic model, showing strong accordance between the experimental trend and literature. Film stiffness and hardness have been measured by nano-indentation tests. Mechanical properties do not degraded during irradiation but improve, thanks to the increase of the H/E ratio. Particularly, the hardness follows a perfect Hall-Petch relation with a maximum around 30GPa, well above the standard values for alumina sapphire.
Having assessed the fundamental role of amorphousness, the final goal of this research has been related to the general control of the crystallization kinetic. Thus, different ceramic compounds have been added to the Al_2O_3 films in the form of dopants: Cr_2O_3 and Y_2O_3 have been selected to anticipate or retard, respectively, the crystallization threshold. Annealing tests have been produced on pure and doped alumina. Cr_2O_3-doped Al_2O_3 crystallizes at least 50°C before the pure counterpart, while the Y_2O_3 dopant delays the crystallization of 150°C. To demonstrate the effectiveness of chemical doping under irradiation, an extensive experimental campaign has been run with an in-situ TEM tandem facility. Each material has been irradiated with Kr and Au ions at different temperatures, up to 5dpa. At 600°C, the presence of chromia dopant reduces the dose needed to crystallize from 0.5/0.75dpa to 0.25/0.5dpa, while yttria increases it to 1/1.25dpa. Nevertheless, the most relevant result has been accomplished at 800°C, above the crystallization temperature of standard alumina. Again, Y_2O_3-doped Al_2O_3 crystallizes considerably after the pure material (around 1dpa instead of 0.25dpa). However, Y_2O_3 dopant is not only able to preserve partially the amorphous matrix, but increases also the overall radiation tolerance, especially after crystallization. Thanks to the stabilization of γ-Al_2O_3 at elevated temperatures, it prevents the formation of the traditional α-Al_2O_3 alumina structure, tacking classical degradative phenomena proper of this material under irradiation.

DATA, TEXT AND IMAGE PROCESSING BY DEEP LEARNING AND EXTREME LEARNING MACHINE FOR PROGNOSTICS AND HEALTH MANAGEMENT

Zhe Yang - Supervisors: Prof. Piero Baraldi, Prof. Enrico Zio

Co-supervisor: Dr. Sameer Al-Dahidi

Recent disruptive technologies, such as internet of things, mobile and cloud computing, advanced big data analysis algorithms and cyber-physical system has enabled a technological revolution that, under the name of Industry 4.0, is driving extensive digitalization and interconnection of manufacturing processes and products.

Prognostics and Health Management (PHM) is a field of research and application aiming at identifying the degradation onset in industrial systems, diagnosing the causes of the degradation, assessing the degradation level, and predicting the remaining useful life, with the objective of increasing the system availability and reducing operation and maintenance costs. PHM methods are generally divided into model-based and data-driven. Model-based methods typically rely on comprehensive physics-based degradation models to describe the degradation process. Since industrial systems are getting more and more complex in the era of Industry 4.0, it is very difficult and expensive to develop these physical degradation models for them. On the other hand, data-driven methods rely exclusively on the availability of data related to the degradation behavior of industrial systems (e.g. vibration, voltage and current) and operational condition (e.g. temperature, humidity and pressure) and are typically based on the training of artificial intelligence models. In the era of Industry 4.0, the increased availability of information coming from different sources and the grown ability of treating the acquired information by intelligent algorithms has opened wide the doors for the development of advanced data-driven methods in support of dynamic maintenance and operation management.

In this context, the present PhD work addresses some of the main challenges that are limiting the application of PHM in Industry 4.0: 1) the large amount of high dimensional data makes difficult the extraction and selection of human-designed features relevant for the PHM tasks; 2) non-numerical data are typically not utilized by existing PHM approaches; 3) evolving environments make unsatisfactory the performance of intelligent models trained using data collected in the past.

These challenges are addressed by developing a novel PHM framework based on advanced artificial neural networks, such as extreme learning machines, autoencoders, and deep and convolutional neural networks.

Specifically, the proposed framework is founded on:

i) The automatic extraction of degradation indicators in evolving environments by using sparse autoencoders-based deep neural networks

We propose a novel fault detection method based on the use of Sparse Autoencoder-based Deep Neural Network (SAE-DNN). The proposed method is able to minimize missed and false alarms in presence of concept drift, with a simplified process of tuning the hyperparameters of the SAE-DNN. Being the degradation process an irreversible monotonic process, the SAE is pre-trained using a run-to-failure trajectory of the monitoring data, and the most monotonic of the extracted features is considered to assess the component degradation. In this way, the hyperparameters are selected during the "pre-training" phase avoiding time-consuming fine-tuning of DNN models.

