



## DOCTORAL PROGRAM IN ENERGY AND NUCLEAR SCIENCE AND TECHNOLOGY

Chair:  
**Prof. Carlo Bottani**

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

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

The specific thesis discussed in this Yearbook are related to the PhD work of:

Binotti Marco	Linear Fresnel Reflectors: Study of the Technology and Steps toward Optimization
Colombo Marco	Experimental Investigation and Numerical Simulation of Two-Phase Flow in the Helical Coil Steam Generator
Della Torre Vittorio	Multi-scale CFD modelling of intake and exhaust systems for internal combustion engines
Fiorina Carlo	The Molten Salt Fast Reactor as a Fast Spectrum Candidate for Thorium Implementation
Gazzani Matteo	Thermodynamic and Economic Analysis of Advanced Process for CO <sub>2</sub> capture
Guerrieri Claudia Renata	Investigation of the dynamic behaviour and of control issues of circulating fuel reactors
Mangili Francesca	Development of advanced computational methods for prognostics and health management in energy components and systems
Piccinelli Roberta	Methods for the Vulnerability Analysis of Critical Infrastructures
Spallina Vincenzo	Mid-long term solutions for coal power plants with near-zero emissions
Tizzanini Alessio	Study and development of new power generation technologies for geothermal low enthalpy resources
Visek Margareta Emilia	Control Strategies, Fault Detection and Diagnosis of Renewable Energy Sources Systems

Visek Matej	Study of innovative techniques aimed at reducing energy consumption in domestic refrigeration system
Wang Hua	A Study of Gaseous Transverse Injection and Mixing Process in a Simulated Engine Intake Port
Zago Matteo	Direct Methanol Fuel Cells modeling: mass transport phenomena and electrochemical impedance spectroscopy
Zani Alessandro	Experimental and theoretical studies on ultraintense laser-driven ion acceleration

Radiation Science and Technology 24° cycle

Ghazy Rasha	A Study on the Key Factors of Nuclear Power Plant Performance
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Their research and most significant results are presented in the following pages.

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# LINEAR FRESNEL REFLECTORS: STUDY OF THE TECHNOLOGY AND STEPS TOWARD OPTIMIZATION

Marco Binotti - Supervisor: Ennio Macchi

## Introduction and Methodology

The PhD thesis focuses on Linear Fresnel Reflectors (LFR) as an innovative solution for Levelized Cost of Electricity (LCOE) reduction in Concentrating Solar Power (CSP) plants. The study purpose is the definition of an effective and efficient procedure to optimize the design of a LFR: a set of calculation tools was developed to model the different aspects of a CSP plant using LFR. LFRs are characterized by a high number of geometrical parameters (number, spacing, curvature, width of the mirrors, height of the receiver, type of receiver, etc.) and thus it is important to determine 'guidelines' that help in the selection of an optimized collector. A simplified analysis is proposed and the minimization of the Levelized Cost of Thermal Energy (LCoTE) is set as objective: the collector with the minimum LCoTE is the collector that optimizes, for a chosen location, the yearly harvest of thermal energy with the minimum investment cost. In order to reduce the number of optimization parameters, only molten salts as heat transfer fluid was considered, while the storage system and the power block were not taken into account. Two CSP plants based on Fresnel and PT technologies

were initially simulated from an overall plant point of view to assess their performance and to determine a reference cost for electric energy generation through CSP. Different models (optical model, thermal model, piping and economic model) were then developed to study the different aspects of a linear Fresnel collector field. All the models were assembled together to determine the dependence of the LCoTE from the different geometric parameters of the collector. Sensitivity analyses on each model are performed to reduce the number of significant parameters. Once the optimization procedure has led to a limited number of collectors with the minimum LCoTE, the entire plant analysis for one year operation could be performed with more specific simulation tools (Thermoflex 22) reducing the computational time.

## Overall plant simulations and LCOE

The Andasol I power plant with Solar Multiple SM=2, nominal power of 50MW and heat storage capacity of 7.7 equivalent hours was chosen as 'benchmark' reference case to determine LCOE for parabolic trough. The software used for the simulation of the whole plant was Thermoflex 22,

together with a VBA code used for the storage management. The obtained yearly solar-to-electric efficiency for the Sevilla site was of about 15.9%, with a corresponding LCOE of about 18.4 c€/kWh. The collector NOVA1 was chosen as 'reference commercial technology' for Fresnel reflectors and a plant based on saturated Direct Steam Generation was simulated. No thermal storage was implemented. The yearly sun-to-electric efficiency for Sevilla site was of about 10.1%. A preliminary economic analysis showed that the equivalent cost of Fresnel technology should be about 45–50% lower than parabolic trough in order to match the same LCOE.

## Optical analysis

To study the optical performance of a Fresnel collector both a built-in ray-tracing code implemented in MATLAB® and the SolTrace software (a code developed by the NREL) were used. The codes can predict optical performances of different Fresnel collectors as a function of the transversal and longitudinal incidence angles ( $q_i$ ,  $q_t$ ), and the heat flux distribution on the absorber tube. Optical performances at different incidence angles are summarized in the Incidence Angle Modifier (IAM) curves. The performance of the NOVA

1 collector obtained with the two simulation tools showed good agreement with the performance guaranteed by the manufacturer. SolTrace was selected as the best candidate for parametric analyses and a suite of MATLAB was developed to manage input-output of the tool.

Sensitivity analyses were performed to investigate: i) the differences between parabolic and circular mirror, ii) the IAM factorization hypothesis and iii) the effect of the variation of the focal length on the performance of a single mirror. An innovative procedure of 'compression' of the weather data was proposed to summarize the distribution of solar radiation from the different directions of the sky in a whole year: in this procedure, the sky is discretized in a grid of  $1^\circ \times 1^\circ$  of transversal and longitudinal incidence angles and the DNI supplied in each time step (the length of the time step can be chosen) of the year is assigned to the corresponding  $1^\circ \times 1^\circ$  grid element. The yearly optical efficiency can be then calculated simply as the product of the obtained DNI map with the IAM map.

## Thermal analysis

A suite of MATLAB implementing the thermal model proposed by Forristal for evacuated absorber tubes was developed. The model allows the sizing of the absorber tube for a chosen mass flow and temperature difference as well as the calculation of the thermal performance in off-design condition. The model was used to investigate the dependence

of the thermal losses on: i) the absorber diameter, ii) the Concentration Ratio iii) the absorber longitudinal discretization and iv) the ambient conditions. The energy hitting the receiver is not only a function of the DNI, but depends also on the optical efficiency. In order to reduce the computational time and not to perform an hour by hour simulation, a proposed simplified approach for the average yearly thermal efficiency estimation was introduced: this procedure allows the calculation of the yearly thermal losses on the basis of a properly averaged energy hitting the absorber tube. The error made with this procedure, compared to the hour by hour use of the Forristal model, was estimated for different cases around 0.6% in average: this value is not negligible, but acceptable for the preliminary selection of the collector design purpose of this work.

## Piping and Economic Model

A MATLAB suite was developed for the solar field piping system sizing: the number of collectors is determined by imposing a target of thermal yearly energy output from the solar field. The model requires as input the nominal HTF mass flow in the collectors, their length  $L$ , the target specific thermal losses (W/m) for the hot and cold headers and the HTF velocity. The code calculates the required commercial tube diameters, the wall thicknesses, the amount of insulating material and the pressure losses for each segment of the piping. A cost data-base obtained from data available in literature was built and simple correlations

were used to relate the geometric parameters variation to the cost variation. The total specific Solar Field cost ( $\frac{\text{€}}{\text{m}^2}$ ) is determined and with the "Fixed Charge Rate" (FCR) method it is possible to calculate the LCoTE with a procedure analogous to the one usually followed for the LCOE.

## Conclusions

LFRs were investigated and studied from different points of view from their optical characterization to the whole plant design. A procedure helpful for the assessment of the optimal LFR configuration as a function of the Levelized Cost of Thermal Energy was developed. The procedure reduces the number of simulation for the optimization of the LFR configuration saving computational time compared to a detailed model. The procedure is based on different models describing each conversion step from solar to thermal energy and defining the correlations between geometric characteristics of the collectors and their costs. The minimization of the cost of the produced yearly thermal energy at the solar field outlet can be set as optimization parameter.

# EXPERIMENTAL INVESTIGATION AND NUMERICAL SIMULATION OF TWO-PHASE FLOW IN THE HELICAL COIL STEAM GENERATOR

**Marco Colombo** - Supervisors: **Antonio Cammi, Luigi Colombo**

Helically coiled pipes are today considered as a primary option for the Steam Generator (SG) of different new nuclear reactor projects of both Generation III+ and Generation IV. The improvement of such an important plant component is vital as much as the research for new technological solutions to reach the goal of improved safety, performance and cost established by the world nuclear community for the future nuclear power plants. Numerous favorable characteristics justify the renewed interest developing in the nuclear field. In particular, helical tubes can provide enhanced heat and mass transfer rates, higher critical heat flux during boiling and evaporation and better capability to accommodate the thermal expansion, in addition to allow a more compact design of the SG. Helical coils are particularly attractive for Small-medium Modular Reactors (SMRs) of Generation III+ which adopt an integral layout. As a matter of fact, compactness and efficiency improvement become particularly important for this type of reactors, being all the primary system component located inside the reactor vessel. Within these respects, the thesis work is the natural prosecution of the recent efforts made by the Nuclear Engineering Division on the thermal hydraulics of

the two-phase flow for SMR SGs. The group has been involved since many years into the IRIS project (International Reactor Innovative and Secure), an integral Pressurized Water Reactor of 335 MWe of power developed by an international consortium. In the thesis work, the single-phase flow and in particular the two-phase flow are thoroughly studied, to improve the knowledge of the thermal hydraulic of the helically coiled SG tube. In particular, frictional pressure drop, two-phase flow structure and void fraction and two-phase flow instabilities are the main subjects. A careful characterization and a precise quantification of all of them is of fundamental importance not only for the design of the SG but of the whole secondary system. To the aim, suitable simulation tools are defined and developed throughout the thesis. Analytical and empirical models are developed for a reliable estimation of the physical quantities under study, which becomes particularly important for the engineers involved in the design process. Furthermore, the helical geometry introduces an additional level of complexity, especially for the two-phase flow. As a consequence, the work is also devoted to an improvement of the understanding of some basic

physical phenomena, as for example the influence of the centrifugal force on the phase distribution and the interaction between the phases. In view of the pointed out diversified necessities, an overall analysis method is employed in the thesis work, based on the application and strict and continuous interrelation between experimental investigation, numerical simulation and analytical and empirical model development. Starting point of the research activity is the availability of a large number of experimental data, which are necessary for model development and validation of numerical results. The data were measured in an experimental facility designed for the study of the helical coil SG for application in a Small-medium Modular Reactors (SMRs) of Generation III+. In particular, the database includes measurements of single-phase pressure drop, two-phase adiabatic frictional pressure drop and instability of the two-phase flow, in particular Density Wave Oscillations (DWOs) and Ledinegg instabilities. The first section of the work is focused on the single-phase flow. The experimental data are compared with some empirical correlations for the friction factor and the laminar to turbulent flow transition.

