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:

Astorino Sonia	Sound absorption measurements with sound intensity method. Investigations at normal and oblique incidence.
Balandeh Mehrdad	Hierarchical Quasi-1D Nanostructures for Photoelecrochemical Hydrogen Production.
Baricci Andrea	A combined experimental and modelling approach for the improved characterization of high temperature pem fuel cells.
Biserni Erika	Silicon Nanostructures for Energy Applications.
Cimina' Susanna	An experimental study on fluid dynamics in straight and bend rib-roughened channels
Cornolti Luca	CFD Modelling Of Turbulent Premixed Combustion In Spark-Ignition Engines.
Eremed Wondwossen Bogale	Increasing energy recovery of waste-to-energy plants.
Garcia Ferre Francisco	Radiation tolerant nanoceramic coatings for lead fast reactor nuclear fuel cladding.
Ghadirzadeh Ali	Nanostructured Oxide Semiconductors for Direct Solar Energy Conversion: Photovoltaics and Water Splitting.
Mandelli Stefano	Strategies for access to energy in developing countries: methods and models for off-grid power systems design.
Moschetti Roberta	Building sustainability assessment and rating: an Italian objective system proposal.
Pistocchini Lorenzo	Development of a Fixed Bed Quasi-Isothermal Adsorption Dehumidifier: from Concept to Optimization, through Experimental and Theoretical Investigation.
Prencipe Irene	Advanced materials for novel laser-driven ion acceleration schemes.
Rocco Matteo Vincenzo	Primary Exergy Cost of goods and services: an Input - Output approach.
Sartori Alberto	Reduced order methods: applications to nuclear reactor core spatial dynamics.
Torelli Roberto	Novel Approaches for CFD Modeling of Diesel Engines.

Energy and Nuclear Science and Technology - 26° ciclo

Gondoni Paolo	Nanostructured Transparent Conducting Oxides for Advanced Photovoltaic Applications

Energetica - 24° ciclo

Parissenti Guido	Waste atomic separation and raw material recovery by application of plasma technology.

Their research and most significant results are presented in the following pages.

SOUND ABSORPTION MEASUREMENTS WITH SOUND INTENSITY METHOD. INVESTIGATIONS AT NORMAL AND OBLIQUE INCIDENCE

Sonia Astorino - Supervisor: **Prof. Livio Mazzarella**

Information on sound absorption and sound reflection properties of materials is of interest for many practical applications both in architectural and industrial acoustics. The characterization of the angle-dependent absorption properties is required for instance to carry out *a priori* analyses of indoor acoustic quality or noise reduction, with the use of acoustic simulation software. These practical needs are the reasons behind the development of several techniques for the measurement of sound absorption over the years, for different kinds of incidence (normal, oblique and random).
This study focuses on the techniques employed for analysis at normal and oblique incidence, with particular reference to the *sound intensity method*. Potentialities and limitations of this procedure are examined carrying out both experimental and numerical investigations.
The first part of the thesis illustrates the analyses conducted at normal incidence. Based on local plane wave propagation assumption, the sound intensity method is characterized by a simple test setup and an easy and practical implementation. Experimental tests for the determination of the normal incidence sound absorption coefficient have been carried out with the traditional sound intensity probe in a semi-anechoic environment. Measurements results in terms of absorption coefficient have been validated by means of comparison with the outcomes of both a macroscopic empirical predictive model and the standardized impedance tube method. Some differences have been observed at low frequencies. The determination of two specific sound field indicators from the acquired signals has also highlighted that both these descriptors can be helpful to perform initial evaluations on measurements carried out with the sound intensity technique.
To complete normal incidence investigations the thesis work includes the development of numerical simulations based on the Finite Element Method. The analyses are conducted at low frequencies with the commercial software COMSOL Multiphysics. First, a virtual impedance tube has been realized to assess the accuracy in the modeling of the sound absorbing material by comparing numerical values in terms of absorption coefficient with experimental results of the real impedance tube. Successively, we have performed preliminary simulations on two different models of the setup used for the measurements with the sound intensity technique, which have then been numerically improved realizing a third model of the computational domain. For all the simulations, it is chosen to perform three-dimensional acoustic analyses so that the effects of the finite dimensions of the rectangular sample can be correctly modeled and taken into account. Sound pressure and particle velocity numerically computed above the sample have been post-processed with different analytical sound field models: the sound intensity method, the Image Source model and the Di and Gilbert model. Differently from the former, the two impedance-based global models of the sound field take into account spherical wave propagation from a point source. For the analysed configuration, results show that the differences between the calculated absorption coefficients are pronounced especially at low frequencies. However, it has been also proven that the observed divergences decrease reducing the probe-sample distance. As a matter of fact, the developed simulations have provided not only a tool for the verification of the subsequent experimental measurements at oblique incidence, but also the possibility to analyse the sound field above the specimen in a point nearer the sample surface than that measurable in practice with the sound intensity probe. In this regard, results show that with a decrease of the probe-sample distance the absorption coefficient estimated under local plane wave assumption is less affected by the sound field characteristics.
The second part of the thesis deals with experimental and numerical investigations conducted in order to estimate the oblique incidence sound absorption coefficient. It is worth noting that, without involving ratios of complex quantities, the intensity-based method has the advantage to be more robust for performing angle-dependent absorption measurements rather than impedance-based methods. The extension of the sound intensity technique to oblique incidence is presented reporting both the general formulation of the theory and the simplified algorithms for specular reflection assumption existing in literature. The former entails the use of a three-dimensional sound intensity probe. Therefore, a 3-D sound intensity probe configured in a 6-microphone array and a calibrator for matching the microphones in amplitude and phase have been developed for the investigations at oblique incidence. The thesis reports a detailed description of the two, together with a qualitative evaluation of design improvements of the 3-D probe spacer. When a 6-microphone arrangement is used, different post-processing methods that can be employed to estimate sound intensity exist; the associated formulations for the application of interest have been derived.
Various experimental activities are performed using the newly developed 3-D sound intensity probe with the final aim of estimating the sound absorption properties of an acoustic panel at oblique incidence. These include some initial investigations on the performances of the 3-D probe. In detail, measurement campaigns to characterize the radiance patterns of both the three-dimensional and the traditional mono-axial probes have been performed in a totally anechoic environment; the analysis of the associated results has allowed a comparative evaluation between the probes. Successively, considerations on the comparison between the two instruments have been made in terms of experimental procedures and outcomes of the sound absorption measurements at oblique incidence. To this purpose, the specular reflection assumption has been adopted. It has been shown that scattering and diffraction issues inherent to the design of the developed 3-D probe itself negatively affect its outcomes. However, remarkable advantages regarding the use of the 6-microphone array compared to the mono-axial probe in the measurement of sound absorption at oblique incidence have been also pointed out.
In view of these considerations, some efforts have been made in investigating possible solutions aimed at improving the performances of the three-dimensional sound intensity probe. In this regard, we have carried out additional analyses considering two different approaches. The first is a mechanical optimization of the probe, entailing the minimization of the interfering objects near the sensors; predictable outcomes of this procedure have been qualitatively evaluated with a trial test at normal incidence. The second is related to the use of signal treatment techniques to improve the response of the self-assembled 3-D probe without changing its design. The main idea is to numerically compensate the interferences between the microphones and the effects of the presence of the fixture holding the sensors: a signal filtering procedure developed in collaboration with the Dipartimento di Elettronica, Informazione e Bioingegneria of Politecnico di Milano has been proposed with this intent. The application of the compensation filter on a preliminary test case has given globally satisfactory results. This constitutes the basis for some of the possible future developments of the thesis work.
Finally, following the same procedure used at normal incidence, FEM simulations have been employed both to model and verify the experimental tests at oblique incidence, and to carry out further analyses at low frequencies. The effects of different sound field models and smaller probe height on the numerical estimate of the absorption coefficient have been evaluated and discussed also for the oblique incidence case.

HIERARCHICAL QUASI-1D NANOSTRUCTURES FOR PHOTOELECROCHEMICAL HYDROGEN PRODUCTION

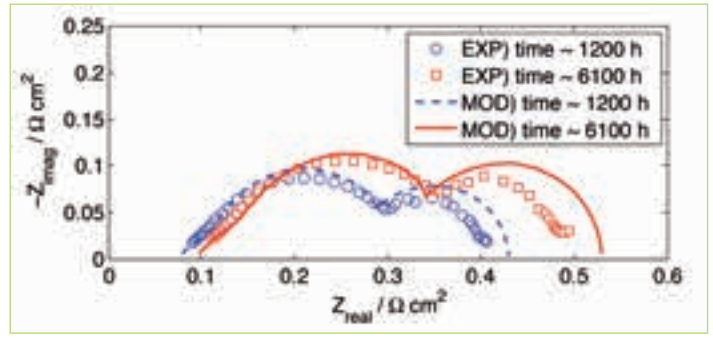
Mehrdad Balandeh - Supervisor: **Dr. Fabio Di Fonzo**

In the last decades there has been an increase in the solar energy efficiency and its contribution to the global energetic production. Although today one third of the world energetic demand is still composed by fuels, that are energy vectors which could be easily stored and moved. While there are no well-established solutions to satisfy the world's energetic request, the production of hydrogen via solar energy stands as one of the most promising solutions for the problem. The process of photoelectrochemical water splitting consists of using a solar-produced driving force to decompose water into its two constituents. This study aims to improve and optimize the efficiency of TiO_2/CdS and WO_3 photoanodes for water-splitting application. The host-guest approach involves decoupling of the optical path and water oxidation center and the electron transport to the substrate by depositing a thin layer of CdS onto a mesoporous TiO_2 host. A TiO_2 hierarchical nanostructured photoelectrode was sensitized with a thin layer of a low energy band gap material. Here cadmium sulphide was chosen due to its apt properties for photoelectrochemical hydrogen production application. The amount of CdS deposited on the TiO_2 scaffold was taken as the main parameter for the study and optimization of the device. The fabrication of the TiO_2 scaffold was performed via PLD technique to obtain hierarchical structures with high roughness factor and light-trapping properties; morphological and crystallographic studies on the TiO_2 substrates showed a nanocrystalline structure with enhanced transport properties thanks to the low density of defects and directional growth of the TiO_2 crystals. The SILAR sensitization technique was employed to deposit a uniform layer of CdS on the TiO_2 scaffold, in order to improve the absorption of the whole device in the visible range. The whole photoelectrochemical device is then completed with a platinum wire as the counter electrode and an electrolytic solution as the supporting electrolyte between the two electrical contacts. The results showed a maximum current density of 6.6 mA/cm^2 for hierarchical TiO_2/CdS which was around 35% higher than reference TiO_2/CdS photoanode made of TiO_2 nanoparticles. Moreover, fabrication and optimization of quasi-1D WO_3 nanostructures photoanode was performed. WO_3 was chosen as a photoanode for photoelectrochemical water splitting process due to its high stability against photocorrosion in acidic environment and also its low energy band gap. Hierarchical quasi-1D WO_3 thin film was deposited by using PLD technique and by tuning the deposition parameters, where hyperbranching and long range crystalline order was achieved. The hierarchical quasi-1D WO_3 photonodes showed efficient light absorption and internal scattering with improved charge collection efficiency despite the large thickness due to the mesoporous structure of the film. Hierarchical hyperbranched WO_3 nanostructures showed current densities up to 1.8 mA/cm^2 with an onset potential of 0.4 V vs RHE, which is significantly lower than the current state-of-the-art. These results are achieved due to the high electron recombination resistance and low charge transport resistance of the hyperbranched morphology. A deep analysis of the both photoelectrodes (TiO_2/CdS and WO_3) was performed to assess their optical, structural, morphological and photoelectrochemical characteristics by using following techniques: SEM and TEM images, Raman and PL spectroscopy, XRD analysis, UV-Vis spectrophotometry, Linear Sweep Voltammometry (LSV), EQE/IQE and Electrochemical Impedance Spectroscopy (EIS).