The main contributions of this work are: *a*) A novel method for DNN hyperparameter setting which allows obtaining improved diagnostic performance with reduced computational efforts and *b*) the development of a novel SAE-DNN-based method for fault detection under concept drifts which allows minimizing false alarms.

ii) The detection of concept drift through the online updating of extreme learning machines

We develop a concept drift detection method able to: *a*) deal with both regression and classification problems, *b*) work with data batches of any size, *c*) does not require knowledge of data stream probability distributions and is not based on hand-crafted statistical features, *d*) automatically determine the amount of data necessary for model updating, *e*) computationally not demanding, and *f*) prompt in the concept drift detection.

The proposed method is based on the use of Online Sequential Extreme Learning Machine (OS-ELM), which is able to periodically update the model output weights by using the one-by-one or batch-by-batch newly collected data, without any requirement on the batch sizes and without using the previously acquired data. The basic idea of the proposed method for concept drift detection is the quantification of how much the OS-ELM model is modified when it is updating using the newly collected data. Since the OS-ELM updating only modifies the output weights, the dissimilarities between two OS-ELM models can be quantified considering the variations of the output weights. A procedure for automatically setting a dynamic threshold for concept drift detection is proposed.

iii) The development of prognostic models based on multi-branch deep neural networks which receive in input numerical and textual data and images

A novel prognostic method based on the use of multi-branch DNNs has been developed. It is able to automatically extract features from both numerical and non-numerical information, such as maintenance records and images, and to predict the degradation behavior of an industrial system by combining the extracted features. The proposed multi-branch DNN consists of some sub-networks designed to extract features from numerical data, maintenance records and images, respectively. The extracted features of the three branches are, then, concatenated together for prognostics. The overall multi-branch DNN is trained with the objective of minimizing the prediction error. The proposed method allows automatically extracting the features to be used for the prognostic task from multimodal data.

iv) Maintenance optimization using convolutional neural networks and multi-state stochastic models considering the information content of maintenance records

A flexible maintenance record analysis method which explores the feasibility and effectiveness of combining CNN and multi-state degradation modeling to analyze maintenance records automatically has been proposed. The method is based on the following steps:

a) Automatic clustering of the short texts of maintenance records into groups each one containing maintenance records which refer to similar maintenance interventions. The clustering is performed using a CNN-based deep feature extraction approach and k-means clustering.

b) Developing a stochastic multi-state degradation model to describe the equipment degradation process where the degradation states are those identified by the first step. The maintenance times are used to estimate the parameters of the model. In multi-state modeling, the transitions among the states are described by stochastic laws (e.g., Weibull distribution, exponential distribution, etc.), representing different aging dynamics. The parameters (e.g., scale and shape factors, failure rates, etc.) contained in these laws must be inferred from data. *c*) Identification of the maintenance strategy which minimizes the maintenance cost using the Monte Carlo method.

The proposed framework is validated using real numerical data extracted from bearing run-to-failure trajectories and wind power production plants, real maintenance records collected from excavator buckets used in mining industry and a synthetic case study inspired by the operation of steam generators in nuclear power plants.

The obtained results show that the proposed PHM framework allows using large amounts of high dimensional multimodal data collected from industrial components and systems working under evolving environments for improving the performance of current fault detection, diagnostics, prognostics and maintenance optimization methods.