The most accurate correlations are identified and they are found to be generally pretty accurate. However, they are not sufficient when a more detailed description of the physical phenomena characterizing the system is desirable, requiring the support of more complex but powerful tools. Therefore, the single-phase flow is characterized in detail with Computational Fluid Dynamics (CFD) numerical simulations. In particular, the effect of the centrifugal force field on the flow and the accuracy of numerous turbulence models are studied. The CFD is selected as the principal simulation tool and is used during all the thesis work. In particular, the ANSYS FLUENT code is adopted for the simulations. Accuracy and consistency of numerical simulations are constantly validated through comparison with the measured experimental data. The large amount of data generated with the CFD are then analyzed to explain the experimental behaviors through a more detailed description of local quantities. The larger part of the thesis work is dedicated to the two-phase flow. A first activity resulted in a new empirical correlation for the prediction of the two-phase frictional pressure drop. The new correlation shows a relatively simple form and satisfy one important requirement initially established, that is the applicability in a large range of geometry parameters and operating conditions, proved by a mean relative error of about 14%. Actually, numerous correlations are available in literature, but none of them is reliable in a wide

range of parameters. At the same time, the CFD analysis has been applied to the two-phase flow. The two-phase flow is modeled through the Eulerian – Eulerian multiphase model. An adiabatic flow is simulated, that is phase change and energy exchanges between the phases are neglected. In addition, only the drag force is considered as a term of momentum exchange between the phases. Initially, an air-water flow at atmospheric pressure is considered. This intermediate step seemed necessary because it allowed a deeper validation of the numerical results through comparison with experimental data, available in a large quantity for the air-water case. The results show a satisfactory 4.5% mean relative error for the void fraction, and about 12% for the frictional pressure drop. After the detailed validation of the air-water results, also the steam-water case has been simulated, comparing the results with the experimental data on the adiabatic frictional pressure drop. The CFD model shows a good accuracy in the prediction of the frictional pressure drop, with a mean relative error of about 15%. Numerical 3-D results allowed also the characterization of the two-phase flow inside the helically coiled pipe and a major understanding of the effect of the centrifugal force field on the structure of the two-phase flow, the phase distribution and the velocity fields. In particular, starting from the CFD simulations, an explanation is proposed for the pronounced peak of the frictional pressure drop profile observed during the experiments. In addition,

numerical results permitted to overcome the shortage of available experimental data on the void fraction for the steam-water case. A new empirical correlation is proposed for the void fraction, based on the drift-flux formulation. The drift-flux model is also successfully used for a further validation of the local velocity field and void fraction distribution, obtained with the CFD. The global approach adopted in the whole thesis is even reinforced for the last subject, that is the study of the DWOs in parallel channels. An existing non linear analytical dynamic model based on the homogeneous flow theory is upgraded to a drift-flux formulation. The empirical correlations developed for the frictional pressure drop and the void fraction are included into the model and the improvement obtained in the results are quantified through comparison with experimental data. At the same time, also an assessment of the results of the RELAP5 numerical code is carried out. A significant code drawback is identified, which requires to use slightly different channel lengths to properly simulate DWOs in parallel helically coiled SG tubes.

# MULTI-SCALE CFD MODELLING OF INTAKE AND EXHAUST SYSTEMS FOR INTERNAL COMBUSTION ENGINES

Augusto Della Torre - Supervisor: Gianluca Montenegro

## Introduction

The present work deals with the multi-scale modelling of intake and exhaust systems for internal combustion engines. The internal combustion engine is a complex system which involves physical phenomena occurring over a very large interval of time and length scales, as illustrated in Figure 1. In the scale framework, the largest one is represented by the engine-scale, related to the characteristic dimension of the pipe system ( $10^{-2} - 10^{-1}$  m). On the other hand, the smallest length scale is related to the dimension of the smallest cavity in which the flow can pass through, such as the pores of porous media, often present with different purposes, e.g. as catalytic substrates for pollutant conversion or as filtering media for particulate removal ( $10^{-5} - 10^{-3}$  m). In addition to the largest and the smallest, other intermediate significant scales can be distinguished, namely component-scale and porous media macro-scale. The aim of the present work is to develop an integrated approach for the CFD simulation of the internal combustion engines, which involves the description of phenomena occurring at the different scales (Figure 2). In this framework, simulation of the smallest scales is performed in order to

enhance the understanding of the physical phenomena, to give optimization guidelines and to extract useful information for the macro-scale modelling. When larger scales are considered, phenomena occurring at smaller scales are modelled, in order to allow the full scale simulation of the device considered with an acceptable computational effort.

## CFD simulation at the micro-scale

CFD numerical simulations have been applied to the study of fluid-dynamics and heat-transfer in open-cell foams and filtering media for after-treatment systems. In particular, different aspects were investigated: application of Image Based Meshing (IBM) techniques for the geometric reconstruction, ideal CAD-based modelling of micro-structural geometries, generation of the computational grid, geometric characterization of porous matrices. Different types of analysis were performed. Unsteady detailed numerical simulations allowed us to describe the development of turbulence and its effects on pressure drop and heat transfer. Moreover, based on these results, considerations were assessed on the turbulence modelling when RANS approaches are applied. The effects of some geometric

properties of the open-cell foam micro-structure, namely porosity and pore density, were investigated, applying mathematical transformation on the real image-based geometry. RANS conjugate heat transfer simulations were used for the characterization of fluid-dynamics and heat-transfer properties of porous media over a large range of flow regimes. These studies confirm how the combination of micro-CT scanning, Image Based Meshing (IBM) and CFD can be an effective tool for the characterization of porous media.

## Derivation of CFD simulation models at the macro-scale

Time- and space-averaging operators were applied on the micro-scale governing equations in order to derive a macro-scale model for the porous system constituted by the fluid and solid phases. The results of the micro-scale CFD simulations were used to calculate the effective contribution of the extra-terms resulting from the averaging process. This allowed to improve the understanding of the physical meaning of these terms and to provide a quantitative evaluation of their influence on the flow behaviour. As second step, models were proposed on the basis of the micro-scale characterization of permeability

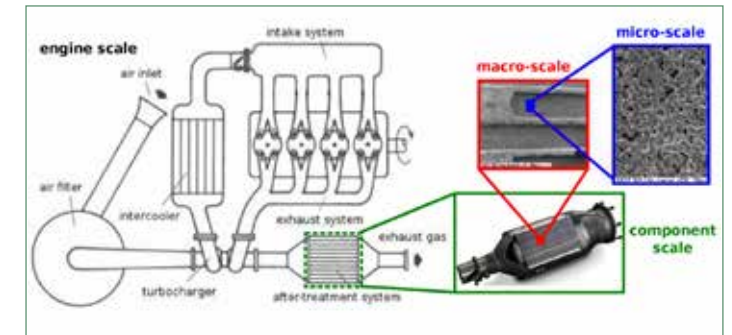
and heat-transfer. Aspects related to the implementation of macro-scale models in a CFD tool were discussed. Validation of the proposed macro-scale approach was provided resorting to representative test cases.

## Quasi-3D engine-scale modelling

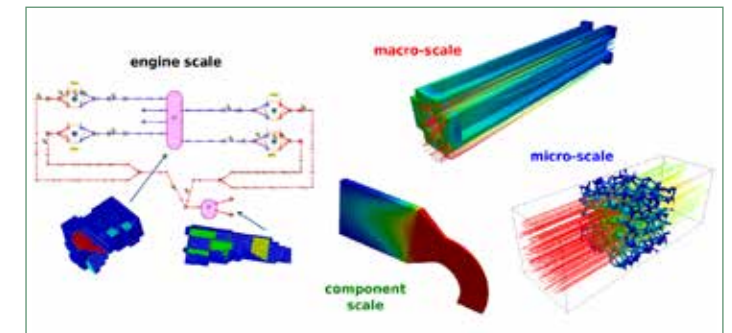
A novel quasi-3D approach, named 3DCell, was proposed as a tool for the engine-scale simulation. It is based on the reconstruction of the geometrical domain by means of a network of 0D elements, defined by two fundamental entities: the cells, which define the volumes, and the ports, which store information about the distance and the flow area between two neighbouring cells. The method has been developed from the foundations and optimized tailoring the best trade-off between accuracy and computational runtime. The approach has been deeply tested on a wide range of test cases taken from the literature or provided by the industry within collaborative research projects, allowing the study and the definition of the range of applicability of this type of tools.

## Conclusions

In this work different approaches have been developed and applied to the fluid-dynamic and acoustic simulation of the intake



1. Schematic of the different scales of the engine system



2. Multi-scale modelling of the engine system: CFD and quasi-3D approaches are applied at the different scales

and exhaust systems of internal combustion engines. These have been applied to the study of the physical phenomena at different scales, ranging from the micro-scale in porous media to the entire engine scale. The present work gives contributions to the specific fields of the internal combustion engine modelling, developing quasi-3D and CFD simulation tools and exploring the possibilities offered by techniques already applied

in different fields, e.g. IBM strategies. On the other hand, the contributions of the present work are not limited to the research on internal combustion engines, but can be of general interest for other fields related to the study of porous media. As matter of the fact, the multi-scale CFD approach can be applied to the optimization of any industrial product or application which includes porous substrates.



## THE MOLTEN SALT FAST REACTOR AS A FAST-SPECTRUM CANDIDATE FOR THORIUM IMPLEMENTATION

Carlo Fiorina - Supervisor: Antonio Cammi

The thesis work investigates the use of thorium in fast-spectrum reactors, with specific reference to the Molten Salt Reactor (MSR) technology.

Fast-neutron-spectrum Reactors (FR) have been developed in the early stages of nuclear technology for the purpose of breeding fissile isotopes from fertile materials. The U-Pu cycle has been preferred over the Th-U cycle because of the better breeding potential in a fast-spectrum and the sounder technical basis available. On the other hand, Th use has been historically investigated to breed fissile material (U-233) in a thermal spectrum, thus avoiding specific technological challenges associated to the development of FRs.

Over the course of the years, interest in fissile breeding has faded, especially in western countries, due to the slow deployment rate of new nuclear power plants and thanks to the availability of natural uranium resources. Concerns related to proliferation of nuclear weapons have also been a powerful deterrent against the production of fissile material. Conversely, waste management has emerged as one of the main problems for public acceptance of nuclear energy. Following these trends, both Th-based thermal reactors and U-based FRs started to be considered

in view of their capability to operate with continuous recycle of all actinides, while potentially burning legacy TRUs (TRansUranic isotopes) from LWR operation, thus drastically limiting the actinide waste to be disposed.

Under this scenario, Th-based FRs can offer specific advantages. The lower mass number of Th fosters a low endogenous generation of TRUs while the low breeding capability of Th cycle may enhance the consumption of an external supply of TRUs. Past studies have also pointed out the Th potential capability to improve safety parameters. Despite the potential advantages, the implementation at an industrial scale of the Th closed cycle needs to overcome several challenges, including difficulties in dissolution and reprocessing of used fuel, and fabrication of highly radioactive recycled fuel. The use of liquid fuel with online reprocessing would avoid most of the issues related to reprocessing, manufacturing and transporting radioactive fuel. The logical technology for the adoption of liquid fuel is the MSR. MSRs were conceived during the fifties for military purposes in the US, and developed for two decades as graphite-moderated reactors for U-233 breeding and power production. After the

selection of the MSR among the Generation-IV reactors in 2001, the concept evolved in the direction of fast-spectrum MSRs, identified as Molten Salt Fast Reactor (MSFR) and mainly developed in the frame of the EURATOM EVOL Project.

Use of Th in fast-spectrum MSRs is a relatively recent proposal and limited studies are available. A first-of-a-kind comparative analysis with solid-fuelled FRs is performed in this thesis work in terms of breeding capabilities, waste management, TRU burning and safety features. The activity has been carried out in the frame of an IAEA Coordinated Research Project (Near Term and Promising Long Term Options for Deployment of Thorium Based Nuclear Energy), to which the Politecnico di Milano participates.

To ease the investigation while excluding major sources of biasing, a common tool is employed to evaluate the performances of the MSFR and of the solid-fuelled FRs. Specifically, an existing ERANOS-based procedure, developed at the Paul Scherrer Institut (Switzerland) for the analysis of solid-fuelled FRs, is employed and extended to allow the simulation of Th-based cycles, the use of fertile blankets and the online reprocessing system of MSRs. In addition, dedicated sub-procedures are set up for

the calculation of radiotoxicity and decay heat of wastes.

Using this tool, the capability of the MSFR to operate with a flexible conversion ratio is first demonstrated, showing the possibility of employing it as breeder, iso-breeder or burner reactor.

Operation of the MSFR as breeder reactor is demonstrated to allow a remarkable doubling time of approximately 40 years, although significant uncertainties exist on the U-233 capture cross-section.

Use of Th in fast-spectrum reactors is found to foster notable advantages in terms of decay heat of wastes, with the caveats of an increased Sr-90 generation of U-233 vs. Pu-239. Waste generation is particularly low in the MSFR thanks to the high average burn-up and lower reprocessing rate allowed by a liquid fuel.