A COMBINED EXPERIMENTAL AND MODELLING APPROACH FOR THE IMPROVED CHARACTERIZATION OF HIGH TEMPERATURE PEM FUEL CELLS

Andrea Baricci - Supervisor: **Prof. Renzo Marchesi -** Coordinator: **Prof. Carlo Bottani**

Significant progress has been recently achieved in the field of polymer fuel cells (PEMFC) that has resulted in increased attention to this technology for energy conversion systems. Several automobile manufacturers are currently undergoing field testing of fuel cell vehicles and few of them have programmed commercialization within 2015. Not only automotive applications have generated interest in PEMFC research, but also stationary residential applications for combined production of electricity and heat.
The interest received by PEMFC technology for direct energy conversion is due to their unique features: high efficiency and power density, low emissions, fast start-up, fast response to load changes, modularity. Nevertheless, several issues have to be addressed yet: the lack of infrastructures for hydrogen distribution, the high cost if compared to competitors, the durability.
A significant cost reduction has been recently achieved by decreasing the loading of noble metals used as catalyst and by increasing the number of units produced. In this view, PEMFC durability is an additional tool to impact the cost: any improvement in fuel cell stability could mitigate the capital cost by distributing it over a wider life time. For this reason degradation of PEMFC components has received increasing attention over the past years. Many degradation mechanisms have been observed to affect the polymer membrane, *e.g.* thinning, or the porous layers, *e.g.* loss of hydrophobicity, but most of the degradation is generally attributed to the catalyst layers, specifically the cathode. Corrosion of the catalyst, corrosion of the support, loss of porosity or onset of heterogeneity are few of the effects of ageing that have been reported by experiments. Characterization of degradation is the crucial step before the proposal of improved materials or mitigation strategies, but unfortunately long term tests are costly and time consuming. In this sense, modelling and theoretical work are expected to assist experimental activity and facilitate technological progress.
The work focuses on durability of high temperature polymer fuel cells (HT-PEMFC) based on phosphoric acid doped polybenzimidazole. Differently from PEMFC that operate at 80°C, HT-PEM fuel cells work between 120 and 200°C and are interesting for stationary applications because of enhanced tolerance to fuel impurities and simplified water management. Unfortunately HT-PEMFC suffer additional problems that are related to the cathode: lower performance and lower durability than PEMFC, therefore efforts in research are motivated toward the understanding of cathode operation and ageing, in analogy with low temperature PEMFC.
The PhD thesis reports a detailed analysis of cathode operation in high temperature polymer fuel cells, taking into account both performance and durability and adopting a combined experimental and modelling approach. A 6100 hours degradation testing has been carried out on a commercial HT-PEMFC. It is reported that cathode is the most critical component for durability: the catalyst electrochemical active surface is observed to reduce to half of the initial value at the end of the test, causing a significant voltage degradation rate (10 $\mu V\ h^{-1}$). The evolution of the impedance spectra during ageing is analyzed by means of a physics-based model.
The conclusion is that about 30% of the degradation rate observed at 0.4 A cm^{-2} is not directly ascribed to a loss of electrochemical active surface, but it is due to increased mass transport.
Therefore the work analyzes oxygen transport in HT-PEMFC components. *Ex situ* characterization of porous media that constitute the Gas Diffusion Media is discussed. The results indicate that Knudsen diffusion constitutes approximately 50% of the mass transport resistance in the catalyst layer without phosphoric acid and 30% in the MPL. *In situ* analysis of mass transport in real operating conditions is carried out by electrochemical impedance spectroscopy and reveals that mass transport affects cathode operation.
Combination of *ex situ* and *in situ* experimental information is carried out by means of an advanced physics-based model validated on experimental data. The effect of phosphoric acid on mass transport is analyzed: simulations indicate that phosphoric acid floods the catalyst layer and causes low catalyst utilization at high current density. Since oxygen is forced to diffuse into the liquid electrolyte that floods the catalyst layer micro structure, the catalyst nanoparticles that are hardly accessible to oxygen (*i.e.* those in the inner core of the agglomerate) do not work at high current density. It is concluded that flooded agglomerate model is a requirement for HT-PEMFC models and average radius of spherical agglomerates has been estimated in 180 nm.
An innovative geometry for flooded agglomerate model has been presented and discussed: the macro pore cylindrical agglomerate geometry. From *ex situ* observations, mass transport in the catalyst layer is reported to occur over macro cylindrical-like pores and, in analogy, a 1D agglomerate geometry that resembles this observation is developed. The flooded agglomerate region is represented as a porous ring that encloses the macro pore. Consequently from this assumption, the geometry of the flooded agglomerate is measured *ex situ* and no model calibration is required. Flooded Agglomerate Model with cylindrical macro pore geometry is finally validated, in support of the physical consistency of flooded agglomerate model in HT-PEMFC.
In a final step, the improved model is applied to the analysis of ageing data. A literature review indicates two characteristics of degradation to be considered in the analysis: catalyst layer thinning and heterogeneity of ageing. Both effects succeed in reproducing the evolution of the impedance spectra during ageing (Fig. 1), but catalyst layer thinning predicts an improvement in proton transport across the catalyst layer that is not consistent with experiments. Heterogeneity of ageing has been studied on two scales: along the channel and across the catalyst layer. The results indicate that non-uniform current distribution induced by ageing is detrimental for HT-PEMFC performance, because the reaction is restricted in a reduced active volume where mass transport becomes critical. As a consequence, mass transport resistance in the active region is responsible for additional increase of the degradation rate.



1. Evolution of the Electrochemical Impedance Spectra recorded at 0.2 A cm-2 during the degradation test: experiments (symbols) and simulations (continuous line) considering the effect of heterogeneity of ageing.

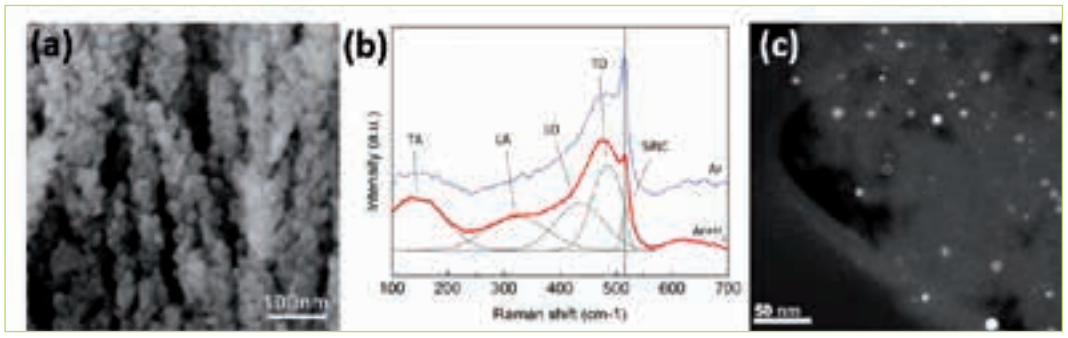
SILICON NANOSTRUCTURES FOR ENERGY APPLICATIONS

Erika Biserni - Relatore: **Prof. A. Li Bassi -** Correlatore: **Dr. P. Bruno -** Tutor: **Dr. M. Passoni**

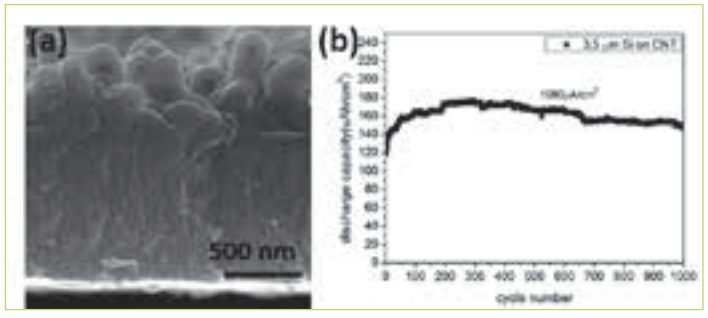
Being silicon the most widely used material in the electronic and photovoltaic industry, thanks to its abundance, low cost and non-toxicity, specific technology has been developed and deep knowledge has been acquired on its properties, especially at the bulk scale.
Only partially, however, have its properties at the nanoscale been investigated and exploited accordingly.
This dissertations reports the research activity done by the author at the Center for Nano Science and Technology (CNST) of the Italian Institute of Technology (IIT) and funded by IIT through a dedicated scholarship. Focus of the work is the synthesis and characterization of silicon nanostructured thin films and their engineering to make them suitable for specific energy applications in the fields of energy production and storage.

The silicon nanostructured films are prepared by Pulsed Laser Deposition (PLD) and characterized by suitable microscopic and spectroscopic techniques to understand their properties and allow for their tailoring by means of a good control over the film features –namely, porosity at the nanoscale and formation of nanocrystals. The synthesis heads for exploitation in innovative devices with a stronger relevance being given to silicon anodes for lithium-ion batteries. In addition, good confidence with the fabrication process opens the way for explorative studies on the properties of the material and the possibilities to tune them to make them suitable for application in photovoltaics and thermoelectrics.
Thanks also to a fruitful network of national and international collaborations, it was possible not only to study and engineer the material properties, but also, in the case of anodes for lithium ion batteries, to realize proper working devices.
Besides nanoporous silicon films, PLD allows to grow hierarchically nanostructured films composed of Si nanocrystals embedded in a columnar porous amorphous matrix, that can be of interest in various energetic fields, with Quantum-Dot photovoltaics being one of the most challenging ones.
Nanoporous silicon, in turn, can be successfully applied in the development of nanostructured porous silicon-based anodes for Lithium-ion batteries, which is the core activity of this dissertation.
In order to address power and energy demands of mobile electronics and electric cars, Li-ion technology is urgently being optimized by using alternative materials, with nanostructuring being a key means to open new opportunities in terms of energy density, high rate of charge and discharge, and better cyclability.
Graphite is commonly used as the standard material for the anodes of Lithium Ion Batteries (LIB), because of its low price, good performances and high processability. Silicon is a potential anode material for high energy density LIB due to its very high theoretical capacity (~3579 mAh/g), which is an order of magnitude beyond that of a commercial graphite anode.
However, the wide spreading of Si has to face two main concerns, i.e. volume expansion and the formation of a stable Solid Electrolyte Intephase layer.
The work reported in this thesis discusses the investigation of innovative solutions to address the two main concerns of silicon anodes in lithium ion microbatteries by means of suitably designed anodes made of amorphous nanoporous Si.
Such porous structures offer a large surface area to volume ratio, which can accommodate the large volume expansion associated with silicon lithiation.
Then, in order to promote the formation of a stable SEI layer and improve conductivity and mechanical stability, Carbon has been coupled to Si, either as a separate capping layer or as integrated in the Si film. In these composite anode architecture, the Si hierarchical nanostructure was deposited by PLD and C either by Chemical Vapour Deposition (CVD) or by PLD.
Thanks to coupling of silicon and carbon, all the proposed anodes show very good stability over cycling, even reaching up to 1000 cycles with very low capacity fade.

In a dedicated study conducted at the Karlsruhe Institute of Technology (KIT) in Karlsruhe, Germany, silicon-graphite anodes have been prepared by slurry-based processes, commonly in use in industrial battery manufacturing. Despite some technological issues related to the nanometric size of Si powders, Si-graphite anodes were fabricated and electrochemical tests showed good cyclability. Feasibility of partial substitution of Si for graphite with a drop-in approach in current productive processes has been proven, but further optimization is surely needed for what concerns slurry composition and fabrication process parameters.
In all cases, the approach to fabrication is driven by the need to minimize the processing effort, both in terms of number of steps required and of temperatures involved, so as to orient the work to possible up-scaling.
Moving to larger scale production, the dissertation involves also the fabrication of silicon-based anodes using methods and techniques typical of the industrial production.
On the way to large-scale fabrication of silicon-carbon anodes, this study can outline a starting point and a strategy for improvement.
Finally, nanoporous silicon can find application in the field of thermoelectric materials, since controlling the porosity provides a means to reduce the thermal conductivity of the material, which is one of the key figures to evaluate a thermoelectric material, while growing the film into an ordered columnar structure can in principle allow for good electronic transport.
Following this direction, the thermal conductivity of silicon films grown by PLD is characterized.