OPTIMAL DESIGN OF URBAN ENERGY DISTRICTS UNDER UNCERTAINTY

Matteo Zatti - Supervisor: Prof. Emanuele Martelli

This thesis addresses the optimal design of urban energy districts, also called Multi-Energy Systems or District Energy Systems, wherein multiple energy demands (i.e., (heating, cooling and electricity) must be satisfied. The MES/DES might feature multiple locations with users, energy conversion and storage systems. Inner networks allow the distribution of energy. A design optimization methodology based on a Mixed Integer Linear Programming (MILP) formulation has been developed.
The first main feature of the model is the participation of the energy district to a two-stage electricity market: a day-ahead bid plus a real-time balance, which entails the handling of the uncertainty associated to the day-ahead forecasts of the energy and the sun irradiance. The model takes also in account the unit commitment inflexibility of slow start-up units and the real-time scheduling adjustment of quick start-up units. The problem has been formulated following the Stochastic Programming approach, leading to a three-stage stochastic mixed integer programming (SMIP) problem with integer recourse.
The second main feature of the optimization model is the possibility to accommodate both parallel and series heat integration configurations, so that it can be applied also to large-size district heating networks (DHNs). Indeed, large DHNs frequently feature a large difference between the delivery and the return temperature, in which a simple parallel heat integration arrangement might not be sufficient to reach the required delivery temperature if low outlet temperature units are involved.
The modelling strategies and assumptions adopted to develop the model are: (i) the linearization of the size effects on costs and performance and the part-load performance maps of the units; (ii) the reduction of the size of the problem to enable its computational tractability, through a novel method for the selection of the representative input hourly profiles (named k-MILP) and the generation and reduction of stochastic scenarios to model the possible real-time realizations of the day-ahead forecasts; (iii) finally, the multiple heat integration configurations have been made possible by the implementation of a temperature intervals superstructure, which, besides the hourly operation of the units, optimizes also their contributions to the single temperature intervals in which the whole delivery/return temperature range can be divided, according to the inlet and outlet temperatures of the considered systems.
Concerning the problem size reduction, the k-MILP has been tested against k-means and k-medoids on the design optimization of the MES of two case studies: a university campus and a single building. While k-MILP systematically outperforms the k-medoids approach, for the university campus case study, k-means and k-MILP have very similar performance in representing the operating costs of the whole year; nevertheless, the extreme days selected by the k-MILP allow decreasing the number and extent of the outages. For the single building case study, the advantages of k-MILP over k-means become considerable in terms of both costs (up to -30% total annual cost) and reliability of the optimized designs. This is mainly due to the extreme days selected by the k-MILP, which turns out to be more challenging in terms of heating demand with respect to those of the k-means. Hence, the novel clustering algorithm turns out to be a valid alternative to well-known clustering techniques for its accuracy in reproducing both the hourly profiles and the integral of the aggregated load duration curves, while automatically identifying extreme and atypical operating periods.
The three-stage stochastic mixed-integer programming (SMIP) problem with integer recourse features a great number of binary variables and constraints, making it computationally intractable rather quickly. Thus, an iterative heuristic algorithm based on the decomposition of the original problem and the addition of an integer cut, in order to explore the performance of different combinations of technologies in a stochastic environment, has been proposed. Tests on a real-world case study (a university campus), comparing a "standard district" (S-D) and a "net zero CO_2 district" (NZCO2-D), show that: (i) the deterministic approach (neglecting the uncertainty) and the stochastic approach find slightly different design solutions; (ii) the design solutions found by the deterministic problem features an increase of Total Annual Costs (TAC = Capex + Opex) equal to 8% (S-D) and 11% (NZCO2-D) when it is operated in the stochastic scenarios with on/off real-time adjustment for the quick start-up units; (iii) the possibility of integer recourse for the quick-start units enables operating costs reductions of 6% (S-D) and 7% (NZCO2-D) with respect to the real recourse for all the units; (iv) the decomposition algorithm, devised to solve the stochastic problem, reaches a design solution that performs better than the deterministic one in the stochastic scenarios (1% and 2% decrease of TAC). Future works should address the extension of the model and solution algorithm for problems with finer time resolution (15 min), in order to consider the aforementioned positive role of the energy districts towards the electric grid, by responding promptly to the electric grid fluctuations.
The limited difference between the optimal design of an energy district found under a stochastic approach and a deterministic approach is due to the capability of the energy district with a deterministic design, when connected to the grid and endowed with fully integrated multi-energy and storage systems, to efficiently cope with the effects of the forecast errors. In light of this, the benefits of the optimization of multi-energy systems has been further investigated neglecting the uncertainty associated to the day-ahead forecasts, considering three case studies: a university campus, a hospital and a residential neighborhood. Indeed, in all of them, the design optimized with the proposed model turns out to be annually less expensive than the existing one (18-20% TAC reduction); furthermore, the design that has been optimized assuming an economic objective function, features also a reduction of the fossil CO_2 emissions (10-32% reduction). If the fossil CO_2 emissions are to be reduced of a further 25%, it appears that the optimal mix of technologies, in the three case studies, features a larger use of heat pumps, photovoltaic panels and/or biomass firing organic Rankine cycles; even so, the optimal selection and sizing of technologies is definitely case-specific.
Finally, the temperature intervals superstructure has been exploited to compare a number of retrofit options for the heating and electricity supply to a large-size energy district, featuring a district heating network with a large delivery/return temperature difference. Results show that the model is capable of accurately representing the optimal operation of the existing energy district and assessing the impacts of different strategic choices on the economic balances of the district heating network operator, the fossil fuel consumption and the greenhouse gases emissions.