Transmutation of an initial TRU loading is shown to be ineffective in traditional U-based FRs, while some benefits appear to be achievable in a closed Th cycle. The relatively soft spectrum of the MSFR partly frustrates the effectiveness of transmutation, but its high specific power combines with the lack of out-of-core cooling time for the fuel to yield a short transmutation time (~50 years). Waste burning via an external TRU feed in the MSFR is limited by solubility issues to ~150 kg/GWe-yr, much lower than the 500-600 kg/GWe-yr of traditional FRs. On the other hand, the MSFR shows the potential of using a Th-MA feed (Th and Minor Actinides, without Pu), leading to a MA burning rate of ~150 kg/GWe-yr, three times higher

compared to traditional FRs. Investigation of Th impact on the safety features of traditional FRs confirms significant advantages in terms of void reactivity and Doppler, with the caveats of reduced core and fuel expansion coefficients, and of a possibly higher number of required control rods. In the MSFR, Doppler and fuel expansion represent the only significant feedbacks. Their combined effect is found to yield a strongly negative feedback, one order of magnitude higher compared e.g. to sodium-cooled FRs. The capability of the MSFR to withstand all typical double-fault accidents is also investigated through prediction of the steady-state reached after the transient. The overall inherent safety of the MSFR appears promising and comparable to that of the traditional FRs here analyzed, both U- and Th-based. In particular, the MSFR has the advantage of featuring only negative feedback coefficients. On the other hand, during certain accidental transients it has to rely on a fuel draining safety system, which is a unique safety measure of the MSR technology, but whose effectiveness is still to be proved.

After characterizing the MSFR through a top-level comparison with the solid-fuelled counterparts, the work concentrates on two specific aspects of the MSFR that differentiate this technology from the others. The first one is the thermal-hydraulics, showing the unique feature of an internal heat generation. A correlation is proposed to

predict the Nusselt number in case of internally heated fluids flowing in turbulent regime in a straight circular channel. Application to the MSFR allows to exclude major impacts of the internal heat generation on design and behaviour of its out-of-core components, though attention should be paid in case of channels with low salt velocities and/or large diameters.

The second distinctive aspect of the MSFR technology is the reactor dynamics, strongly affected by the presence of a circulating fuel. A multi-dimensional model of the reactor primary circuit is developed envisioning a node-wise coupling of the various quantities at play. The model is assessed against a similar model developed in the same period at the Technical University of Delft (Netherlands), showing a good agreement. Three recirculation zones are observed in the core, causing excessive temperatures and accumulation of delayed neutron precursors in low flux regions, with detrimental effects on the  $\beta_{\text{eff}}$ . Transient simulations demonstrate a generally benign response of the MSFR to major accidental transient initiators. The new asymptotic state reached by the reactor can be considered as representative of the reactor worst conditions in an accidental transient, thus confirming the promising inherent safety features of the MSFR already pointed out in the thesis.

# THERMODYNAMIC AND ECONOMIC ANALYSIS OF ADVANCED PROCESS FOR CO<sub>2</sub> CAPTURE

Matteo Gazzani - Supervisor: Ennio Macchi

## 1. Introduction

Rising world energy demand has mostly been met by expanding the use of fossil fuels, resulting in higher concentrations of carbon dioxide in the atmosphere. The possible consequences of these trends, in particular global warming, have driven the search for alternative electricity generation technologies capable of limiting CO<sub>2</sub> emissions. It is very likely that carbon dioxide reduction will have to be achieved while fossil fuels continue to be the major source of primary energy for several decades to come. Carbon dioxide capture and storage, is recognized as one of the most promising options because it addresses the impact of the largest primary energy sources and the largest source of CO<sub>2</sub>.

## 2. Thesis overview

The final goal of the PhD research activity was the techno-economic assessment of fossil fuelled power plants with carbon capture by two different innovative technologies: one based on advanced sorbents (Sorption Enhanced Water Gas Shift) and one based on membranes (hydrogen selective membranes). Both the technologies were developed in two FP7 projects: Caesar and Cachet II. The PhD work was exclusively theoretical but with input from experiments carried out by the projects partners (ECN, SINTEF). The features of both the

considered technologies are:

- **Sorption Enhanced Water Gas Shift:** SEWGS comprises of multiple fixed beds operating in parallel that adsorb CO<sub>2</sub> at high temperature and pressure, and release it at low pressure. The combination of CO<sub>2</sub> conversion and removal enhances H<sub>2</sub> production and the purity of the stream feeding the Gas Turbine combustor, whilst a separate CO<sub>2</sub> by-product can be recovered from the adsorbent by regenerating the bed.
  - **Hydrogen membranes:** hydrogen permeable membrane reactors are an attractive technology for pre-combustion carbon capture in both coal and gas fired power stations because they combine the simultaneous production and separation of hydrogen while capturing the remaining carbon dioxide. The carbon dioxide is produced at high pressure, reducing the compression energy for transport and storage
- In order to study advanced technologies together with innovative power production configurations, different investigation levels have been considered:
1. **Detailed reactor model:** it aims at reproducing the behavior of the most critical reactors involving detailed chemical kinetic mechanisms. Two different reactors have been investigated using the single reactor model: the coal gasifier and the hot gas clean-

up system.

2. **Specific process model:** it is focused on the most important processes adopted in a defined configuration. Single system model has been adopted to reproduce the behavior of hydrogen fuelled gas turbine and to the coal gasification processes (Shell and GE).
3. **Overall techno-economic plant simulation:** the thermodynamic evaluation is based on mass and energy balances and it allows integrating all the components required for power production with CCS. All the data obtained in the single reactor and process modeling are implemented in this step.

## 3. Methodology

All the analyses have been carried out using several software: the overall integration and the single process simulations were developed with the proprietary code GS or the commercial tool Aspen Plus whilst the single model simulations are based on brand new code written in Aspen Custom Modeler (gasification reactor) or in Matlab (Hot gas clean up). Finally, overall economic evaluation is based on excel VBA with calculation of the Levelized Cost of Electricity according to the IEA method.

## 4. Detailed Reactor Models

### 4.1 Gasifier reactor

This activity was carried out at the Massachusetts Institute of

Technology under the Rocca project agreement. Being SEWGS and hydrogen membranes pre-combustion technologies, their application to coal plant requires a coal gasification process. A reduced order model (ROM) has been developed in order to predict the performance of the Shell-Preflo gasifier. ROM involves the representation of the gasifier by a Reactor Network Model (RNM) which is used to reduce the computational simulation expense, compared to CFD models. As result of the Shell ROM modeling, several parameters were calculated for a gasifier of about 3000 tons per day, for example: i) syngas, particles and gasifier wall temperature, ii) syngas and particle composition and, iii) overall gasification temperature and pressure. Sensitivity analyses were used to further investigate effects of main variables: i) oxygen to coal ratio, ii) coal feed amount and, iii) CO<sub>2</sub> feed as carrier gas.

### 4.2 Hot gas clean up

The implementation of hot gas desulfurization is a key issue for successful application of not sulfur tolerant technologies. A kinetic model of the system was developed to design the reactor at different operating conditions and estimating its cost. The process is based on fluidized beds: the desulfurizer, which must accommodate a large syngas mass flow, is a fast fluidized bed while the regenerator, which has a low gas flow, is a bubbling fluidized bed. The model has in input the system conditions which are defined by the gasification technology adopted and the desulfurization level to be achieved. The desulfurization and the regenerator design is based on kinetic equations and

it is obtained through several modules accounting for: i) sorbent properties, ii) syngas and regeneration air properties, iii) thermodynamic data of circulating solids, iv) sizing data as provided by Technip and, v) cost computation.

## 5. Specific Process Models

### 5.1 Gasification process

Shell and GE gasification process, which accounts of several reactor and recirculations, have been reproduced by calibrating the property O-D code (GS) in order to match the available data (experimental for Shell, literature for GE) at the end of the process.

### 5.2 Hydrogen fuelled gas turbine

With respect to natural gas, hydrogen combustion causes a variation of the flame properties, mainly temperature, speed and geometry and a higher water concentration in the product gases. All these variations, along with the change of the fuel flow rate due to a change in the LVH, bring about a modification of the machine design specifications. One of the main concerns is limiting the NO<sub>x</sub> emissions provided that: i) lean premixed combustors used with natural gas, at present are not commercially available for hydrogen because of technical hurdles posed by the very high reactivity of hydrogen; ii) the flame temperature of hydrogen is significantly higher than natural gas. These issues could affect the operating conditions of the blades, eventually resulting in a lifetime reduction, or alternatively, in a reduction of the blade metal operating temperature to mitigate their effects. An hydrogen fuelled GT was simulated and a comparison between diffusive and premixed combustor was carried out on the basis of

homogeneous assumptions.

## 6. Techno-Economic Plant Simulations

Concerning the SEWGS process, the PhD activity has been focused on its application in power plant either natural gas fired (Natural Gas Combined Cycles) or coal fired (Integrated Gasifier Combined Cycle) and in steel production plant. On the other side, the integration of Pd-based H<sub>2</sub>-selective membranes was studied only in integrated gasifier combined cycles. SEWGS technology has shown good thermodynamic results both in NGCC and IGCC power plant with a consequent efficiency gain of about 3 percentage points when compared to the commercial ready CO<sub>2</sub> capture technology. From an economic point of view, the application of SEWGS to NGCC does not show evident advantages compared to commercial ready technology. On the other hand, its application to IGCC leads to a decrease in the cost of CO<sub>2</sub> avoided in the order of 35%. SEWGS adoption in integrated steel plant features substantial thermodynamic benefits compared to other technologies. Hydrogen membrane application to IGCC showed an efficiency improvement in the order of 3-4 percentage points compared to the reference pre-combustion technology. The economic evaluation underlined that the cost of CO<sub>2</sub> capture through this technology with the present features is higher than the commercial ready process. Nevertheless there are several future possibilities to reduce the membrane performances which would make this technology more competitive.

## A STUDY ON THE KEY FACTORS OF NUCLEAR POWER PLANT PERFORMANCE

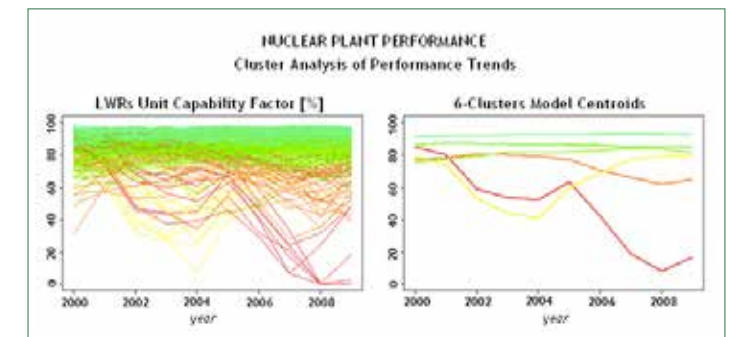
Rasha Ghazy - Supervisors: Paolo Trucco, Francesco de Falco, David Stuart Gilchrist

In the late 1970s and early 1980s a certain number of analysts reviewed the operating performance of Nuclear Power Plants (NPPs), not only to establish the level of performance that the plants were achieving, but also to identify the factors underlying the wide variability that characterized plant performance. Discrepancies observed in the first analysis were mainly attributed to differences in economic and safety regulation, as well as to technological differences in nuclear plants. Regression estimation of capacity factors related to plant characteristics, as learning-by-doing effects, size, age, and total years of construction, is reported in early literature; results were still raw, given that operating experience was reduced at that time and estimates resulted biased by autoregression and other factors. Poorness in availability of data, and in a solid methodology to be employed, added difficulties in discriminating and interpreting the most relevant aspects influencing performance. Nearly a decade later, the IAEA conducted an investigation and as a result of their analysis, factors related to reactor technology, assumed as affecting in previous works, did not look so determinant. The most

significant finding was that top-quality management supporting disciplined operation is the key to achieving overall plant safety, reliability, and economic performance objectives. A comprehensive understanding of the determinant reasons that lead NPPs to successful operation relies on three things: an extended and updated database, a well defined, accurate and integrated classification of key factors, and an adequate statistical methodology able to allow an interpretable analysis of the data. Thus, an effort is done in this thesis for outlining the factors that are involved in the determination of nuclear performance, as well as for estimating the range of variability that the nuclear performances are affected by. In cooperation with the Enel Nuclear Technical Area, international nuclear operational experience is investigated and, according to a thematic classification, the key factors of reactor performance are summarized under five main categories: technical, operational, managerial/organizational, economic and external aspects are all likely to influence NPPs performance. In such a context, the statistical computing code R is employed to analyze the