1. a) Scanning Electron Microscope image (taken in cross section) of a porous silicon algae-like film, b) its Raman signature, and c) an image of embedded nanocrystals evidenced by a Transmission Electron Microscope



2. a) SEM picture of a Si-C composite anode and b) an example of discharge capacity curve of a Si-C composite anode, reaching 1000 stable cycling

AN EXPERIMENTAL STUDY ON FLUID DYNAMICS IN STRAIGHT AND BEND RIB-ROUGHENED CHANNELS

Susanna Ciminà - Supervisor: **Alfonso Niro**

Forced convection heat transfer inside rectangular channels is a matter of interest for industry. Its involvement varies from compact heat exchangers to more critical applications such as turbine blade cooling.
During the design of compact heat exchangers, a high value of the surface-to-volume ratio is pursued; however, the increasing of this ratio beyond a certain value causes a worsening of the thermal performances. The increase of heat transfer area per unit volume causes the narrowing of the area as well as a lower gas velocity in order to maintain an acceptable pressure drop value. Both effects cause a weak turbulent or laminar flow, which is characterized by a lower convective coefficient which reduces the benefits derived from the increased area. To overcome this limit, designers have enhanced heat transfer by means of specially configured surfaces which can properly affect fluid-dynamics while maintaining cost-effectiveness and reliability. These configured surfaces use many passive enhancement mechanisms: periodic deflection of streamlines, interruption of the growth of the boundary layer, swirl, and flow destabilization. Moreover the surfaces also promote turbulence and contribute to increasing of heat transfer by several hundred percent, since their characteristic elements have sizes close to those of the structures to be stimulated.
In the present work, ribbed surfaces have been used. Enhancing heat transfer in these situations would mean the operating limits are increased and thus a more efficient and compact device is created.
In detail, concerning modern Gas turbine blades, to improve thermal efficiency and power output it is necessary to operate at high inlet temperatures or TIT (1100 - 1350 °C).
Nowadays the increasing of TIT has a limitation due to metal melting temperature, but recent studies have demonstrated that developments in achieving a better cooling of the turbine blade can allow the increasing of the TIT. Therefore, the cooling of the blades is becoming an engineering challenge. The blades are cooled with extracted air from the compressor of the engine. Since this extraction incurs a penalty on the thermal efficiency and power output of the engine, it is important to choose and optimize the cooling technology for a given turbine blade geometry under specific thermodynamic conditions. In detail, within a blade, the leading edge is cooled by jet impingement, the trailing edge by pin fins and the middle region is cooled by rib-roughened coolant passages. Moreover, due to the sharp turn, the pressure loss in the curvature section can be as high as 25% of the pressure loss in the entire cooling system. The reason could be that the flow field in a such area is very complex. It is strongly three-dimensional, unsteady, and viscous, with several types of secondary flows, vortices and separation phenomena. The better knowledge of the overall phenomena could be extraordinary important to improve the design of the device. Also, for all the above reasons turbine blade cooling mechanisms have been studied. Therefore, the main concern of the doctoral thesis has been to experimentally and statistically investigate the fluid dynamics and heat transfer in straight and bend channels enhanced by different geometries of ribs, which remotely recall rib-roughened coolant passages for industrial applications.
In particular, the first part of the work has been focused on the fluid dynamics and heat transfer investigations of a straight ribbed channel.
In this context, starting from the huge data-base, belonging to the ThermaLab Group, relating to 49 different rib configurations arranged on a straight channel of D_h= 40mm in 8 different Reynolds numbers with 3 different non dimensional pitches (PR10, PR20, PR40) with 2 different rib heights (2mm and 4mm), the aim of this study has been to find clusters of configurations with almost the same performances in term of heat transfer coefficient and friction factors, using a special mathematical tool. Thus, the statistical agglomerative hierarchical clustering analysis has been performed and it has been, also analyzed, the weight of the each parameters, influencing the performance of the different configurations. Experimental tests, by using PIV and CTA anemometry, have been conducted in order to confirm statistical results.
Fluid dynamic investigations of the flow, show that different configurations, but belonging to the same cluster, have almost the same performance with different fluid dynamics behaviors.
The present research include also an experimental analysis about pressure drop reduction and heat transfer enhancement in a U bend geometry, by the employment of various configurations of guide vanes and two different shape of ribs on the endwall. Eleven different cases of guide vanes were tested, including the baseline one, without vanes. The working Reynolds number have been 8000, 10000, 26000.
Definitively, the present doctoral work has been addressed the following conclusions.
Concerning the explorative statistical analysis and the experimental tests in fluid dynamics on the straight channels: starting from the huge database described previously, it has been achieved a unified classification in three different clusters of configurations (dendogram) with almost the some performances in term of heat transfer and pressure drops. Then, by means of correspondence analysis tool and focusing on the main parameters influencing the performances of the different configurations: height of the rib, pitch, arrangement and design, it has been evaluated the weight of each by the use of a Fischer's exact test. As a result, from statistical point of view the height of the rib represents the most meaningful parameter, it follows the pitch, then the arrangement and design. In order to confirm the statistical results, it has been experimented fluid dynamic investigations by means PIV (uncertainty 10%) and CTA anemometry (uncertainty 4%)on fluid flows in different configurations.
Fluid dynamic investigations on secondary flows, by using PIV and CTA, in order to show as configurations with different shapes, but belonging to the same cluster, have almost the some performance but different fluid dynamic behaviors.
As regards, the heat transfer and pressure drop, experimentally, measured in the outer region of a U-bend channel with and without the presence of guide vanes and ribbed endwall, it has possible to stress: the use of particular devices, like guide vanes, inside a bend geometry can effectively reduce the pressure drop but whit the cost of lower heat transfer compared to the baseline. Comparisons of 10 different cases of placement of guide vanes have been performed. Concerning this study, the application of two different types of guide vanes inside the turn, reduces, prominently, the overall pressure penalty till a maximum of 31%. The different position of guide vanes has a big importance on the pressure drop performance. The combination of ribs and guide vanes allows the thermal performance to be significantly increased. In fact, because of the local heat transfer is dominated by the jet impingement on the endwall: guide vanes switch off this effect, while ribs help it. On the other hand the presence of ribs on the outer wall causes a meaningful pressure penalty inside the bend geometry, respect to the baseline case. With particular type of guide vanes and the presence of ribs on the endwall, heat transfer is enhanced till a maximum of 35% but at the penalty of higher pressure drop respect to the baseline case. The V 45° downstream endwall ribs coupled with a special configurations of guide vanes, gives the best thermal performance.
Definitively, the use of different types of arrangements, strongly depends on the need of the turbine blade cooling system.

CFD MODELLING OF TURBULENT PREMIXED COMBUSTION IN SPARK-IGNITION ENGINES

Luca Cornolti - Tutor: Prof. **Angelo Onorati -** Supervisor: **Dr. Tommaso Lucchini**

Introduction

The present work focuses on the development of computational tools to model turbulent premixed combustion for spark-ignition (SI) engine applications in the context of RANS simulations. Given the prospect of easy improvements in terms of efficiency, Diesel engine has been developed a lot in the last twenty years. Its prevalence has increased over the time, going from an almost exclusive use for commercial vehicles, like trucks, to cover half of total vehicle fleet. Nowadays SI engine is starting to regain the attention of automotive companies for various reasons: the mature level of development reached by Diesel engine, which requires much more resources to be further improved; the need of balancing the vehicle fleet with respect to the products of the fractional distillation of oil; the use of SI engine in hybrid propulsion applications. Considering the limits of actually available experimental techniques to study combustion, theoretical and computational fluid dynamics (CFD) studies are becoming very important support tools. Moreover, because of the increasing development costs of internal combustion engines, the concept of virtual development supported by computational fluid dynamics is becoming more and more important. In particular, in SI engines, the pressure profile inside the combustion chamber is strongly influenced by the position of the piston and timing is very important. As a consequence, the development of the flame has to be modeled since the first stage after ignition. Therefore, in this work, a new premixed combustion model which describe in details also this phase of combustion is proposed. The model is implemented within the OpenFOAM framework.

Characterization of turbulent premixed flames

As turbulent premixed combustion has been studied over the past 60 years, the amount of literature on this topic is impressive, dispersive and sometimes contradictory. As a consequence, the first part of the work is focused on the description of the physical mechanisms which characterize the development of premixed flames. These information and the different modeling strategies employed by various authors, were used to define a sequence of theoretical logical steps which allows the reduction of a turbulent reaction problem, which is complex and numerical demanding, into a simpler hydrodynamic problem. This is the theoretical base of most of the employed turbulent combustion models. Moreover the definition of these steps also helps to delineate strengths and weaknesses of actually employed models and the aspects which require further investigations.

Comparison of RANS turbulent combustion models available in literature

In literature many models describing turbulent premixed combustion are available. Currently, none of them is clearly considered superior to the others. As a consequence, a comparison of the numerical behavior of the most employed models was carried out in order to identify which of them is more suitable for the purpose of modeling combustion in SI engines since the first stage. In particular, these models are the Flame Surface Density method (FSD), the Flame Speed Closure model (FSC) and the G-equation approach. After this comparison, the G-equation model was selected as the most promising approach, as its results show a lower dependence on initial conditions. Moreover it decouples the main properties of a turbulent flame (structure, propagation speed and flame brush thickness), allowing their explicit modelling. This is important in RANS approaches especially when the transient behaviour of the flame has to be modelled.

A comprehensive combustion model for spark-ignition engines

The previous concepts were used to develop an original combustion model based on G-equation approach. The model takes into account spark discharge process and early flame propagation by means of a Lagrangian description of the spark channel, as the mesh size is too big to allow an Eulerian representation of the problem. A set of particles is introduced in the computational domain; each of them represents the geometrical centre of a flame kernel. These particles expand with a velocity computed through various sub-models, which take into account spark energy deposition, stretch effect and the turbulent properties of the flow. The previous set of flame kernels is converted into the G-field. This operation guarantees the coupling between the Lagrangian approach and the Eulerian description of turbulent combustion. To check its predictive capabilities, the model is tested against the experimental data provided by a laboratory engine with optical access. This comparison showed that the model is able to represent many features of the considered experimental case. In particular it is able to reproduce the interaction between the mean flow and the spark channel, which is an aspect usually neglected in other models. Moreover, the effect of discharged energy and mixture composition were correctly reproduced. In particular, for stoichiometric mixture the results were quantitatively good, while for lean mixtures the predictions were less accurate. Uncertainties related to the adopted value of the laminar flame speed are probably the main reasons for this lower accuracy.

Conclusions

In the present work a detailed analysis regarding premixed combustion modelling in spark-ignition engines is proposed. As a result of this analysis, a new combustion solver was proposed and implemented within the OpenFOAM framework. This model describes premixed combustion in SI engines since the very early stages of flame development. The model was tested against the experimental data provided by a laboratory engine with optical access. The results obtained by the model are promising, but further validation is still required in order to better evaluate the model performances.

INCREASING ENERGY RECOVERY OF WASTE-TO-ENERGY PLANTS

Eremed Wondwossen Bogale - Supervisors: **Prof. Stefano Consonni, Prof. Federico Viganò**

1. Introduction

When seeking sustainable energy systems, Waste-to-Energy plants play a great role. However, bringing a long-term solution in solid waste management that are highly efficient, environmentally friendly, socially acceptable, extremely reliable and cost effective is a very challenging task. Particularly, the energy performance of these plants is highly affected by the low quality of the fuel and the small scale adopted. Besides, the unfavorable nature of the waste fuel leads to relatively low boiler efficiency, high auxiliary consumptions and the presence of highly corrosive species in the combustion products limits the maximum pressure and temperature adopted in the steam cycle. Hence, the efficiency of these plants decreases significantly and their investment cost becomes very high. Despite the large efforts dedicated to better use waste as a resource, there is a technological gap that needs to be filled by having a novel and reliable plant configuration. Thus, different innovative plant configurations have been proposed, modeled and simulated.

2. Research objectives

The main objectives of this PhD research are summarized below:

- To investigate and propose a possible and reliable Waste-to-Energy plant configurations that can increase the efficiency, reduce the cost of electricity production, avoid corrosion problems of boiler tubes and minimize environmental impact.
- To perform off-design analysis of Waste-to-Energy plants.
- To perform thermoeconomic optimization so as to find a cost optimal plant configuration.

3. Methodology

All the evaluations proposed in this research project have been carried out by using a number of commercial and in-house computer programs. In order to evaluate the on-design performances of the various technologies GS (Gas-Steam cycles) code has been used. For particular applications, like, off-design and economic analysis Thermoflow software packages has been used.

4. Innovative Waste-to-Energy plant configurations

The main simulation results and the various methods adopted to achieve the main objectives have been presented below by highlighting the original contribution of the authors.

4.1 External superheating and reheating

A literature survey on ways to increase the efficiency of these plants highlights that increasing the steam parameters of the steam turbine increase efficiency of the plant. However, these parameters are highly subjected to chlorine induced corrosion of boiler tubes. Thus, to increase the efficiency and to avoid corrosion problems, a new configuration has been proposed and a set of highly innovative technologies has been considered, modeled and compared. Each of these plants has been calibrated carefully and a lot of sensitivity analysis have been performed. The proposed configuration, which is based on internal superheating and reheating, results in net efficiency over 33 % on LHV basis (30 % is the maximum efficiency now achieved in Waste-to-Energy plants).

4.2. Reheating with flue gas quench concept

Due to shift of thermal load from the radiative part to the convective part of the boiler, Waste-to-Energy plants with steam reheat configuration is highly affected by corrosion problem of boiler tubes. Thus, to avoid the problem of corrosion, reduce the boiler cost and take advantage of the benefit of reheating, the authors proposed a novel configuration based on reheat with flue gas quench concept. A moderate amount of flue gas has been recirculated inside the grate combustor and the remaining flue gas recirculation has been mixed with the flue gas that exits the radiative part to limit the maximum temperature to be 650 °C. Thus, considering 200 MW thermal input and operating parameters of P_{eva} =130 bar and T_{sh} = 450 °C, 32.17 % net electric efficiency has been achieved i.e., that is 3.16 percentage points increment compared to conventional plant. The economic analysis shows that the extra electricity generated brings a positive economic return due to the selling of electricity and green certificate incentives. Besides, it avoids higher amount of CO_2 .Thus, the new configuration will benefit the plants by allowing them to be efficient, economical, reliable and environmental friendly.

4.3. Innovative cogeneration as a means to increase the efficiency and off design analysis

The modified CHP configuration with external superheating further increases the overall efficiency of the plant ultimately. It is important to note that a considerable amount of latent heat is lost at the stack depending on the moisture content of the waste and the heat can be recovered by using flue gas condensation. Thus, a combination of measures has been used to further increase the efficiency of the plant. However, depending on the heat demand from the users, the amount of steam extracted is variable and this affects the performance of the steam turbine greatly. Hence, a detailed off-design analysis of cogeneration plants has been performed.

4.4. Cost optimal configuration based on thermoeconomic optimization analysis

In this part of the thesis, thermoeconomic optimization of Waste-to-Energy plant has been performed by using Proper Orthogonal Decomposition and Radial Basis Function approximation procedure. By varying the evaporation pressure and the amount of flue gas recirculation, the optimal configuration has been obtained. Considering the challenges posed to these facilities, thermoeconomic optimization analysis provides crucial information to find cost optimal plant configuration.

5. Conclusions

In this PhD thesis, innovative configurations to increase the energy recovery potential of Waste-to-Energy plants have been proposed. The main findings are presented below:

- The net electric efficiency of these plants can be increased by about 3 percentage points compared with state of the art and highly efficient Waste-to-Energy plants by using high steam parameters of 135 bar/ 540 °C without facing corrosion problem. However, to increase the reliability and availability of the plant, another new reheating configuration with a flue gas quench concept has been proposed. Among the configuration considered, reheating with flue gas quench concept appears to be the most appealing and can be considered as a potential candidate for these facilities. Especially, steam reheat cycle with flue gas quench configuration with evaporation pressure of 130 bar and T_{max} of steam 450°C appears to be a promising option to maximize the efficiency and reduce the cost of electricity production depending on the gate fee. At this operating parameters, the net electric efficiency is increased by 3.60 percentage points, cost of electricity production is minimized, larger amount of CO_2 is avoided and corrosion of boiler tubes is avoided compared with the benchmark case. Hence, the results of this PhD thesis indicate the possible measures that allow the plants to be more efficient, economical, reliable and environmentally friendly.
- The main findings of the off-design analysis show that part load analysis not only affects the performance of the plant but also the proper functioning of the plant. Compared to the plant that produce only electricity, it appears that cogeneration plant is highly affected by part load conditions.
- Based on the results of the thermoeconomic optimization, it appears that combining exergy analysis with economics it is possible to find an optimal configuration that increases the efficiency and reduce the cost of electricity production.

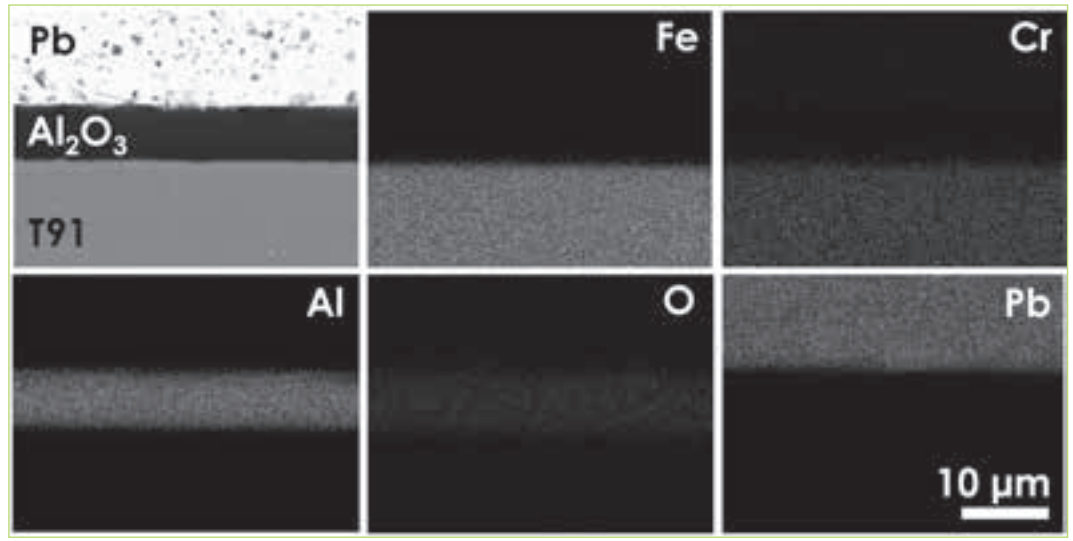
In summary, the overall results show that there are still rooms for significant improvements of the energy performances of these plants. Improving the energy performance, not only increases the economic return of the plant but it also improves the overall environmental outcome since higher energy efficiency means higher avoided emissions.

RADIATION TOLERANT NANOCERAMIC COATINGS FOR LEAD FAST REACTOR NUCLEAR FUEL CLADDING

Francisco García Ferré - Supervisors: **Marco G. Beghi** and **Fabio Di Fonzo**

Over the past decade, several advanced reactor concepts have been explored as the potential fleet of next-generation nuclear systems -else known as Generation IV (GIV). Among these systems, lead fast reactors (LFRs) are particularly interesting owing to inherent safety features and to possible configurations as nuclear waste incinerators or adiabatic reactors that burn self-generated nuclear waste. The major bottleneck for the development of LFRs regards the quest for suitable structural materials. Some of the most prominent issues in this regard are common to nuclear energy systems in general, and are typically found in high-level radiation damage GIV concepts. Anyhow, the most important problem is specifically related to the use of lead as a coolant-namely, corrosion degradation of steels. The very feasibility of LFRs ultimately depends on the development of high-performance materials that are capable of withstanding high-levels of radiation damage in an extremely corrosive environment. While self-passivation through oxygen injection and control is an effective corrosion protection method up to roughly 500 °C, other strategies are required for protecting components in service at higher temperatures, including fuel cladding. Most of these options are incompatible with or require the injection of considerable amounts of oxygen into the coolant. On the contrary, some types of oxide coatings are both independent from and compatible with oxygen injection, which might be necessary anyhow for protecting components in service below 500 °C. In this case, the coatings would allow decoupling the problem of corrosion protection at low and high temperatures. However, ceramic coatings have always been regarded as a taboo in the nuclear field, mainly due to the lack of self-healing properties, among other intrinsic drawbacks. The lack of self-healing properties is a daunting problem. On one hand, fuel cladding is exposed to an extremely harsh environment, in which the combination of high temperatures with an intense neutron radiation field ultimately results in ever growing stress and dimensional instabilities. On the other hand, the structural integrity of the coating-substrate system as a whole must be guaranteed at all times, meaning that a coating must be able to withstand high-level radiation damage, and to accommodate the stresses and strain imposed by fuel cladding.

In this framework, this Ph.D. Thesis deals with the design, the processing, the characterization and the testing under LFR-relevant conditions of a corrosion resistant and radiation tolerant nanoceramic coating as an enabling technology. In order to meet requirements, a custom process -namely room temperature Pulsed Laser Deposition (PLD)- is proposed according to a bottom-up approach. The main advantage of PLD is that it allows tailoring the structural features and the mechanical properties of the coatings through nano-scale engineering. The process is first optimized for coating plates of the steels of interest (1515Ti austenitic steel or T91 martensitic steel), and is then upgraded to coat tubes up to 10 cm long, proving that an industrial scale-up is possible in principle with proper process engineering. Recent studies have highlighted the outstanding radiation tolerance and mechanical properties of nanomaterials. Following these results, the coating -namely, a bi-phase Al_2O_3 nanocomposite- is designed to evolve towards a nanoceramic structure during irradiation in-service. This structure is meant to overcome the major intrinsic problems associated with the use of Al_2O_3 as the coating material, such as void swelling-induced micro-cracking and low fracture toughness, among others. The characterization of the coating in the as-deposited state is performed by a wide variety of techniques, including SEM, TEM, XRD, and nanomechanical and micromechanical methods. Overall, the coating attains an unusual ensemble of metal-like mechanical properties which can be explained in terms of structural features. Detailed analyses by TEM reveal that the nanostructure of the coating consists of a homogeneous dispersion of randomly-oriented Al_2O_3 nanodomains in an amorphous Al_2O_3 matrix. Importantly, this nanostructure is shown to be stable upon annealing up to 800 °C. The remaining analyses show that the fracture strength and the adhesive strength are remarkable, and that the latter is likely higher than the former. The effectiveness of the coating is evaluated under LFR-relevant conditions with specific concern for corrosion and high-level radiation damage. As a general statement, PLD-grown Al_2O_3 performs effectively as a corrosion barrier under the investigated conditions -namely, short tests at 550 °C and 600 °C in stagnant lead (see figure 1). The evolution of structural features and mechanical properties following heavy ion irradiation up to 20, 40, 150, 250 and 450 dpa is analyzed by SEM, TEM, XRD, and nanomechanical and micromechanical techniques. The analyses reveal that the changes in the mechanical properties of the coating are due to athermal radiation-induced crystallization, which drives the evolution of the initially bi-phase nanocomposite coating towards a radiation tolerant nanoceramic structure. This type of structure is able to accommodate radiation-induced stresses through grain boundary-driven deformation modes. Importantly, the exposure to end-of-life levels of radiation damage does not compromise the structural integrity of the coating-substrate system. In conclusion, PLD-grown Al_2O_3 is a suitable and promising coating material for LFR nuclear fuel cladding.