NPPs Performance Indicators (PI) data using different statistical methodologies; PI are studied with reference to the PRIS database developed by the IAEA, at which utilities annually provide their complete performance records. Unit Capability Factor (UCF) is employed as dependent variable into an ordinary least squares (OLS) regression analysis performed on a sample of 14 electrical firms. Operational and technical factors data (*Reactor technology, NSSS supplier, Plant size and Age*) of 135 Light Water Reactors (LWRs) operating in five different countries with an age between 10 e 40 years are used in this first analysis as independent factors. Results show that a modest proportion of UCF variation is accounted for by the four independent variables: *Plant size and Age* don't help predicting plant performance; despite the role *Reactor technology* seemed to have played in the past, and even though PWRs result generally less performing of 7% on average with respect to BWRs, it doesn't result in accounting for effective variation in UCF. Alternative and nonconventional methodologies are investigated to allow a more significative, innovative and useful interpretation of NPPs performance data. Indeed, OLS

regression technique applied to PI data demonstrates to be less consistent when compared to more robust and flexible analytical methods, such as Cluster Analysis (CA) or Classification And Regression Trees (CART). CA technique is applied for analyzing performance data of an enlarged dataset including all the LWRs operating in 2010 excluding plants in their running-in phase, and its outcomes used in the CART analysis. The results show that six clusters are adequate to represent the different evolution in time of all the reactors considered in the sample for the last decade: each group is characterized by a unique and defined trend that summarizes the general progression and development of the included plants performances (Figure 1). Clusters composition is analyzed from several perspectives, with the aid of representative conditional barplots, and its results contribute to explain reasons of success for those plants characterized by a performance positive growing trend. Technical and physical aspects that don't result as relevant in the regression analysis, when used to classify NPPs into the clusters, show however to play a significant role, contributing in classifying the plants; on the



1. 6-Clusters Model for Nuclear Performance Trends

basis of the these variables, CART analysis finds the best partition of the plants that depicts their cluster affiliation. Late works findings show that the role of the utility in determining NPPs performance is crucial; therefore, in this thesis the variation in the performances considers managerial and organizational issues as well, used in the CART analysis to predict the cluster determination of a new plant. A group of nuclear electric utilities operating in six different countries have agreed to support this research project and provided answers to a questionnaire addressing issues related to plant management systems and organizational initiatives within the plants, other than relevant economic aspects. The survey outcomes help creating decision rules for growing classification trees that determine the clusters

composition according to these aspects. CART analysis results show the considerable effects on performance of implementing a managerial model within the nuclear utility, and discriminate between a proprietary model and the recognized NEI SNPM; date of implementation is also studied in the clusters classification. Further examples show the importance of the issues dealing with the strategies hold by the organization and the management in the outage control outage programme, in the oversight function and so on. Although a more exhaustive analysis is likely to be developed through a wider utilities participation, this study represents the first attempt, based on a voluntary participation of the nuclear utilities, to analyze aspects and issues related to the plants daily activities and directly correlate them to the PI trends.



# INVESTIGATION OF THE DYNAMIC BEHAVIOUR AND OF CONTROL ISSUES OF CIRCULATING FUEL REACTORS

**Claudia Guerrieri** - Supervisors: **Antonio Cammi**

The aim of this thesis work is the investigation of the Circulating Fuel Reactor (CFR) dynamics and the discussion of some control issues concerning these class of nuclear reactors. In particular, reference is made to those CFRs adopting molten salt as primary coolant, namely the Molten Salt Reactors (MSR). The first efforts in the development of this technology were carried out during the sixties at the Oak Ridge National Laboratory (ORNL), with the construction of the Molten Salt Reactor Experiment (MSRE), an 8 MW<sub>th</sub> MSR prototype, and the subsequent design of the Molten Salt Breeder Reactor (MSBR). The interest in MSRs, that faded out after the closure of the Molten Salt Reactor Program in the USA, met a true revival in the last decade. Since 2001, MSRs have been included among the Generation IV systems, an ensemble of six innovative nuclear reactors selected by the Generation IV International Forum (GIF-IV) to be developed in the medium/long term in order to meet the future challenge of a safe, sustainable, economic competitive and proliferation resistant nuclear energy production. Nowadays, the activities carried out worldwide on MSRs are focused on the study of different designs. Among these, an important role is played by

the Molten Salt Fast Reactor (MSFR), a new reactor concept developed in the framework of the Euratom EVOL (Evaluation and Viability of Liquid Fuel Fast Reactor System) Project, which has been adopted by GIF-IV as MSR circulating-fuel reference configuration. The different MSR designs share common features, typical of the molten salt technology. In particular, the presence of a liquid fuel that circulates in the primary circuit acting simultaneously as primary coolant leads to a complex and highly coupled dynamic behaviour, which requires a careful investigation, as a consequence of some unusual characteristics, like the drift and the decay of delayed neutron precursors (DNP) in the out-of-core part of the primary circuit and the phenomena involving heat transfer with internally heated fluid. Throughout the work, classical tools for dynamics analysis were re-formulated and applied to the study of poorly-known features of systems involving circulating fuel. Innovative approaches were developed as well, like the Multi-Physics Modelling (MPM), that allowed important breakthroughs in the dynamic and transient analyses. The first intent of the thesis work was to provide a systematic and complete evaluation of the stability

properties of molten salt reactors, adopting approaches consolidated in the theory of linear systems, according to the common practice in the field of nuclear reactors. A theoretical analysis of the zero-power point kinetics of circulating fuel reactors was carried out for a rigorous treatment of the effect related to the transport of the fuel salt outside the core on the dynamic characteristics of the system. Proved tools in the dynamics analysis of conventional nuclear reactors were re-formulated in this work and applied to the study of liquid fuel systems. The developed approaches have been assessed against the experimental data available for the MSRE. The effect of the fuel velocity on the balance of delayed neutrons was investigated, and its importance in terms of reactivity was compared with the neutronic temperature feedback. A power threshold was identified, which is related to a change of the system behaviour. It was found that, when operating at lower power, transients caused by a velocity variation are dominated by the effect related to the variation of DNPs that decay out of the core, whereas temperature feedback dominates at higher powers. These results are important looking at a control strategy that

involves a variable flow rate in the primary circuit, as well as to evaluate any operative transient involving a variation of the fuel velocity. Also, a detailed analysis was carried out for the stability margin evaluation of the MSFR operating in the entire range of power.

The evaluation of the MSR transient behaviour was carried out considering two complementary approaches. First, simplified non-linear models were developed considering zero- or one-dimensional geometries. These models allowed the analysis (both in the time and frequency domain) of the entire plant in different working conditions, and were useful for a preliminary evaluation of single-component dynamic behaviour and control-oriented analyses. The second class of models are based on an innovative Multi-Physics Modelling (MPM) approach. Thanks to the capability of solving all the partial differential equations that govern the system behaviour, by managing simultaneously the different quantities at play without requiring the interface of dedicated codes, the MPM stands as a unique and natural environment of simulation for complex systems, like MSRs, where strongly coupled phenomena (neutronics, thermal-hydraulics and DNP transport) interact. In particular, a full-core Multi-Physics (MP) model of the Gen-IV MSFR was developed. This model allowed notable advances in the understanding of peculiar aspects that characterise the system dynamics (e.g., during full-power steady-state operative conditions). Important

indications for the finalization of the system design were obtained, concerning the DNP distribution and the flow field inside the core. Among the available commercial software, COMSOL Multiphysics® was chosen thanks to the possibility to be interfaced with MATLAB®. Integrated simulations between these two software platforms could be useful for future control-oriented analyses, where the control action computed exploiting dedicated tools of MATLAB® (e.g., the Control System Toolbox) can be directly applied to the MP model, which provides a detailed and accurate description of the dynamic response of the system. Furthermore, the modularity of COMSOL Multiphysics® is convenient when dealing with large models involving a number of different physical phenomena. The last part of the thesis work aims at analysing some controllability issues related to molten salt systems, paying particular attention to the MSFR. A traditional approach was adopted, considering a decentralized feedback scheme of control based on the use PID (Proportional-Integral-Derivative). Molten salt reactors, and nuclear power plants in general, can be considered Multiple-Input-Multiple-Output (MIMO) systems, since a number of quantities must be controlled in order to guarantee a correct operation of the plant, using a set of manipulated variables. Therefore, more than one possibility exists for the choice of the control loops, when a decentralized feedback scheme of control is adopted. Usually in the industry, the pairing of the controlled and manipulated

variables is based on the knowledge gained through the observation of the transient behaviour of the plant. An emerging approach is to look for objective criteria for this selection. In this thesis work, a technique based on the analysis of the Relative Gain Array (RGA) was applied to the study of the degree of coupling of the input and output variables of the modelled MSFR, in order to provide an objective criterion in choosing among all the possible pairing options for decentralised control. Based on these results, a set of possible control schemes was selected and implemented, integrating the simplified models developed for the purpose of the dynamic analyses with an ad-hoc set of PI controllers. Finally, different control strategies for the operation of the MSFR plant at partial load have been evaluated and discussed.



## DEVELOPMENT OF ADVANCED COMPUTATIONAL METHODS FOR PROGNOSTICS AND HEALTH MANAGEMENT IN ENERGY COMPONENTS AND SYSTEMS

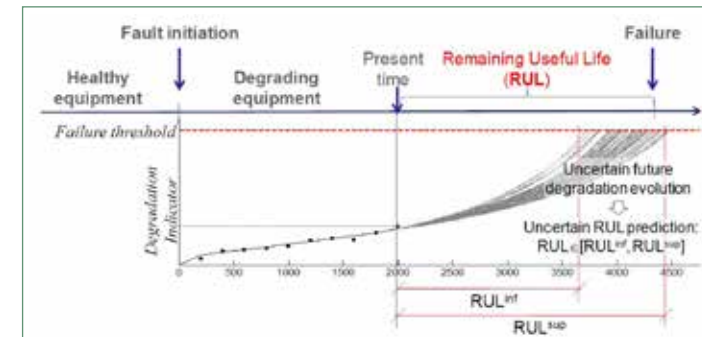
Francesca Mangili - Supervisor: Enrico Zio

For industry, unforeseen equipment failure is costly, both for repair and lost revenue. The maintenance strategies that are set up to face this problem traditionally fall into two categories: preventive maintenance and corrective maintenance (after failure). The former may result in unnecessary maintenance; the latter may take long times and result in significant lost revenue. In recent times, a third strategy, predictive maintenance, is emerging, based on assessing the actual equipment condition and predicting the optimal time at which performing maintenance. The underlying concept is that of failure prognostics, i.e., predicting the Remaining Useful Life (RUL) of the equipment defined as the time left before it fails to perform its function according to design specifications (Figure 1). Many diverse prognostic methods have been proposed in the last decades, primarily due to the wide variety of systems and applications they have been designed for. Those methods can be classified in model-based methods, which make use of an explicit mathematical model of the degradation process, and data-driven methods, which base their predictions on models learned from time series of observed degradation states, or

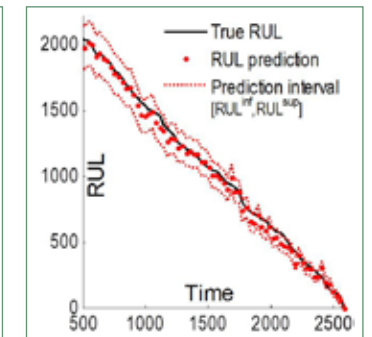
on directly mapping the relation between observations and equipment RUL. Two of the main open issues that remain in the field of prognostics are how to efficiently use different types of information available and how to correctly treat the uncertainty affecting this information. Indeed, depending on the different forms of information and data that may be available about the evolution to failure of degrading equipment, different prognostic approaches may be applied to project the current equipment condition in time, in the absence of future measurements about its degradation state and the operational conditions. This leads to propagating large uncertainties which need to be assessed and managed, by associating uncertainty estimates to the RUL predictions, so to measure the expected mismatch between the real and predicted equipment failure times, and use this information to confidently plan maintenance actions, according to the desired risk tolerance. In this context, the goal of this PhD work has been to identify the most representative situations of information available, develop properly tailored prognostic approaches, and provide a critical investigation of the capabilities of different prognostic

approaches to deal with various sources of uncertainty in the RUL prediction. The work has been performed within a cooperation between the Laboratorio di Analisi di Segnale ed Analisi di Rischio (LASAR) of Politecnico di Milano, and the Institute for Energy Technologies, OECD Halden Reactor Project, Norway, which has financially supported the PhD grant.