1. Cross-sectional SEM micrograph of the coated surface of a T91 steel sample after exposure to stagnant molten lead at 550 °C for 500 h (a). No signs of corrosion are found, as confirmed by the EDX maps for Fe, Cr, Al, O and Pb.

NANOSTRUCTURED OXIDE SEMICONDUCTORS FOR DIRECT SOLAR ENERGY CONVERSION: PHOTOVOLTAICS AND WATER SPLITTING

Ali Ghadirzadeh - Tutor: **Prof. C.E. Bottani -** Advisors: **A. Li Bassi, F. Di Fonzo**

Objectives of thesis work

I performed my doctoral research in Energy and Nuclear Science and Technology at the Center for Nano Science and Technology (CNST) of the Italian Institute of Technology (IIT), with an IIT scholarship on "Nanostructured Semiconductors for Direct Solar Energy Conversion: Photovoltaics and Water Splitting", focusing on the synthesis and characterization of nanostructured metal oxides mainly as photoelectrodes for hybrid heterojunctions as solar cell and water splitting devices.

Motivation and Originality

Low-cost semiconductor materials and facile fabrication routes for photovoltaic (PV) junctions have been longstanding goals for photovoltaic materials research. New materials or fabrication procedures that could reduce the cost of PV electricity sustainability could help to drive a rapid expansion in implementation of photovoltaic technology. In the field of solar energy conversion, hybrid organic/inorganic devices represent emerging alternatives to standard photovoltaic devices in terms of exploiting the specific features of both organic nanomaterials and inorganic semiconductors. In hybrid devices, an organic material is mixed with an inorganic material to form a photoactive layer. Utilization of intrinsic properties of the inorganic materials such as charge selectivity behaviour and advantages of nanostructuring such as increase of interfacial area are the two main objectives of current research in this field.
In hybrid devices, including hybrid organic/inorganic solar cells and water splitting cells that are the target of this project, interface between the organic and inorganic materials plays an important role in the power conversion efficiency (PCE) of the device. In both photovoltaic (PV) and water splitting (WS) configurations, currently there are two major issues that are highly under investigation: first is the proper choice of material selection and the second is the organic/inorganic mixture design at nanoscale that greatly affects the performance of the final device.
In the framework of this project, I am aimed to synthesize novel nanostructured materials, mainly transition metal oxides (TMOs), as hybrid device photoelectrodes, and perform complementary optical, electrical, compositional, and morphological characterizations in order to gain well understanding of the material and device behaviour and features, which make us capable of tuning properties by means of better control over the fabrication process.
Experimentally, I will focus on developing and characterizing different aspects (e.g. morphology, structure, optical properties) of nanostructured thin films, mainly TiO_2, MoO_3, and PdO as charge selective contacts by means of pulsed laser deposition, in order to meet the most important requirements for the desired hybrid PV and WS applications.

Hyperbranched TiO_2 nanostructure

In the field of PV, a quasi-1D hyperbranched nanostructure of titanium dioxide was synthesized and characterized and its application as photoanode in hybrid organic-inorganic solar cells was explored. P3HT was used as the hole conductive organic couple. Hybrid solar cells were made by evaporation of silver and the cells were measured by a solar simulator set up. Performance of the cells was optimized by focusing on the film thickness, film porosity, and the molecular weight of the infiltrated polymer. In parallel and as a reference, mesoporous titania paste based cells were fabricated and the photovoltaic performances of both type of devices in terms of open circuit voltage (Voc), short circuit current (Jsc), and fill factor (FF) were compared. A maximum power conversion efficiency exceeding 1% for the champion PLD-fabricated cells under air mass (AM) 1.5 illumination has been obtained for 800 nm thick cell, deposited at 7 Pa of oxygen. This result represents a 130% increase with respect to an optimized device obtained with a standard architecture based on a mesoporous titanium dioxide photoanode (0.43%). The efficiency gain arises mostly from a tremendous increase in Jsc from of 1.55 mA/cm^2 to 2.7 mA/cm^2 for the standard and the hierarchical photoanode respectively. This is mainly attributed to the peculiar optical properties such as light scattering of the novel acceptor phase and to the close-to-optimal interpenetrating morphology obtained as confirmed by quantitative electron tomography, as well as an increase in the crystallinity of the infiltrated polymer which was demonstrated by XRD analysis and by transient absorption measurements.

2D nanolamellar α-MoO3 structure

As mentioned before, in the frame of PHOCS project, nanostructured hole-selective materials were the target of the research. MoO_3 and V_2O_5 have the highest values of work function (6.9 and 7 eV respectively) among the TMOs. Since V_2O_5 is a highly soluble material, MoO_3 was chosen as the starting material. MoO_3 has a hierarchical structure upon deposition in a background atmosphere and annealing up to 350°C (β phase) and it converts to α phase by further annealing and forms a nanolamellar structure due to the 2D nature of the α-MoO_3. Physical, structural, electrical, and optical properties of high purity α-MoO_3 nano-lamellar structures produced by PLD were investigated. Ultra-thin lamellar structure was realized for films annealed at 400 °C where a mixed α/β phase is present prior to complete crystal growth in single α phase where thick lamellas can be observed. An innovative technique based on the differential etching rate of the two phases was used to achieve pure α phase. The films are being characterized by means of Scanning electron microscopy, Raman spectroscopy, X-ray diffraction, Kelvin probe force microscopy, and UV/Vis spectrophotometer to understand the morphology, crystallinity and relative phases ratio, surface energy and optical behaviour variation by phase transition. Ability of intercalation between the lamellas for tuning material band gap is studied by annealing in H_2 atmosphere. For hydrogen production, the structure was coupled with P3HT:PCBM blend and the photoelectrochemical behaviour was studied. A maximum current of 50 μA at the positive potential of 0.35 V vs RHE was extracted for this system. However in spite of the good photoelectrochemical activity of the system, due to the reducing tendency of the oxide by negative swap, at which it tends to get reduced to MoO_2 at 0.24 V, and to the narrow range of stability by pH (between 0 and 1), other materials, namely Palladium oxide, became in the focus of our attention.

Hierarchical PdO nanostructure

Palladium oxide has been reported to be a p-type semiconductor with high work function which makes it a suitable choice of selection as a photocathode for a hybrid device. In addition, PdO has long been known for its high insolubility, good thermal stability, non-toxicity, as well as ideal corrosion resistance in wide range of pH values, acidic to basic, and relatively cheaper in comparison to the very few other metal chalcogenides with similar stability characters such as IrO_2 and PtO. Once being nanostructured, high surface-to-volume ratio could be obtained which is a key parameter in hybrid devices in order to maximize the charge generation in the organic molecules, and its interfacial extraction to the charge-selective inorganic compound. Hierarchical nanostructure of PdO was synthesized by using a Pd target and further annealing in air. An example is depicted in Figure 2.a. Among all investigated pristine and blended bulk-heterojunctions, APFO-3:PCBM attained the highest photocathodic current. By analysing photoelectrochemical measurements, this systems failed to produce hydrogen due to the reaction of the generated electron with oxygen in the water Precise degasation of electrolyte revealed that the photogenerated current decreases with the amount of outgoing oxygen.

NANOSTRUCTURED TRANSPARENT CONDUCTING OXIDES FOR ADVANCED PHOTOVOLTAIC APPLICATIONS

Paolo Gondoni - Supervisors: **Dr. Carlo S. Casari, Prof. A. Li Bassi**

The attention of research in the field of solar energy has been lately focused on Hybrid and Organic PhotoVoltaic (HOPV) cells, as promising low-cost and high efficiency flexible energy harvesting devices. A key component in any HOPV cell is constituted by transparent electrodes, whose main purpose is to let the solar light enter the device and the photogenerated charges exit to an external circuit. Such electrodes, in the form of compact Transparent Conducting Oxides (TCOs), have been investigated for a long time, leading to the development of highly performing materials among which Indium-Tin Oxide (ITO) is the most widely employed. However, a number of major problems have emerged which make compact TCOs - and ITO in particular - unfit for future HOPV devices. Novel properties are required, including effective light management, low temperature synthesis, large surface area and low priced constituents. A promising candidate which can meet all these requirements is Aluminum-doped Zinc Oxide (AZO). ZnO-based materials are inexpensive and easy to synthesize in different forms with peculiar structures at the nano- and micro scale. One powerful deposition technique to obtain AZO and ZnO thin films is constituted by Pulsed Laser Deposition (PLD), whose versatility allows control of morphology, structural and functional properties down to the nanoscale.

In this framework, this project was first dedicated to understanding and achieving control of the relation between structure and functional properties of nanostructured AZO layers grown by PLD at room temperature. Subsequently, this knowledge was employed to develop novel nano-and mesostructures combining all the desired properties in one low cost, large surface area, transparent, conducting and light scattering material, compatible with flexible substrates.

The deposition of AZO layers by PLD at room temperature was performed in the presence of oxygen as a background gas. O_2 pressure during deposition proved to be a critical parameter, whose variations cause dramatic effects on morphology, structure, stoichiometry, optical and electrical properties. Two main deposition regimes were identified based on the O_2 deposition pressure: compact layers with low oxygen content (from now on, "compact films") are obtained at low pressures, whereas above 10 Pa O_2 it is possible to achieve mesoporous forest-like structures (from now on, "porous films"). Examples of these structures are presented in the Scanning Electron Microscope images shown in figure 1.

At an optimal deposition pressure value of 2 Pa O_2, a compromise between local structural order and defects beneficial for carrier concentration leads to the state-of-the-art resistivity of 4.5×10^{-4} Ω cm was found, with a mean visible transmittance of 85%. Unlike compact films, porous AZO layers showed an extremely significant light scattering capability, with a haze over 80%. Still, due to their open morphology, and possibly also to the saturation of oxygen vacancies, porous films have much higher resistivity (of the order of MΩ cm). The deposition process of both porous and compact films was calibrated in order to permit adhesion on flexible substrates, namely Ethylene-TetraFluoroEthylene (ETFE), which is of significant interest for HOPV devices as discussed above.

The identification of the importance of oxygen content in compact films, together with the optimized light management properties obtained in porous films, allowed to devise two approaches to obtain electrically conducting nano-forests by PLD at room temperature.

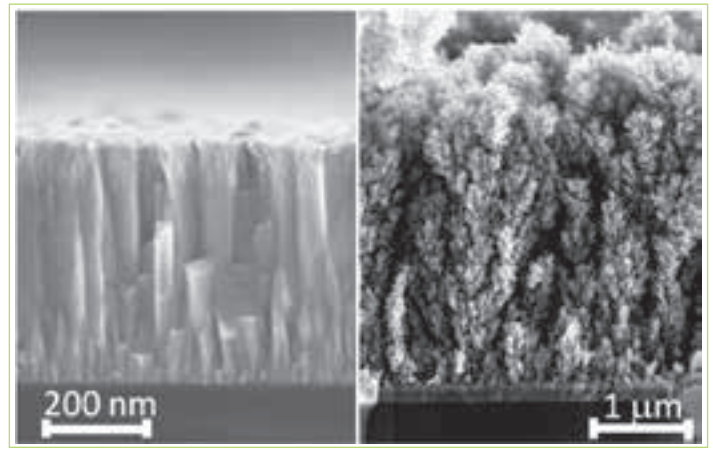
In order to achieve this result, PLD was first performed in a mixed $Ar:O_2$ atmosphere rather than in pure oxygen: in these conditions it is possible to uncouple the effects of the background gas on morphology and stoichiometry. The results in terms of electrical properties are promising: the electrical resistivity of AZO layers grown at a total pressure of 100 Pa, with oxygen partial pressures ranging from 2% to 10%, are 5-6 orders of magnitude lower than films with similar morphology grown in pure O_2 atmosphere: this means that it is virtually possible to synthesize a hierarchical AZO layer with controlled resistivity, optical transmittance and haze by adjusting the O_2 partial pressure and the thickness.

The second approach involves the spatial separation of electrical conductivity and light scattering, i.e. the realization of a multifunctional, multilayer architecture combining the properties of compact and porous AZO films. The versatility of the PLD technique allows to synthesize this kind of structure in one single deposition step, in which the transition from compact to porous AZO (and vice versa) occurs as a consequence of a variation in the O_2 pressure during deposition.

The identification of multiple trade-offs between conductivity, transparency and light scattering allowed to devise an optimal deposition condition: mean visible transparency of the order of 80%, haze of 40% and resistivity of the order of 3 mΩ cm. In terms of comparison, the light scattering capability of the nanoforests is combined with an electrical resistivity which is 9 orders of magnitude lower.

The benefits deriving from light scattering have been tested by evaluating the enhancement of absorption in a low bandgap polymer (PCPDTBT) employed in HOPV devices as an electron donor. A 40 nm PCPDTBT layer was spin-coated on an optimized graded AZO structure, and the absorption profile of the polymer in these conditions was compared with that of an identical PCPDTBT layer deposited on compact AZO. The results are shown in figure 2, where the black curve shows the PCPDTBT absorption on a compact AZO layer (shown as a reference): the region of low absorption is clearly visible in the 450-550 nm spectral region. The red curve corresponds to the absorption of an identical layer deposited on a graded AZO architecture: the increase in the same spectral region is as high as 100%, both on glass substrates and on ETFE flexible substrates.

This project demonstrates the room temperature synthesis of a nanostructured, flexible transparent conducting layer based on low cost materials for photovoltaic applications. Compact, transparent and highly conductive AZO layers combine the functionalities required for conventional solar cells with mechanical flexibility, whereas nanostructured forest-like layers can provide enhanced light harvesting capability (up to 100% for flexible polymer-based photovoltaic cells).



1. Cross-sectional SEM images of a compact sample grown at 2 Pa O_2 (left) and of a mesoporous sample grown at 160 Pa O_2 (right)

2. (left) A flexible transparent conducting scattering AZO layer on an ETFE substrate. (center) Cross-sectional SEM image and corresponding scheme of a graded AZO layer constituted by a compact conducting layer on a porous scattering layer. (right) Increase in optical density of a 30 nm PCPDTBT: the black curve shows the polymer absorption profile when it is deposited on a compact AZO layer, the red curve reports the absorption of an identical PCPDTBT layer grown on a graded AZO architecture.

STRATEGIES FOR ACCESS TO ENERGY IN DEVELOPING COUNTRIES: METHODS AND MODELS FOR OFF-GRID POWER SYSTEMS DESIGN

Stefano Mandelli - Supervisors: **Prof. Emanuela Colombo, Prof. Marco Merlo**

This doctoral thesis copes with methods and models for sizing, analysis and evaluation of small-scale power systems for off-grid implementations. This theme is specifically developed within the frame of rural electrification in Developing Countries with a particular emphasis on Africa.

The thesis theme refers to the field of research in "Energy for sustainable development in Developing Countries". *Developing Countries* are affected by the lowest per capita values of energy supply as well as electricity consumption. These conditions are exacerbated in rural areas where many scattered villages are characterized by no access to any kind of service. Dealing with the *problem of access to energy* means to study the problems of electrification and traditional biomass dependence.
The thesis also considers the concept of *sustainable development*. This aspect is quite important in Developing Countries where the impact on local development due to enhancing access to energy is more tangible.

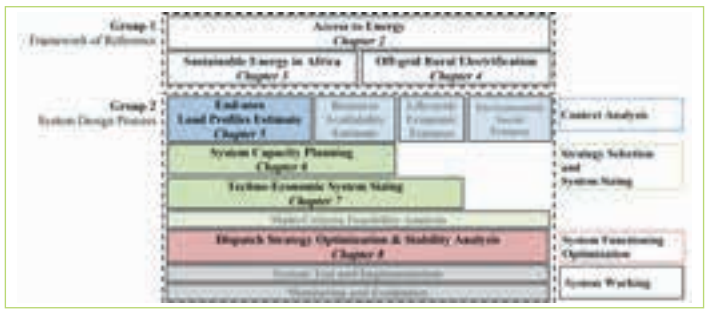
Within this frame, three main observations can be recognized as general motivations of the research activities:

1. off-grid small-scale power systems based on Renewable Energy sources are often the most viable strategy for rural electrification. Nevertheless the design of these systems is not straightforward and several issues can be investigated;
2. the development of methods and models to tackle these issues contributes to promote electrification. Moreover, achievements in Developing Countries can have favourable spin-off on applications in the developed world;
3. the research field of small-scale power systems has experienced a growing interest in the past few years. This theme addresses a number of engineering disciplines leading to the development of several research areas. This thesis revises the literature and capitalizes its main fundamentals in order to provide scholars with a reference framework.

By looking at the different elements of a rural electrification intervention based on small-scale power systems – from the features of the intervention context, to the aspects about the development of the technological solution – seven main issues have been identified:

1. when aiming at sustainable energy development, it is required to understand the relationships between energy issues and sustainability;
2. the energy framework where the electrification action takes place has to be analyzed. This means, at country or macro-region, to acquire a picture of the energy situation and to measure the progress towards a sustainable energy system;
3. it is required to study the features of rural areas, i.e. to identify the typical energy needs and to acquire the state of the art of the technology solutions for rural electrification;
4. looking at the analysis of the technological solutions, energy resource availability and electric consumption patterns have to be evaluated according to the intervention context;
5. the technology solution has to be selected and sized. This involves the planning of systems components capacity according to local consumption patterns and energy resources. Moreover, sizing may also embrace economic features to assess system feasibility;
6. the real interactions between the identified system components have to be analyzed. This refers to the optimization of dispatchment strategies and stability analyses;
7. finally, rural electrification interventions require monitoring and evaluation in order to understand to which extent local development has been promoted.

The highlighted issues can be arranged in two groups: those which deal with the *Framework of Reference* of the targeted theme (i.e. issues 1, 2, 3), and those which are the building blocks of the *System Design Process* (i.e. issues 4, 5, 6, 7). This thesis addresses some of these issues in accord with these two groups. Fig. 1 shows a schematic overview of this framework and it highlights the thesis contributions.
Chapter 2 introduces the theme of access to sustainable energy with particular reference to Developing Countries. It focuses on the issues of access to electricity and traditional biomass dependence as regards the topic of sustainability.
Chapter 3 depicts the current energy situation of Africa as far as the concept of sustainable development is concerned, and it analyzes if and how local energy policies fit with this asset. In particular, emphasis is given to the situation of rural electrifications.
Chapter 4 deals with off-grid small-scale power systems which often are the most appropriate energy solution to address rural electrification. It deepens the analysis of rural electrification issue in Developing Countries and it reviews the literature about small-scale off-grid power systems. The review is the basis for the development of methods and models which address system design process and which are introduced in the following chapters.
Chapter 5 describes the development and implementation of a stochastic procedure to estimate electric load profiles in rural areas. The procedure allows developing user load profiles which are required as input data for the most advanced system sizing techniques. This procedure, as well as the ones introduced in the following have been implemented in Matlab and Matlab SIMULINK.
Chapter 6 describes a novel mathematical procedure for system capacity planning of both on-grid and off-grid systems. It identifies the best mix of energy sources available in a targeted context in order to meet user load profiles. Moreover, it computes the power sources and storage system sizes according to specific objective functions.
Chapter 7 introduces an appropriate techno-economic system sizing approach for rural areas. Indeed, in addition to energy sources and user load profiles, it embraces in the system sizing process also local costs of traditional and modern energy systems. It has been applied for PV system sizing in Uganda.
Chapter 8 deals with a new approach for electro-mechanical modelling of off-grid systems capable to analyze system operation and dynamic behavior. A model for a micro hydropower plant in Tanzania has been implemented and analyzed.
This doctoral thesis deeply analyzes and revises the framework of rural electrification in Developing Countries. Moreover it contributes in improving the design process of off-grid power systems by means of a number of new methods and models.



1. Schematic overview of the topics concerning rural electrification interventions via off-grid small-scale power systems and thesis contributions

BUILDING SUSTAINABILITY ASSESSMENT AND RATING: AN ITALIAN OBJECTIVE SYSTEM PROPOSAL

Roberta Moschetti - Supervisor: **Prof. Livio Mazzarella**

The thesis fits in the broad research topic of the sustainability assessment and rating systems for buildings.
The main result concerns an innovative approach for the development of a new protocol, with a focus on Italian residential buildings.
One of the main motivations of the research work is related to the absence of a uniform and complete evaluation tool at national level, whose parameters are substantially founded on the principles of objectivity and measurability. Moreover, the lack of a life cycle approach in national sustainability evaluation protocols is also pointed out, meaning the almost total absence of criteria referred to all building life stages, with a consequent lack of related benchmarks.
In the first part of the thesis, given the existence of many evaluation tools in addition to several standards on building sustainability issue, a careful study of the state of the art was executed, leading to the choice of few tools to take into consideration for a further deep analysis. Therefore, according to the usual framework of criteria-based tools, the new rating system was supposed to be characterized by the presence of: evaluation areas, assessment criteria, performance indicators and related computation methodologies. Hence, the potential evaluation areas to be included within the new protocol were chosen as a result of the investigation of the areas contained within the analyzed existing systems and Standards. Furthermore, in order to recognize interdependencies among the different identified areas a mathematical multi-criteria method, the Decision Making Trial and Evaluation Laboratory (DEMATEL), was applied. Thereafter, another mathematical multi-criteria technique, the Analytic Hierarchy Process (ANP), was implemented, in order to define a scale of priority among the analyzed areas. The final choice of the evaluation areas resulted from the calculation of the 'Preference Index' taking into account the results of both DEMATEL and AHP methods.
It is worth to notice that, in order to face the complexity of several heterogeneous scientific areas, a panel of experts was established. Its members belonged to the university field and represented a valuable support for the application of the multi-criteria methods used within the research work.
The following step regarded the definition of the assessment criteria to be included in the established evaluation areas. This involved an extensive comparative analysis of the criteria included in the existing sustainability protocols and Standards, identifying similarities and repetitions, detecting possible gaps and proposing adaptations or extensions. The main selection principle was the actual measurability and objectivity of each criterion.
Afterwards, both evaluation areas and criteria were weighted in order to characterize their importance within the protocol structure. The weight of the evaluation areas derived from the combination of the results got from DEMATEL and AHP, by applying the Analytic Network Process (ANP). Instead, the criteria were weighted through the AHP, with a new consultation of the panel of experts.
Subsequently, each criterion was associated to performance indicators, derived by a critical analysis of the potential existing ones, with the suggestion of possible combinations, adaptions or additions. Next, calculation methodologies were defined for each criterion, by the analysis of the existing procedures and the proposal of revisions, extensions or new methods.
The quantitative information obtained from the computation of the performance indicators needed to be referred to predefined baseline values, in order to rate the achieved performance. Therefore, the indicators were related to scales of reachable values, built on the basis of limit and reference values. This led to the second part of the thesis, where the benchmark concept was introduced, underlying its importance for the setting of the new protocol structure.
In particular, the absence of reference or limit values for some performance indicators was emphasized and, to compensate for this lack, specific computation methodologies were proposed. In particular, reference values were calculated for: 'Use phase' energy, Life Cycle Impacts (LCI), Life Cycle Costs (LCC), and Indoor Quality (IAQ). For this purpose, detailed analyses on reference buildings were performed, referring to the European project TABULA for the definition of 36 Italian residential building archetypes. The analyzed buildings were chosen within the after-2005 construction age, so that they all presented the typical envelope components of the most recent construction period. Furthermore, the archetypes were differentiated on the basis of the combination of three variables: the building typology (single-family house, terraced house, multi-family building, and apartment block); the climatic zone (Italian E climatic zone, 2100-3000 degree-days; Italian D climatic zone, 1400-2100 degree-days; Italian C climatic zone, 900-1400 degree-days); the building systems (heating, cooling, and domestic hot water (DHW) plants). Three main analyses were performed: (1) 'use phase' energy evaluations, through dynamic energy simulations by EnergyPlus software; (2) LCI assessments, with the application of LCA methodology, through SimaPro 8 software; (3) LCC assessments, by means of economical evaluations based on the global cost approach, as suggested in EN 15459. First, the analyses related to the 'use phase' energy were performed and then the results were integrated in the LCA and LCC analyses, leading to the final definition of the investigated life cycle indicators. Thereafter, another methodology was set for the definition of benchmarks concerning the IAQ criterion.
In particular, a reference single family house, derived from TABULA project, was subjected to specific indoor airflow and pollutant analyses, through the multizone airflow and contaminant transport analysis software CONTAM. In particular, the last drafts of UNI 10339 and EN 15251 were examined for a comparison on the suggested supply and extraction airflows, with regard to the minimum air quality class.
The last part of the thesis focused on the implementation of the developed protocol on a case study, in order to practically test and validate its applicability. Furthermore, to assess the coherence of the developed protocol with others actually in use, a widespread Italian system, ITACA protocol, was also implemented on the same case study. In conclusion, the results obtained by both protocols were critically discussed and compared.
It is worth noticing that the implementation of a sustainability assessment and rating system represents a manifold process, requiring a plenty of data on the analyzed building, with reference to different life phases. Nonetheless, this phase was highly required for the examination of the consistency of the proposed Protocol structure and of the trustworthiness of the defined evaluation methodology.
The thesis results are aimed at providing a contribution to the national and international development of methods and guidelines, supporting the sustainability management and optimization in the building sector. Indeed, the research provided an effective methodological and operative tool for decision makers in the field of sustainability assessment systems. In fact, the study illustrated a detailed methodology that could be followed in the definition of new assessment systems, showing an objectification procedure for the definition process, with a parallel reduction of the subjectivity margins in its inner content. Finally, the developed benchmark values, related to several sustainability criteria, could be used as a comparison base for future similar studies, or could be also employed in Italian sustainability rating systems for residential buildings, as soon as the analyzed indicators will be introduced in their structure.