As first undertaking, we have identified three practical situations with decreasing information available for the prognostic task, and developed prognostic methods properly tailored to tackle each of them. We have supplied methods for the quantification of the RUL prediction uncertainty and characterized their performance in a case study with simulated data concerning prediction of the RUL of a turbine blade in which creep damage is developing (Figure 2). This case study has allowed performing a consistent analysis about the impact of the uncertainty affecting the prognostic information and models on the accuracy of the RUL prediction, thus contributing to the way of investigating the capabilities of prognostic methods to deal with the RUL prediction uncertainty. Furthermore, we have studied how the performance of the three proposed approaches varies depending on the quantity



1. Pictorial view of the prognostic task



2. Example of turbine blade RUL predictions obtained at different time steps during the creep growth process

and quality of the available information. From this analysis, we have been able to provide guidelines for the choice of a prognostic approach based on the available information. However, when multiple approaches can be applied, the combination of their outcomes is an alternative strategy to the choice of the best performing one. In this context, ensemble techniques have been introduced as an effective tool for aggregating different sources of information and achieving high prediction accuracy and reliable confidence estimate. In the industrial application of the prognostic approaches investigated in this work, one may very likely have to face additional problems related to the limited and unreliable information available about the equipment degradation state

or about its future operating conditions. We have tackled these problems in two case studies with data collected from real industrial applications. In the first case study, we have faced the problem of deriving exploitable prognostic information from noisy and unreliable data taken from eroding choke valves used in the oil & gas industry, and provided a solution for data pre-treatment based on a hybrid ensemble of physics-based and data-driven models. In the second case study, we have considered the problem of predicting the RUL of clogging filters which are used to clean the sea water entering the condenser of a Swedish nuclear power plant. To tackle this problem in the absence of physics-based information about the degradation mechanism, we have developed two

advanced data-driven prognostic approaches based on Gaussian process regression and similarity-based regression. In order to increase the robustness of the RUL prediction, we resorted to the belief function theory for treating the large uncertainties due to the unpredictable variations of the external conditions affecting the clogging process, and combining the different types of uncertainty measures provided by the two approaches proposed. The results obtained with real data have proved the effectiveness of aggregating multiple pieces of information treated by complementary methods, within an ensemble approach.

# METHODS FOR THE VULNERABILITY ANALYSIS OF CRITICAL INFRASTRUCTURES

Roberta Piccinelli - Supervisor: Enrico Zio

The subject of this PhD thesis concerns methods for the analysis of critical infrastructures with respect to their vulnerabilities to random failures and targeted attacks.

The work has been performed at the Laboratorio di Analisi di Segnale ed Analisi di Rischio (LASAR Laboratory of Signal Analysis and Risk Analysis) of the Department of Energy of the Politecnico di Milano.

Critical infrastructures (CIs) are large scale, spatially distributed, engineered complex systems which provide vital services for modern society, such as energy supply (electricity, oil and gas supply), transportation (by rail, road, air, shipping), information and telecommunication (such as the internet), drinking water distribution, including wastewater treatment. Outages or mishaps in CIs cause disruption or incapacitation of fundamental services and result in diverse consequences with economical and social implications.

For this reason, a comprehensive vulnerability analysis of CIs requires not only identifying the logical and functional relationships among the large number of spatially distributed, interacting elements but also accounting for a broad spectrum of hazards and threats including random failures and intentional attacks.

The conceptualization of critical infrastructure vulnerability assessment implies system analysis for (figure 1):

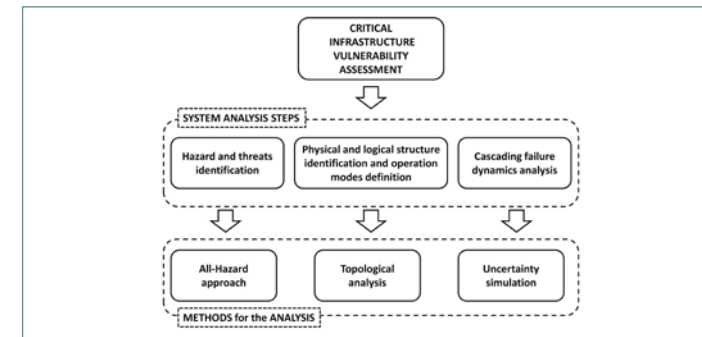
- hazards and threats identification;
- physical and logical structure identification and operational modes definition;
- cascading failure dynamics analysis.

In this thesis, three methods for the analysis have been devised to perform the vulnerability analysis:

- the all-hazard approach to address issue a;
- the topological analysis to address issue b;
- uncertainties analysis to address issue c.

CIs are especially attractive targets for malevolent attacks because today's societies operate heavily on their reliance. In risk and vulnerability analysis, random accidents, natural failures and unintentional man-made hazards are typically known and categorized by emergency planners. The likelihood of their occurrence is traditionally addressed within a probabilistic framework. On the other hand, terrorism poses a hazard that eludes a quantification by probability theory due to the intentional and malevolent planning it implies. Therefore, there is the need of an all-hazard approach encompassing a broader view

on the hazards, that threaten CIs. The all-hazard approach is intended to provide the basis for addressing unexpected events of any nature such as deterioration and random failures, natural disasters, accidents, and malevolent acts. In this PhD thesis, an *All-HAZard ANalysis* (A-HAZAN) is developed. It aims at identifying the features, operating conditions and failure modes relevant to CI vulnerability, and capturing the CIs vulnerability sources and issues, given their technical and physical features, and the dependencies and interdependencies on other CIs. CIs are engineered complex systems and can be modeled as hierarchies of interacting components. In this view, the actual structure of the network of interconnections among the components is a critical feature of the system. In a topological analysis, a CI is represented by a graph  $G(N, K)$ , in which its physical constituents (components) are mapped into  $N$  nodes (or vertices) connected by  $K$  edges (or arcs), representing the links of physical connections among them. The focus of topological analysis is on the structural properties of the graphs. In order to quantify the structural importance of the network components, several centrality measures have been introduced: commonly used



1. Pictorial view of the critical infrastructure vulnerability assessment presented in the present PhD thesis

centrality measures identify the most important elements in networks of components, based on the assumption that physical/communication/service among nodes flow follows the shortest paths in the network. In spite of the usefulness and appealing simplicity of the topological analysis of the network underpinning a CI and of the insights it provides, empirical results show that it cannot capture the rich and complex properties observed in a real infrastructure system, so that there is a need for extending the models beyond pure structural topology. While the topological approaches for identifying critical components are capable of highlighting structural vulnerabilities, they are limited from the point of view of the functional vulnerability of the CI. In real network systems,

another important dimension to add to the vulnerability characterization refers to modeling the dynamics of flow of the physical quantities in the network where physical law and operational rules drive the physical/communication/service flow. This entails considering the interplay between structural characteristics and the dynamics, in order to provide indications on the elements critical for the propagation process and on the actions that can be performed in order to prevent or mitigate the undesired effects. In the final step of the CI vulnerability analysis developed in this PhD thesis, the characterization of uncertainties related to the physical flow through the network has been undertaken and exemplified with respect to the electric infrastructure. Failing to

incorporate uncertainties in system planning may lead to an overestimation of risk reduction barriers and of system capabilities to maintain acceptable levels of reliability. In order to quantify the impact that the propagation of the identified uncertainties has on the reliability of the electric infrastructure a stochastic model that simulates the operations of an electric transmission network was developed. This event based model, embedded in the Monte Carlo Simulation framework, and has shown the ability to represent daily hourly changes in power requests at customer side of the system, ambient temperature, wind speed and wind power generation. The increasing variability in the operating conditions lead to an increase in the generated power that cannot be supplied to the customers.

# MID-LONG TERM SOLUTIONS FOR COAL POWER PLANTS WITH NEAR-ZERO EMISSIONS

Vincenzo Spallina - Supervisor: Giovanni Lozza

The present PhD project has been focused on the investigation of two different novel concepts, based on the use of IGCC with carbon capture to determine the evolution of clean coal technologies in the future years.

The first system is based on the use of chemical looping combustion (CLC) with packed bed reactors (PBRs); it would represent a **mid-term** solution: the CLC combustion has been considered in the recent years for pilot plants and the combined use of PBRs with CLC is at the early demonstration stage.

The second system is based on the integration of SOFCs in an integrated gasification plant: since the technological level of SOFCs development is not yet ready for industrial applications, SOFCs stack for multi-MW is expected to be proved in the **long-term** scenario.

For both systems the study is based on different levels of investigations:

## Components modelling:

*Packed Bed Reactors for CLC:* PBRs 1-D model is presented with kinetic model description based on the use of ilmenite as oxygen carrier, discussing the effects of both gas-solid and heterogeneous reactions; the thermal model is discussed

to include the effects of solid and gas composition; different strategies for heat management are studied in order to define the more favorable operating conditions of PBRs.

*Solid Oxide Fuel Cells:* a pseudo 2D model is described with a proper kinetic model implemented for pressurized systems, working with syngas from coal gasification and high CH<sub>4</sub> content; the electrochemical model is also discussed with new set of equations based on CO direct oxidation.

## Components integration in coal-fired power plants:

*PBR-IG-CLC:* according to the strategies discussed for the heat management in the previous stage of investigation, different plant layouts with thermal balance are evaluated in order to provide the best performance (net electric efficiency, CO<sub>2</sub> emissions, etc.). This analysis concerns the integration of different sections, such as Gasification Island, acid gas removal (AGR), GT and heat recovery steam cycle (HRSC). *IG-SOFC:* the presence of SOFC working with coal-syngas is discussed and different systems are proposed:

*IG-SOFC-base:* IG-SOFC without CO<sub>2</sub> capture system to predict the potential of fuel cell integration in coal-based power plant; *IG-SOFC-cryo:* IG-SOFC based on

oxy-combustion of SOFC anode exhaust gas with CO<sub>2</sub> capture through a cryogenic system and pressurized CO<sub>2</sub> cooling system; *IG-SOFC-meth:* IG-SOFC is based on the production of syngas with high CH<sub>4</sub>-content to exploit SOFC cooling through internal reforming and improve thermal integration with GT cycle; CO<sub>2</sub> capture is carried out by using physical absorption while an H<sub>2</sub>-fired gas turbine system is considered for the combined cycle.

Comparison of novel technologies with reference power plants: the technologies here discussed are compared with the reference systems for IGCCs with and without CO<sub>2</sub> capture. Related to the system with CO<sub>2</sub> capture, a pre-combustion technology with physical absorption through Selexol™ from coal syngas, following a water-gas shift reactor, is considered.

## Mid-term technology for fossil fuel power plant with CO<sub>2</sub> capture: Chemical Looping Combustion (CLC)

The CLC concept is based on the indirect oxidation of a fuel, by means of a solid metal which is alternatively oxidized and reduced by sequential contact with air and a fuel respectively. Thus, the solid metal, easily separable from the gaseous

stream, behaves as an oxygen carrier, taking oxygen in an air reactor (AR) and releasing it by oxidizing a fuel in a fuel reactor (FR). While the metal oxidation reaction is always exothermic for the chemical species investigated in the literature, its reduction can either be exothermic or endothermic, depending on the metal and the fuel involved.

Chemical Looping Combustion (CLC) can be competitive, in applications for power generation from gaseous fuels, if operated at high pressure (>15 bar), in configurations where the stream from the air reactor is expanded in a turbine. The technology here presented is based on dynamically operated packed bed reactors. With this configuration, the solids are always kept in the same reactor, which is alternatively exposed to reducing and oxidizing conditions by properly switching the inlet gas between air and fuel streams. Results have shown that the use of CLC in IGCC can lead to a penalty efficiency of 7% points which is 2% points higher than the conventional CO<sub>2</sub> capture system with coal.

## Long-term technology for fossil fuel power plant with CO<sub>2</sub> capture: Integrated Gasification Fuel Cells

Important international projects are focusing on the development

of advanced power cycles using fuel cells and gas turbine cycles, integrated to a coal gasification plant (e.g. the FutureGen Vision 21 projects of the US DOE). R&D activities are pushed by the exploitation of a low cost fuel and by the perspective of applying such technology (Integrated Gasification Fuel Cell cycle – IGFC) to high efficiency electricity generation with CCUS. A distinctive advantage of this concept is given by the electrochemical oxidation of the syngas occurring in the fuel cell, which acts like an oxygen combustor avoiding the dilution of exhaust gases with nitrogen. An analysis of a pseudo 2-D finite volume model for the prediction of the performance of an intermediate temperature (800°C) planar SOFC fed with syngas from coal gasification was carried out under different configurations. Different systems have been performed with and without CO<sub>2</sub> capture providing an electrical efficiency of 47-51.2% with near zero-emissions.