WASTE ATOMIC SEPARATION AND RAW MATERIAL RECOVERY BY APPLICATION OF PLASMA TECHNOLOGY

Guido Parissenti - Supervisor: **Alfonso Niro**

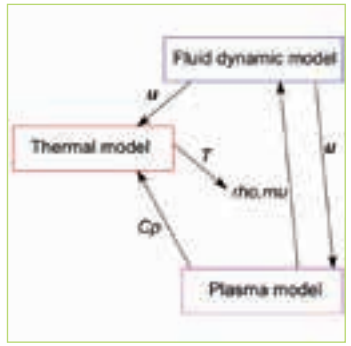
Our society's economical model, in terms of the western way of living based on consumerism, is presently no longer sustainable. The present goods production rate requires a constant supply of raw materials, which results in a continuous draining of the Earth's fossil and renewable resources. Attempts are being made to improve our environmental responsibility. Ecological lifestyles, improved production processes and better waste management are some examples of policies introduced to reduce our environmental impact. Nevertheless wastes are still one of the most devastating results of human activities because of its twofold drawback: on one side they represent a reduction of available raw material for goods production, and on the other side they occupy space and mass, polluting natural resources, and creating additional costs for proper disposal. The obvious best solution to get rid of the waste problem is not to produce wastes, improving reusability and reducing packages. Unfortunately this solution can only be gradually implemented, and the problem remains for the already produced wastes, which are mainly managed in three ways: disposal in dumps, destruction/incineration, recycling.

Of the three methods the first is the one with the largest drawbacks. The second is an attempt to recover at least the energy contained in the waste at the expense of destroying any possibility to reuse the material. The third is the more environmentally friendly option, because the energy required to produce goods starting from recycled material is many times lower that starting from raw materials.
Despite recycling, mixed wastes which cannot be separated, special wastes, and ashes from incinerators still represent a tremendous potential source of raw material that cannot be exploited but shall inevitably be disposed in dumps.

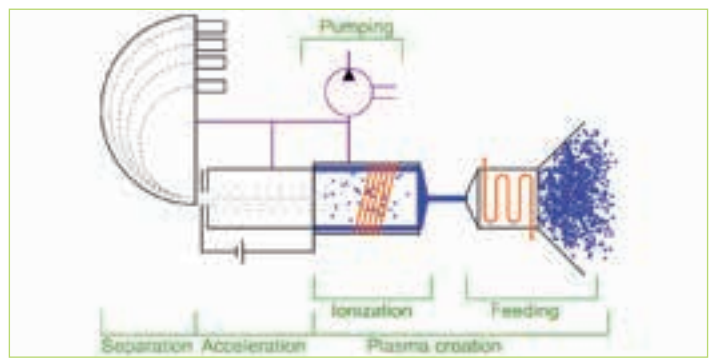
In this frame, the present research investigates the possibility of obtaining raw materials as pure elements starting from multiple not refined sources, such as wastes, minerals and other sort of low grade materials, by using plasma means. The concept has been proposed in the past, for very specific applications, in very different fields ranging from nuclear physics to space science. The process implies the ionization of the source materials and the separation of its constituents by electromagnetic means in a single production step, with the advantage of shortening the overall production chain respect to traditional production processes, at the expenses of a high quantity of electric energy. In this work the problem is analyzed in the special case of silicon production starting from silica, which traditional production method involves many production steps and the usage of large quantities of energy, water and chemicals. The possibility to directly separate silica into its constituents in a single passage would provide benefits in terms of energy consumption, logistics and environmental impact.

The problem is initially set to evaluate synergies with previous technologies, and the preliminary configuration of a demonstrator plant is proposed with its main constituents. The proposed idea relies on the concept of mass spectrometry, which is a chemical analysis device that measures the mass-to-charge ratio and abundance of ions in the gas phase. It works by ionizing chemical compounds to generate charged molecules or molecule fragments and measuring their mass-to-charge ratios. The proposed demonstrator plant resembles the main parts of a mass spectrometer, but with the consideration that a much bigger throughput is required for the separation operation to be convenient and able to be performed in a reasonable amount of time. The silica vaporization and plasma generation is provided by a particular self-feeding plasma torch concept identified within the study, which does not need an external supply of working gas.

A numerical multiphysics 2D axisymmetric FEM model, capable of simulating the actual torch geometry and the thermochemical processes in each point of the domain, is then developed to analyze the process, allowing to perform a more detailed design of the overall device.
The model comprises a fluid-dynamical model, a thermal model and a plasma model coupled one to each other.
Ions and neutrals are supposed to have a single temperature, different from the electrons one. This implies that a single fluid model is used, where the plasma is seen as a unique conducting fluid and globally neutral, that reacts to external inputs. The modeling of the plasma decomposition of the inbound gas mixture is the most complex physics taken into consideration. It comprises both plasma reactions, which involve electrons impact, and chemical reactions, which are responsible of the heating of the neutral mixture.
A big effort was put in identifying an exhaustive set of equations capable of simulating silica decomposition and thermal behavior. Other than the physics of oxygen, which reactions are commonly available, the plasma reactions involving silicon and its oxygen compounds were very difficult to gather. The majority of the papers found in literature focus on Plasma Enhanced Chemical Vapor Deposition (PECVD), which involves hydrogen, or on the production on nanometric silica, in plasma torches where silica reaches only fusion temperature. In order to collect the fundamental equations to build the model, reaction has to be found in astrophysics and atmospheric related papers.
It has to be underlined that apparently no complete kinetic models of silica plasma decomposition are available in literature, therefore this set of reactions can be a useful source of rate constants and references for those involved in building similar models.
After the numerical calculations the power consumption of the device's constituent parts is estimated, with the preliminary design of a particular section if needed. The demonstrator plant is then globally evaluated from the energetic point of view, and its sustainability is compared with traditional production processes.
Results show the feasibility of the approach, but also an overall energy consumption unfortunately higher than the traditional production process. Nevertheless the overall environmental impact is limited to the electric energy demand, with no chemicals involved in the process. Areas of optimization are identified, which may lead to substantial improvements in the energy consumption.



1. Multiphysics model logic



2. Demonstrator concept simplified schematic

DEVELOPMENT OF A FIXED-BED QUASI-ISOTHERMAL ADSORPTION DEHUMIDIFIER: FROM CONCEPT TO OPTIMIZATION, THROUGH EXPERIMENTAL AND THEORETICAL INVESTIGATION

Lorenzo Pistocchini - Supervisor: **Prof. Mario Motta**

Research goals

The research focuses on the development of a heat driven adsorption dehumidifier for waste heat recovery and solar air conditioning applications. It is based on the batch operation of two finned tube heat exchangers, where silica gel grains are packed between the fins. Quasi-isothermal adsorption and desorption processes are achieved respectively by rejecting and supplying heat within the fixed beds, thanks to the alternative flow of cool and hot water through the heat exchangers. The novel dehumidifier has the purpose to be a cheaper system than existing desiccant systems for air conditioning application, being made by standard components. Moreover, it aims at providing a suitable dehumidification rate even at low regeneration temperatures, thanks to the quasi-isothermal operation.

Main results

First step of system development is the optimization of the packed bed, mainly focused on the minimization of the pressure drop, by means of a theoretical and experimental study of its peculiar geometry. This is characterized by the little ratio of fin pitch to silica gel grains diameter, which affects the porosity ε of the adsorption bed and consequently the pressure drop in the air side. To carry out such analysis, an experimental apparatus is realized on purpose.
First result is the development of a semi-empirical formula to calculate the volume fraction of monodisperse packed beds – made by randomly pouring spheres between the fins – as a function of the ratio of fin distance (p) to spheres diameter (d). This formula corrects, by an empirical coefficient γ, the theoretical model of Pansu et al. for the case of finite pressure exerted by the bed walls on the spheres. At p/d <= 1.707 the volume fraction is
1 – ε = π3γ pd41 – pd – 12 – 1
An optimal range of p/d_{av} is identified even for a polydisperse packed bed of spheres, made by a distribution of diameters in a range $d_{min} \div d_{max}$, where $d_{min}/d_{max} > 0.75$. In such an optimal range, identified by theoretical considerations and validated by experimental results, porosity of the packed bed is maximized: $p/d_{min} = 1.5 \div 1.63$; $p/d_{max} = 1.13 \div 1.23$; $p/d_{av} = 1.29 \div 1.40$, if $d_{av} = (d_{min}+d_{max})/2$.
A new semi-empirical formula for pressure drop calculation is developed, to adapt the Ergun equation to the specific geometry of the packed bed between the fins. The new formula provides very good accuracy and indicates that pressure drop, besides being inversely proportional to porosity - as already shown by Ergun equation - is directly proportional to the p/d_{av} ratio. This means that pressure drop is minimized at lower values of p/d_{av} than those which maximize the porosity.
ΔPvL = α*μ1 – εSv + 2p2ε3 + β*pdavnρfv1 – εSv + 2pε3
α, β and n are empirical coefficients;
Sv is the specific surface of solid particles in the bed [m^{-1}].
Based on the results of packed bed analysis, a prototype of the dehumidifier is realized. It is specifically designed to be tested in different operating modes, in particular with regard to the direction of the air flow through the adsorption heat exchangers during the different stages of the operating cycle.
To carry out the testing campaign of the prototype independently of the actual climatic conditions, a new laboratory and the related monitoring and control systems are designed and realized.
Experimental evaluation of the prototype is aimed at determining the main energy performance indicators – dehumidification rate, the Coefficient of Performance (COP) and the Energy Efficiency Ratio (EER) – on varying the humidity by mass (x_{in}), temperature (T_{in}) and flow rate ($\dot{m}$) of the air at the inlet of the heat exchangers, and the inlet temperature of the cold (Tc) and hot (Th) water flow.
Test results show that the energy performances strongly depend on the operating conditions, which need to be optimized. Anyway the prototype guarantees a significant dehumidification in all the tests, despite the narrow thickness (108 mm) of the heat exchangers and the low regeneration temperature. As a reference: it provides an average dehumidification rate up to 5 g/kg with a cooling water temperature Tc = 25°C, a regeneration temperature Th = 50°C, an air flow rate V=1850 m3/h and a "parallel flow" regeneration, meaning that the airstream flows through the heat exchangers in the same direction during the dehumidification and regeneration stage. Proving the effectiveness (in terms of performances) of "parallel flow" regeneration, which allows to simplify the prototype design and control, is an important result of the testing campaign.
Two semi-empirical formulas are then developed to calculate the energy performances (dehumidification and COP) as a function of the operating conditions. Development of these formulas is not only based on the fitting of experimental data, but on the assumption of proportionality between the performances of the prototype in actual and ideal operation. Thanks to such approach the accuracy of the formulas results to be remarkable.
They are a suitable tool to optimize the control of the dehumidifier, since a dehumidification target can be achieved by different combinations of some operating variable, as ṁ, Tc, Th, to which different energy performances correspond. Suitable combinations can be computed by one formula and the resulting energy performances by the other one, so the best operating conditions can be selected on the basis of different control strategies.
Last step of the research work is the optimization of the dehumidifier design.
A numerical model of the prototype is developed to simulate the operation of revised configurations and assess the improvement of the performances. It is based on integral models of the main physical phenomena (not stationary heat and mass transfer, adsorption and desorption) in specific reference volumes, where average values of the relevant quantities are considered rather than the three-dimensional fluid dynamics. Due to the diameter of silica gel grains, the effect of vapour diffusion within the grains is not considered negligible. Thus an isotropic diffusion model is coupled to the integral model, which applies the hypothesis of instantaneous adsorption just to the external layer of the grain.
The numerical model is based on empirical formulas, available in literature, to compute the convective heat and mass transfer coefficients and vapour diffusivity. Such coefficients are calibrated on the basis of test results. Then model reliability is verified by means of further experimental results, and exploited to quantify the performances of a revised design of the prototype: by increasing (up to twice) the thickness of the heat exchanger and reducing the air flow rate, with the condition of keeping the same flow regime, both the COP and dehumidification are significantly improved. It must be noted that in such an operating mode, the conditioned flow is mixed to an unconditioned flow to regain the overall air renewal rate.
The promising results of this research push in the direction of an integration of the optimized layout of the dehumidifier in a "conventional" Air Handling Unit. This is the rational, but not trivial, main future development of the work.