## Conclusions and final remarks

CCUS technology is expected to play an important role in the next years due to the need of reducing greenhouse gases. The integration of CCUS technologies in coal power plant need to be investigated due to the high CO<sub>2</sub> emissions

associated to the high C content of coal. In the mid-term future the use of CLC is a valid alternative to the technologies currently studied, at the demonstration stage: the low penalty efficiency with the relatively simplified CO<sub>2</sub> capture system make this technology interesting especially if some other plant simplification can be included due to the improvements in materials, components, catalysts, etc... When considering the use of SOFC, the power plant efficiency is expected to increase especially when CO<sub>2</sub> capture is accomplished. Hence, the integration of SOFC in large scale power plants, whose economic applicability in such configurations and size has to be proven, would represent a very attractive option, but, according to the economic analysis, this technology will be suitable if relevant research activities and investments will improve SOFC costs and reliability.

# STUDY AND DEVELOPMENT OF NEW POWER GENERATION TECHNOLOGIES FOR GEOTHERMAL LOW ENTHALPY RESOURCES

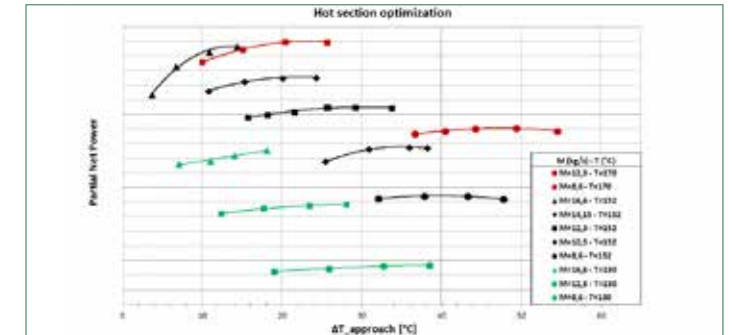
Alessio Tizzanini - Supervisors: Macchi, Campanari

The recent international focus on the value of increasing renewable energy supply highlights the need for reevaluating all alternatives, particularly those that are large and well-distributed. In this context, low enthalpy geothermal water dominant fields (with a brine temperature ranging between 130°C and 170°C) represent a high potential energy source for the electricity generation. The most efficient and cost-effective way to exploit this type of reservoir is based on the use of binary ORC cycles. In 2007 ENEL acquired the rights for the exploitation of four low enthalpy geothermal fields located in Western United States, which are expected to add about 150MW of electric capacity in the next years. Currently, two ORC cycles are already in operation. The purpose of this work was to select, design and demonstrate an advanced ORC technology to be applied to the exploitation of water dominant geothermal resources acquired by ENEL. The main targets to be reached via this new technology were: (i) high performance in terms of maximum power, in order to maximize the annual energy production for a certain geothermal source and (ii) high operating flexibility in terms of negligible performance decline due to external condition

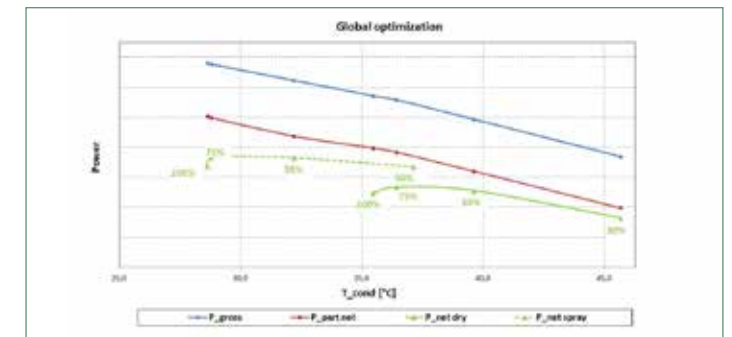
variability, such as brine temperature and mass flow rate, as well as environmental air temperature (flexibility is also a key-point for a future integration of binary plants with a solar field). During the preliminary selection of the working fluid and cycle configuration, carried out in collaboration with Massachusetts Institute of Technology and Politecnico di Milano, different Rankine cycles using hydrocarbons or refrigerant as working fluid were extensively studied and optimized in order to maximize the overall conversion efficiency. This analysis allowed the assessment of both subcritical and supercritical cycles and showed that in a supercritical cycle the possibility to operate outside the fluid saturation curve during the heat addition phase guarantees a higher operational flexibility compared to subcritical cycles. Results pointed out that, in the considered range of geofluid temperature, the best ORC configuration is represented by the supercritical ORC cycle using a refrigerant as working fluid. Based on the theoretical analysis results, it was decided to demonstrate the identified advanced, high efficiency binary cycle at the pilot scale (500 kWe). This activity was developed in the framework

of a collaboration agreement between ENEL, Politecnico di Milano and Turboden. The power plant was built at ENEL's experimental area in Livorno (Italy), and an extensive experimental activity, which lasted more than 700 hours, was carried out in 2012. Due to the flexibility of the experimental facility, a wide range of brine temperature and mass flow rate was simulated, thus testing the application of the supercritical ORC technology to different types of low enthalpy geothermal resources. Moreover, experimental activities covered the Winter and Summer period, thus also the influence of the ambient conditions on the ORC performance was assessed. The experimental data obtained were analyzed in order to: (i) validate the design criteria of the main components of the cycle and thus reduce the risks related to the evaluation of the studied technology on the full scale, (ii) check the nominal cycle performance, (iii) assess the reliability of the thermodynamic database available for the working fluid, (iv) optimize the cycle performance and verify the optimal operating parameters for different operating conditions (see figures 1 and 2), (v) verify the thermal stability of the working fluid, (vi) verify the control system stability for different operating conditions,

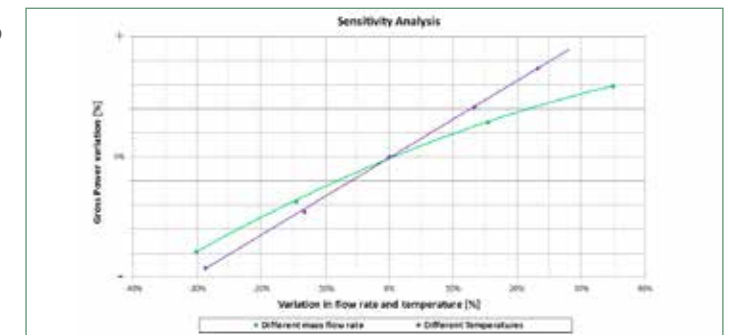
(vii) assess the reliability of the most critical components of the cycle, (viii) carry out a sensitivity analysis of the supercritical ORC performance as a function of the geothermal brine characteristics (see figure 3). Expected performance were experimentally confirmed. A detailed model of the power plant was developed via Aspen Plus and Aspen EDR. The model was validated on the basis of experimental data, and resulted to be consistent with them, thus demonstrating the reliability of the codes and thermodynamics libraries used. The experimental results showed a high performance level in terms of power production (a specific work higher than 44kJ/kg<sub>BRINE</sub> for the full scale application, e.g. for the 10MW scale) and a high operating flexibility (good performance for all the considered values of brine temperature and mass flow rate). Thus, the developed technology was demonstrated to be commercially competitive.



1. Hot section optimization for different values of temperature and mass flow rate of the geothermal resource



2. Hot section optimization for different values of the condensing pressure/temperature



3. Sensitivity analysis of the ORC performance as a function on the geothermal resource characteristics



# CONTROL STRATEGIES, FAULT DETECTION AND DIAGNOSIS OF RENEWABLE ENERGY SOURCES SYSTEMS

**Emilia M. Visek** - Supervisor: **Mario Motta**

According to IEA (2011) less than 20% of energy was produced by renewable resources. The field of exploitation of these resources interferes abundantly with research and scientific world and the development of renewable energy sources systems is accelerated. Increasing of renewables usage can be accomplished by developing new methods and new technologies or by polishing the ones existing.

Large amount of energy is wasted in building systems because of unsuitably installed equipment, incorrectly implemented control algorithms, missing, failed or non calibrated sensors and inappropriate maintenance of systems. Wasted energy can be reduced by applying predictive control strategies, fault detecting techniques for system and sensors and by optimizing the diagnosis of the building systems. Fault detection and diagnosis – FDD – is engaged already for decades in lots of research fields like automotive, aerospace, manufacturing, national defense, nuclear and so on. In the last decade predictive control strategies and techniques together with FDD applied to HVAC systems expanded the research interest due to large saving possibilities which could be achieved. However, ample

research still needs to be done to develop new methods or to convert the ones existing in other fields in order to match the requirements of HVAC systems. Much of the research and development is performed in the universities and national laboratories while commercial tools are only beginning to merge the markets.

This research purpose is to identify and combine known and highly developed techniques for control and FDD with new HVAC system (solar cooling and a heat pump); to prove the effectiveness and applicability of the methods but also to adjust them in order to be used for the specific systems proposed. The efficiency of the systems is evaluated in terms of methods used. Conclusions are drawn based on simulation of TRNSYS model of a solar cooling system with absorption chiller in the case of controls. The controls applied are programmed in Matlab and Simulink connected to TRNSYS Simulation Studio. For the fault detection parts the conclusions are drawn based on methods programmed in Matlab and validated using laboratory measurements of a reversible heat pump subsystem in a test stand.

A trivalent renewable energy sources system refers to a system which converts direct or indirect solar to thermal energy,

respectively cooling, space and domestic water heating. Starting from the assumption that energetic and economical losses can be reduced by predictive control strategies and techniques and fault detection and diagnosis I defend the following challenges:

- Identify methods of control from sensitivity, quickness of reaction and complexity point of view;
- Spot the influences on the performances and degradations of HVAC's when using different control techniques;
- Distinguish possible failures and techniques to avoid, adjust and detect them;
- Spot the influences of failures and also of using detection methods on HVAC's performances.

Other benefits of correct and predictive control and fault detection methods applied to HVAC's are that it would improve the reputation of the producers and it could enhance further development of the technologies under discussion. This PhD study is structured in 2 main parts: part A regarding the control strategies and part B regarding fault detection and diagnosis.

The objective of part A regarding controls was accomplished by comparing and analyzing 3 control methods: on/off, PID

and fuzzy PID. The reasoning for this choice is not random, in fact on/off is the most used method and the major problem identified is that the on/off cycling affects the reliability of system components and accuracy of control. Instead PID control improve the system reliability and accuracy, but the performances are depredated due to the fact that the parameters applied are fixed and don't permit the flexibility of control when condition of running the HVAC system are changing. It reacts slowly when system is transient and it proved time consuming to adjust the parameters which define the method. Therefore, arrives the need to identify robust way of adapting the parameters and fuzzy logic has the proper characteristics to accomplish the need. This strategy allows non-linearity and disturbances in the system, is a linguistic based method and requires a-priory knowledge of system possible outputs and needs. I generalized an optimum strategy to adapt PID parameters using fuzzy logic for a solar cooling system. Actually this method proves to be a compromise between *accuracy* and *reliability*, *quickness of reaction* and *range of applicability*. The assertion from which I started when defining part B of my work was that during the running period of a HVAC system the efficiency and reliability can decrease for unknown reasons, although the desired output is achieved with the same accuracy all the time. This is a result of highly developed control strategies and techniques which shade some failures. They are called hidden

because they are difficult to determine, mostly at the time when the user will receive the energy consumption bill. The sensor measurement failure is of such a kind.

The goal is to identify and provide an adapted method to be used in proactive control procedure, in the case a sensor is failing. This can be thought later on as an automated fault detection and diagnosis and prognostics procedure. I tested some sensor signal reconstruction techniques, widely used in other fields: principle component analysis, fuzzy principle component analysis and complex fuzzy principle component analysis. Prior to analyze the methods, an evaluation of the impact of failure on system performance and reliability of the methods is provided. The application consists of several tests on a reversible heat pump subsystem on a test stand (HPTS) in Emerson Climate Technologies, Mikulov, Czech Republic. The failure was simulated by moving one sensor from one part of the system to another where the difference of measurement was low enough not to damage the system but still detectable. The failed sensor was doubled in both states: failure and non-failure in order to be able to permanently monitor and analyze correctly the system behavior. The results of evaluation shown that the 3 methods proposed are eligible for use in HVACs. PCA shown less accuracy in reconstruction and less computational effort, FPCA shown more accurate but also more computation effort is needed, while CFPCA doesn't show improvements

compared to FPCA but is even more computational requiring. However, because of data clustering characteristic is expected that FPCA and CFPCA, perform better in non stable conditions than PCA. Considering that the calculation of reconstructed signal is based on non failed data, the hypothesis of not having available measured non failed data occurs. In this case usage of extrapolated data from measurement instead of measured non-failed proves compliance if the new data is calculated properly for each condition of running the system. The offline analysis of the experimental results showed that ~3% of efficiency loss could be avoided if the reconstructed value would be used in the control mechanism instead of failed sensor reading. Further on, the reconstructed value can be compared with reading value and failure announced. This PhD is catching one track of failure possibility and 3 failure detection methods. In reality during the lifetime of a HVAC system a lot of interconnected failures occur and many other detection methods can be used. Thus it is recommended that a database of possible issues, failure, performance degradations and their correlations is created especially when a new product is to be released on the market. Existence of such database is the keystone for application of more complex methods for failure detection.

# STUDY OF INNOVATIVE TECHNIQUES AIMED AT REDUCING ENERGY CONSUMPTION IN DOMESTIC REFRIGERATION SYSTEM

Matej Visek - Supervisor: Cesare Maria Joppolo

Cold domestic appliances consume approximately 15% of residential electricity consumption which accounts for remarkable 122 TWh/year only in EU. Thus governments all around the world are promoting energy efficiency and are strengthening energy consumption standards in the domestic refrigeration field. Largely diffused initiative is energy labeling which informs customers about energy efficiency of the products. The most popular domestic refrigerators on the market are the combined refrigerator-freezer appliances (2 doors) which are composed of two compartments with very different operating temperatures; freezer compartment (FC) operating at  $-18^{\circ}\text{C}$  and refrigerator compartment (RC) at  $4^{\circ}\text{C}$ . Marketed appliances (except the two compressors ones) are cooling both FC and RC by evaporating refrigerant at single temperature. Hence high temperature lift during RC operation is causing significant thermodynamic losses. Innovative sequential dual evaporator (SDE) circuit operates FC and RC cooling in alternative mode and allows two evaporation temperatures with single compressor. High evaporation temperature during RC operation increases

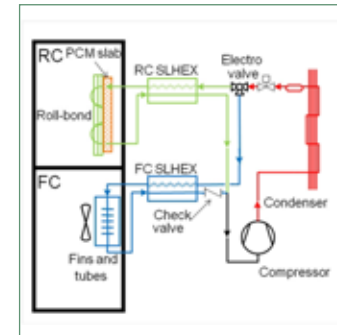
compressor COP and improves overall efficiency of the appliance. The principal problem of the SDE system is an extremely large cooling capacity provided by volumetric compressor and decreased heat transfer rate to the evaporator at increased RC evaporation temperature. Hence variable speed compressor is usually utilized to decrease cooling capacity and forced convection fan is employed in the RC to increase heat transfer rate to the evaporator. However forced convection has negative effect on the quality of the fresh food stored in the RC. Therefore two innovative refrigeration circuits based on the SDE technology employing variable speed compressor and preserving natural convection heat transfer in RC were proposed in this PhD activity. The first concept was to place phase change material in contact with visible RC evaporator and freeze it by high cooling capacity. Then the PCM can absorb heat load from the RC continuously at much lower natural convection heat rate. In addition to the positive effect on the fresh food preservation, also the RC air temperature is much more stable and resistance of the RC to grid power failure is improved. Selection of PCM temperature has a strong effect on the amount of heat being absorbed

from RC air and also impacts the evaporation temperature. PCM has to meet criteria such as compatibility with food environment, low supercooling/ superheating effect, cyclic stability, availability, cost and many others. One of the promising fluids meeting many criteria is pure water. Phase changing temperature  $0^{\circ}\text{C}$  gives high potential for increasing RC evaporation temperature but limits heat absorption rate from RC air.

The overall SDE appliance COP depends on the COPs of individual compartments and on the RC heat load ratio ( $x$ ).

$$COP_{SDE} = xCOP_{RC} + (1-x)COP_{FC}$$

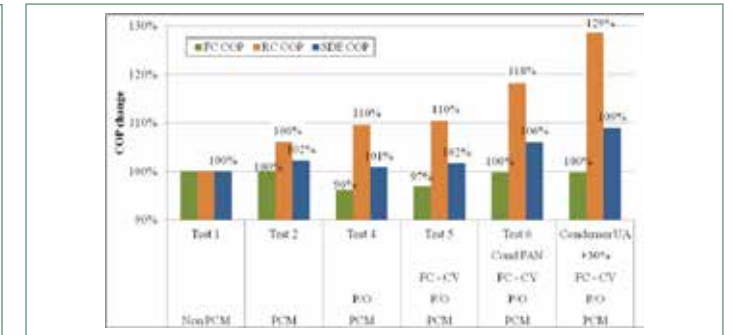
The higher the RC heat load ratio the closer is the system COP to the higher RC COP. Hence the second conceptual idea was to implement supplementary loop attached to the freezer liquid line, which by passing through RC PCM can additionally subcool liquid refrigerant and shift load from the FC to RC. The idea was considered innovative and patent application was submitted. The two innovative concepts were turned into two bottom-mount refrigerator-freezer appliance prototypes. The first prototype included SDE circuit with PCM pocket in RC directly attached to one side of the



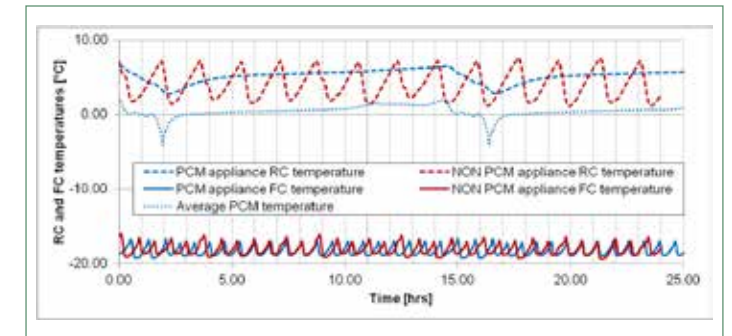
1. SDE-PCM refrigerator-freezer concept

visible roll-bond evaporator is showed in Figure 1. The second prototype included also extra FC subcooling loop. Low thermal conductivity vacuum insulation panels were implemented in the RC walls to decrease compartment heat load and match it with small heat absorption rate of the PCM (water).

One of the disadvantages of the SDE circuit is a necessity for refrigerant mass charge migration between FC and RC evaporators. To deal with migration issues two components were added to the system. Electronic block valve was attached to the liquid line after the condenser to be able to perform pump out of the refrigerant from the evaporators. Check valve was placed on the FC suction line to avoid refrigerant back flow to the evaporator.



2. COP improvements of SDE-PCM versus simple SDE



3. Air temperature fluctuations for PCM and non PCM appliance

Experimentally measured energy efficiency of the prototypes at various setups was compared to the performance of the baseline SDE circuit without PCM as showed in Figure 2. The SDE-PCM concept showed significant improvement in the RC COP and overall SDE COP by up to 29% and 9% respectively. It was also understood that refrigerant migration components and

condenser design play essential role in reaching high efficiency. Air temperature fluctuations in RC were reduced in the SDE-PCM prototype and the RC compressor OFF period was extended from 1 hour to almost 13 hours, Figure 3. Wide support of Whirlpool Corporation during this research activity is duly acknowledged.

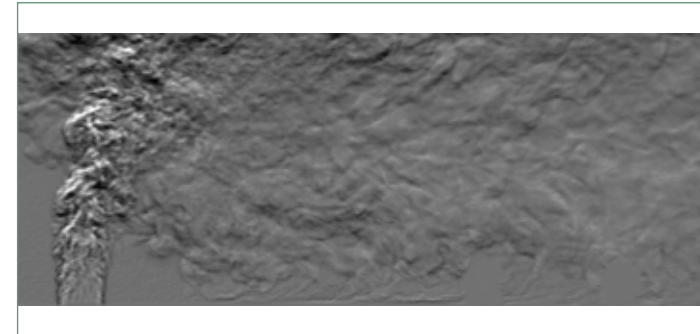
## A STUDY OF GASEOUS TRANSVERSE INJECTION AND MIXING PROCESS IN A SIMULATED ENGINE INTAKE PORT

Hua Wang - Supervisor: Aldo Coghe

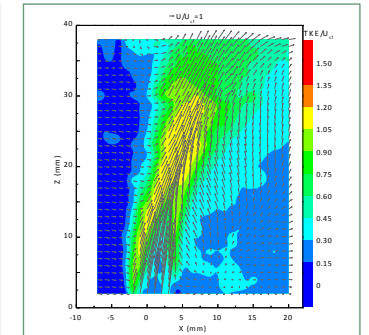
Transverse injection into crossflow has been studied over many years, due to its great relevance to many engineering applications, particularly in energy and propulsion systems, as a consequence of the near field enhancement of the entrainment of crossflow and superior molecular mixing, when compared with the free jet issuing into quiescent surroundings or co-flow jet. Recent applications in automotive industry include port fuel injection (PFI) for internal combustion engines fueled with non-conventional gaseous fuels, such as methane, hydrogen,  $\text{CH}_4/\text{H}_2$  mixtures or synthetic fuels. PFI of gaseous fuels has advantages in air-fuel mixing compared with in-cylinder direct injection, since it has been proved that in-cylinder direct injection may be affected by incomplete mixing due to the short available time in the speed range 1000-5000 rpm. In this study, the flow field resulting from injecting a gas jet into a crossflow confined in a narrow square duct has been studied under steady regime using both experimental and numerical methods. A transparent duct is built, intended to simulate the intake port of an internal combustion engine fueled by gaseous mixture, and the jet is issued from a round nozzle.

Schlieren imaging, laser Doppler velocimetry (LDV) have been applied for the experimental study as well as hot wire anemometry (HWA). The schlieren images show that the relative small size of the duct would confine the development of the transverse jet, and the interaction among jet and sidewalls strongly influences the mixing process between jet and crossflow. The mean velocity and turbulence fields have been studied in detail through LDV and HWA measurements, at both the center plane and several cross sections. Fig.1 shows the schlieren image at one representative condition while Fig. 2 gives the corresponding velocity and turbulence kinetic energy at the center plane of this duct for the same condition. Several important phenomena have been identified with these techniques and analyzed in depth, including the well-known counter rotating vortex pair (CVP), which starts to appear at the jet exit section and persists far downstream contributing to enhancing mixing process. Again, it has been observed that the confinement from the duct plays a critical role in the development of flow field, particularly when  $R$  is high. It stops the transverse development of jet, forcing the jet to move laterally. The

mixing is greatly influenced by the confinement, since the transverse movement of CVP is also confined. In addition, jets of different gases have been investigated with various injection orientations, aiming to fully understand the behaviors of transverse jet and the mixing process in the simulated intake port under wide practical conditions. Particularly, the jet injection against crossflow has been found favorable in this study. The results show that the injection direction can influence the flow field remarkably, while the effect of injected gas is negligible, when the appropriate scaling is applied. Moreover, a numerical study has been performed as well with FLUENT, which shows well agreement with the experimental results acquired. The numerical results could present the concentration field, and consequently directly show the mixing process between the jet and the crossflow. According to the author's knowledge, this is the first study concerning gas jet injection into confined crossflow, attempting to simulate the gaseous fuel-air mixing process inside the intake port of a PFI engine using gaseous fuel. A comprehensive description of the flow pattern of jet into confined crossflow, under various injection



1. Instantaneous schlieren images of jet into crossflow:  $R=6.1$ ,  $U_{ci}=1.7\text{m/s}$ ,  $\text{CO}_2$  injected, normal injection ( $R$  is jet to crossflow momentum flux ratio)



2. Mean velocity vectors and TKE field at center plane,  $R=6.1$ ,  $U_{ci}=1.7\text{m/s}$ , air injected, normal injection (TKE: turbulence kinetic energy, defined from the RMS of velocity measured by LDV)

conditions, has been obtained from the study. The main outcome is that different mixing strategies may have sensible effect on the mixture formation and the related in-cylinder combustion process and thus fuel gas injection should be optimized to improve the overall engine performance.

# DIRECT METHANOL FUEL CELLS MODELING: MASS TRANSPORT PHENOMENA AND ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY

Matteo Zago - Supervisor: Renzo Marchesi

Direct Methanol Fuel Cells (DMFC) are a promising energy source for portable and automotive applications, mainly due to the direct use of a liquid fuel and low emissions. However the widely use of the DMFC technology is still hindered by some technological issues, among which water management is one of the most important. Water crossover through the membrane may cause two problems named anodic water consumption and cathode flooding. Moreover water management can affect DMFC lifetime, that is limited by several interconnected degradation phenomena. The only way to monitor the system internal losses during real operation is the Electrochemical Impedance Spectroscopy (EIS). Despite the potentialities of this in situ measurement technique, the analysis of experimental observations is still object of discussion. In the literature, the interpretation of impedance spectra has mostly been carried out by means of equivalent electric circuit method (ECM), but in this way only few useful qualitative information are achieved.

This work aims to propose a combined experimental and modeling analysis in order to provide an insight into the basic principles regulating water transport and impedance

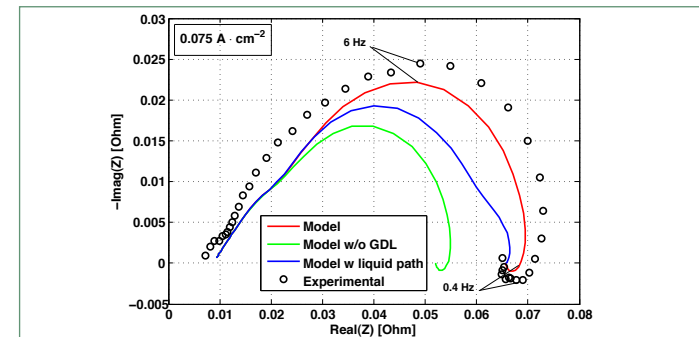
behavior in DMFC.

From the experimental analysis of water flux at cathode outlet, that has been carried out in a wide range of operating conditions and with different configurations of both anode and cathode gas diffusion layer (GDL), it is possible to presuppose the main involved phenomena regulating water management. Subsequently the proposed interpretation has been implemented in a DMFC model. In particular the water crossover through the membrane is considered as the sum of electro-osmotic drag and liquid diffusion and convection, while the water crossover through the membrane, along with that generated in the cathode catalyst layer, are transported through the cathode GDL by gas diffusion and liquid convection. Instead flooding effects are modeled considering two contributions: superficial obstruction, due to the condensation of drops of water on GDL surface facing the channel, and bulk pores obstruction, due to the liquid flow that obstructs GDL pores. To take into account flooding effects two suitable correlations were developed.

The developed model has been validated on the entire data set (264 measurements points) with respect to three different typologies of measure

at the same time: performance, water transport and methanol cross-over. This triple validation constitutes an innovative aspect in DMFC modeling: in the literature more detailed models can be found, but none of them is validated on different typologies of measure, considering such a wide range of operating conditions. The model reproduces experimental data with high accuracy and therefore the proposed interpretation of DMFC water transport is reliable. Moreover the validated model provides an accurate estimation of local fluxes and concentrations, that is necessary to develop a model for a quantitative interpretation of DMFC impedance.

Therefore, after the complete characterization of DMFC steady-state operation, a systematic experimental analysis of anode and cathode EIS has been carried out. This investigation aims to elucidate the main relevant phenomena governing impedance behavior and to provide an insight into the development of quantitative interpretation models. Initially, an existing interpretation methodology has been adapted and locally integrated into the previously developed DMFC model. The cathode simulations show good agreement with experimental data, while the anode ones present



1. Comparison of the simulated and measured anode EIS

inconsistencies, mainly due to complicated two-phase mass transport through the GDL and proton transport losses within the catalyst layer. For this reason a new approach has been adopted and a detailed physical model of anode impedance has been developed from scratch. Particular attention has been given to the understanding of the mechanisms regulating liquid convective fluxes. The GDL is not assumed to be always flooded with fully liquid pathways; in fact recent studies show that liquid paths are intermittent and breakthrough locations change with time. These flow visualizations suggest that the liquid transport within the GDL is a process of capillary pressure buildup and breakthrough at the interface of GDL intersecting fibers. When the liquid pressure exceeds the breakthrough value, the liquid expands rapidly through this interface until the

fluid contacts the next fiber intersections interface. Then the process of pressure buildup and breakthrough begins again. When the fluid reaches the electrode interface, the liquid is quickly removed from GDL pores, that become empty. The dynamic of liquid emergence and detachment from GDL surface is very fast and the liquid accumulation terms in the GDL are present only for perturbation frequencies higher than tens of Hertz.

The transient perturbation solution of the DMFC anode can be obtained by linearizing the system and perturbing each of the variables with a sufficiently low sinusoidal disturbance, in order to obtain a system of linear equations for the complex perturbation amplitudes. Fig. 1 illustrates simulation results (red line): there is a good agreement with experiment and the model is able to reproduce the linear branch due to proton

transport limitations. The green line represents impedance simulation without the effect of GDL: its contribution has a relevant influence even at low current density. Instead the blue line shows impedance simulation performed with the assumption that GDL is always flooded with fully liquid pathways: the model predictions are inconsistent with the experiment and confirm that liquid convection through the GDL is an intermittent phenomenon.

The developed model has been also validated on experimental data of a DMFC with micro porous layer (MPL) at anode side. Model results evidence that the inductive behavior is enlarged by the presence of MPL: the increased mass transfer resistance through the GDL amplifies the oscillations of methanol and water concentrations at GDL-electrode interface enhancing the phase delay between voltage and current.

Finally the physical model of anode impedance has been used as a diagnostic tool to investigate the origins of few temporary degradation effects. In particular the decrease of inductive loop and the extension of linear branch might be caused by a reduction of methanol concentration and electrode dehydration, respectively.



## EXPERIMENTAL AND THEORETICAL STUDIES ON ULTRAIINTENSE LASER-DRIVEN ION ACCELERATION

**Alessandro Zani** - Supervisor: **Matteo Passoni**

The main topic of my thesis work deals with the study of ion acceleration driven by ultraintense and ultrashort laser pulses, having power densities (intensities) in excess of  $10^{18}$  W/cm<sup>2</sup> and durations between  $10^{-12}$  and  $10^{-14}$  s. In such regimes of process parameters, the interaction between laser pulses and matter evolves with a dynamics dominated by nonlinear relativistic effects. Among the consequences arising from the interaction in this unconventional regime, the experimental observations have shown the emission of both radiation and matter having peculiar properties, and known as laser-plasma "secondary sources". In particular, the emission of multi-MeV ions has been observed when linearly polarized laser pulses ranging in intensity from  $10^{18}$  to  $10^{21}$  W/cm<sup>2</sup> impinge on solid foils with thicknesses ranging from few nm to tens of  $\mu\text{m}$ . The mechanism able to account for most of the so far recorded experimental results is known as Target Normal Sheath Acceleration (TNSA). The first cycles of the pulse create a blow-off plasma where part of the total pulse energy is transferred to a population of target electrons via some collisionless absorption mechanisms, giving them an average energy of the order of

tens of MeV. These electrons are able to travel through the target reaching the non-irradiated side and, expanding in vacuum for a Debye length (of the order of  $\mu\text{m}$  for these energies), they set up a longitudinal electric field of the order of MV/ $\mu\text{m}$ . This field is maximum around the solid-vacuum interface: hence it promptly ionizes and accelerates hydrocarbon and H<sub>2</sub>O contaminants located on the target surfaces. Protons, being the particles with the most favorable charge-to-mass ratio, gain most of the field energy and are more efficiently accelerated with respect to heavier ions. The typical recorded proton spectra are continuous and exponentially distributed with a cut-off energy. So far the highest maximum proton energies ever obtained are around 60 MeV and have been obtained exploiting picosecond duration petawatt laser systems. Moreover recent results have reported 40 MeV protons obtained exploiting the same intensity value but with a femtosecond 200 TW laser pulse. This result is in particular of great interest, since 100s TW laser class guarantees compact dimensions ("table-top") and lower costs with respect to huge and expensive PW class facilities. The laser-accelerated proton bunch has been observed to own high beam quality thanks to

small transverse and longitudinal emittance,  $< 0.004$  mm mrad and  $< 10^{-4}$  eVs, respectively. The foreseen improvements in these beam properties might lead to the application of ion sources in several fields. The most promising ones deal with proton radiography of extreme systems, fast-ignitor proton-driven scheme of inertial confinement nuclear fusion and medical applications such as hadrontherapy and radioisotopes production for PET. Every cited application of laser accelerated ions requires the optimization of one or more beam parameter and in general these are different passing from one another. To optimize a quantity a general procedure would be to get a fundamental theoretical understanding of the system, combined with novel experimental approaches. My doctoral activity focuses the attention on one of proton beam parameters, that is to say the maximum energy. The goal is achieved by a two-steps methodology: first a theoretical study of maximum proton energy dependencies on laser properties in TNSA has been performed. The second part of the project has dealt with an experimental activity aimed to improve TNSA mechanism in a smarter fashion, i.e. not demanding further laser performances but

properly engineering the target properties at the nanoscale. During this work the production, characterization and testing of innovative targets for TNSA have been tackled.

To achieve the first goal of my PhD project, an extended theoretical study of TNSA has been carried on. First, six different analytical models published in literature have been classified (as "fluid" "quasi-static" or "hybrid" approach) and implemented in order to calculate maximum ion energy as a function of process parameters: the lower the number of external dependencies the more accurate the prediction. In particular we have calculated the maximum energy with all the analyzed models using the external inputs reported in an experimental database, where several data belonging to different experiments in literature are reported. We have been able to perform the comparison between models with respect to the capability to predict the experimental maximum ion energy data as a function of laser intensity, which is extremely important to extrapolate guidelines for future experiments. As a result, the so-called quasi-static approach appears to better reproduce proton cutoff energy from experiments, since in those models the physical description is limited to the very first instants following laser-target interaction, i.e. when the electric field is established and the most energetic protons are accelerated. One of the model, which I have contributed to develop has been then adopted to study in detail the non-trivial

problem of maximum energy dependency on laser intensity. The resulting scaling have to be considered after the convoluted dependence on both laser intensity and laser energy which are not independent. The key role of these two parameters have been enlightened by the comparison of the model results with those from 2D-Particle-In-Cell (2D-PIC) simulations, and different scaling of maximum ion energy with intensity have emerged, by changing or not pulse energy content.

The second aim of my PhD has started with a feasibility study for the realization of a multi-layered target configuration composed by a solid foil and a low density coverage, assisted by 2D and 3D PIC simulations. In fact it has been recently observed how laser energy absorption is enhanced by reducing the density of the interacting material down to the order of critical density ( $\sim \text{mg}/\text{cm}^3$ ). A campaign devoted to the production with pulsed laser deposition of such low density carbon films (so called "foams") on different substrates depending on their employment (Si for characterization and Al for acceleration experiments) has been carried on. Morphological and structural characterization, performed by scanning electron microscopy and Raman spectroscopy, respectively, have revealed the nature of carbon films being very open and porous down to tens of nm, being the size of the elementary constituents of the foam. The measurement of mean density has been carried on by means of the classical technique of quartz-crystal microbalance (QCM). Since this

characterization is crucial for our purposes, we have developed a novel and more reliable method to measure film density exploiting energy dispersive X-ray spectroscopy, which have allowed to confirm the QCM results within a limited range of deposition parameters and to address foam densities to values nearly three orders of magnitude lower than solids typical values. An experimental campaign at the UHI100 laser facility at CEA Saclay has allowed us to collect a wide set of maximum proton energy data accelerated from our novel targets, whose preliminary evidence is the existence of different interaction regimes depending on the laser and foam parameters. At intensities well below the limit of  $10^{18}$  W/cm<sup>2</sup>, widely reported in the literature as the TNSA onset, proton maximum energies with foam have been measured in excess of 1 MeV. That proves that by exploiting the smart target configuration aim MeV regime of proton acceleration becomes accessible already with  $10^{16}$ - $10^{17}$  W/cm<sup>2</sup> laser intensities.