ADVANCED MATERIALS FOR NOVEL LASER-DRIVEN ION ACCELERATION SCHEMES

Irene Prencipe - Advisor: **Dr. Matteo Passoni -** Tutor: **Prof. Carlo E. Bottani**

Since it was first observed in 2000, ion acceleration driven by ultra-intense (>10^{18}W/cm^2) ultra-short (10-100 fs) laser pulses interacting with thin solid foils has attracted increasing interest as a unique tool to investigate new laser-plasma interaction regimes and because of a number of possible application fields. The potential of this technique is related to the possibility of producing multi-MeV protons and ions with a high degree of laminarity and very low emittance. Accelerated ion bunches are short (ps), have a fs synchronization with the driving laser pulse and contain 10^{11} to 10^{12} ions per bunch. The experimental apparatus required by this technique is relatively compact and cheap compared to common acceleration systems. Laser-driven ion sources have been successfully employed for proton probing and proton heating and the possibility of employing them for hadron therapy and for the fast ignition of inertial confinement fusion targets has been widely investigated. However, these foreseen applications require energy up to several hundreds of MeV per nucleon, much higher than the maximum energy of particle beams currently produced by laser-driven acceleration. Thus, great effort is being devoted to enhance the efficiency of the acceleration process and different strategies have been adopted to this aim. A detailed insight of the laser-ion acceleration physics in a variety of experimental conditions has been pursued through both theoretical and numerical studies. Moreover, advanced laser systems have been designed to achieve pulses with super-high intensity (above 10^{20} W/cm^2) and ultra-short duration (30 fs) in order to explore new laser-plasma interaction regimes and acceleration mechanisms.
Finally, novel nano-engineered targets have been studied to properly control the laser-matter interaction phase and to enhance the efficiency of the acceleration process. In this frame, my PhD thesis was devoted to the investigation of novel and enhanced ion acceleration mechanisms through the design, production and employment of engineered nanostructured targets.
The emission of accelerated protons and ions produced by the interaction of ultra-intense ultra-short laser pulses with matter can be due to different physical phenomena depending on the experimental conditions, i.e. the pulse parameters and the target properties. Thus, the design of nano-engineered targets for laser-driven ion acceleration should always take into account both the properties of the specific laser system and the target requirements imposed by the acceleration mechanism under analysis. Target Normal Sheath Acceleration (TNSA) is currently the most investigated and efficient acceleration mechanism. The acceleration process in the TNSA scheme is due to the generation of fast electrons in the interaction between the incident laser pulse and the plasma produced on the surface of a thin solid foil by the pulse itself. As fast electrons propagate beyond the non-illuminated surface of the target, they produce a quasi-static sheath field which in turn accelerates light ions adsorbed on the rear target surface. Thus, the number and the maximum energy of ions produced by TNSA can be increased by enhancing laser absorption and fast electron production. Many target configurations have been recently considered to this aim exploiting different physical processes. During my doctorate, in particular, I've studied the possibility of exploiting the enhanced laser absorption in ultra-low density materials and the resonant excitation of plasmonic surface waves for the design of targets for ETNSA have been investigated.
Multilayer targets composed by a μm-thick Al foil with a low-density C layer (*foam*) on the directly illuminated surface were considered in my PhD activities to exploit the enhanced laser absorption in ultra-low density materials. According to recent numerical studies, the ranges of interest for the foam density and thickness are 3-10 mg/cm^3 and 5-15 μm, respectively. The production and characterization of extremely low density C foams required the development of advanced material science methods. A general approach based on Pulsed Laser Deposition was developed to produce C foams with controlled density and thickness, with satisfactory uniformity on large surfaces and complete substrate coverage. An innovative density evaluation technique based on Energy Dispersive X-ray Spectroscopy (EDS) was experimentally developed and validated exploiting compact coatings and nanostructured thin films with various compositions, a large variety of mesoscale morphologies and density ranging from the density of solid to a few mg/cm^3. A proof-of-concept laser-driven ion acceleration experiment was performed at the UHI100 laser system of the LIDyL facility (France) to test foam-attached target at moderate pulse intensities (25 fs, 5×10^{16} W/cm^2-5×10^{19} W/cm^2) while the role of target properties and pulse parameters was extensively investigated at high intensity (29 fs, 7×10^{19} W/cm^2-5×10^{20} W/cm^2) at the PULSER I laser system of the GIST institute (South Korea). These experiments showed the existence of optimal foam properties for which a significant enhancement of the maximum energy of accelerated ions (from 30% to 250% depending on the experimental setting) was systematically observed with respect to bare Al targets. Maximum H^+ and C^{6+} energies up to 26 MeV and 120 MeV, respectively, were achieved and the possibility of a further enhancement for optimum target-laser coupling is expected. However, these results are interesting in view of some of the foreseen applications of laser-driven ion sources: provided that a high repetition rate configuration is adopted, 10s MeV protons can be employed, for instance, for the production of radioisotopes for medical diagnostics, for material irradiation or radiation detector testing.
A secondary goal of my PhD activities was the participation to a laser-driven ion acceleration experiment performed on grating targets with the aim of completing a previous study by extending the range of explored target properties (different resonance angles and different thickness values) and by analyzing the angular and spectral electron distribution to achieve a deeper comprehension of high field plasmonics effects (for which a relativistically correct theory is not available yet). The experiment was performed at the above mentioned UHI100 laser system (25 fs, 5×10^{19} W/cm^2, 10^{10} contrast ratio). Preliminary results showed clear indications of the production of accelerated electrons along the target irradiated surface, consistent with the excitation of plasmonic surface waves.
In conclusion, in this thesis the possibility of exploiting novel and enhanced ultra-intense ultra-short laser driven ion acceleration schemes through the design, production and employment of engineered nanostructured targets was investigated. This study draws attention to the importance of achieving a suitable coupling between target properties and laser parameters to enhance the efficiency of energy conversion from the incoming laser pulse to accelerated ions, thus exploiting to the highest degree the development of advanced ultra-intense laser facility. Therefore, the development of advanced target concepts, as those described in this thesis, will give a decisive contribute to the worldwide efforts towards the development of advanced laser facilities for laser-driven ion acceleration.

PRIMARY EXERGY COST OF GOODS AND SERVICES: AN INPUT – OUTPUT APPROACH

Matteo Vincenzo Rocco - Supervisor: **Prof. Emanuela Colombo**

Among the large multiplicity of natural resources, the class of *non renewable primary energy-resources* (i.e. fossil fuels) plays a crucial role in sustaining human economies and their production activities. Indeed, the prosperity and the stability of modern societies is inextricably linked to the extraction and consumption of fossil fuels, and the most authoritative projections clearly shows that this trend will hold for the future decades. Political initiatives as well as research efforts are thus facing the issue of the increasingly scarcity of fossil fuels acting in two main directions: (1) claiming a *transition* towards alternative power sources and (2) promoting a rational use of primary fuels through the so-called *energy saving* practice. This thesis focuses on the latter objective: it aims at providing a comprehensive and novel methodology to assess and to reduce the total fossil fuels requirements due to production of goods and service.

Emerging needs in Environmental Impact Analysis

Today, the concept of energy-resources consumption is undergoing a radical re-evaluation, in response to the acknowledged interdependency of the productive sectors with both the environment and the society at large. Indeed, all the production processes of modern economies are sustained, in a both *direct* and *indirect* way, by flows of fossil fuels extracted from natural environment. Therefore, all the goods and services produced within a given economy are characterized by a *primary energy-resources cost*, which is here defined as the *direct* and *indirect* amount of primary fossil fuels required to deliver the considered products and to sustain their Life Cycle (LC). Many efforts are focused on the definition of methods to account for the overall fossil fuels contribution to individual products. From the analyst perspective, two major issues emerge from the literature:

- *Identification of a standardized accounting method.* Although several methods have been proposed, consensus about the most appropriate resources cost accounting scheme is still nonexistent. Indeed, LC methods are often based on arbitrary assumptions and are not unambiguously defined, making results of different analysis of a same system hardly comparable. Moreover, such methods relies on extensive data collection procedures, resulting very expensive in terms of time and data requirements;
- *Evaluation of real efficiency of energy systems*. Performances evaluation of energy conversion systems by means of traditional First and Second Law indicators neglect the indirect effects linked to the indirect consumptions due to non-energy related products and externalities. Novel thermodynamic based indicators are claimed in order to obtain useful insight for the optimization procedure.

In response to these limitations, literature claims to (a) *deepen system analysis and resources cost accounting methodologies* and to (b) *define criteria for primary energy-resources cost assessment suited for analysis and optimization of energy conversion systems.*

Objectives of the research

The general objective of the research is to define and to formalize the *Exergy based Input – Output framework* in order to integrate cost accounting methods and thermodynamic analysis into one comprehensive method for system analysis and optimization. The main features of the developed framework are aimed at dealing with the lacks and the emerging issues highlighted by the literature review, which become the specific objectives of this research:

1. Primary energy-resources cost is defined as the total *non-renewable primary fossil fuels requirements*, expressed in terms of *exergy*, caused by the considered system or product within a given economy;
2. The mathematical formulation of the *cost accounting approach* is based on *Input – Output analysis*, which establishes standard time and space boundaries for any analyzed system or products, encompassing the whole LC. The approach relies on standard and freely available data sources, avoiding extensive data mining processes and resulting in simpler and faster application with respect to traditional process based LCA. Moreover, a specific model is developed to evaluate the side effects that *working hours* requirements have on primary exergy cost of products;
3. The developed approach establishes specific indicators in order to *identify* and to *optimize* the primary exergy efficiency of energy conversion systems in a LC perspective.

The research lies in the broad discipline of *Industrial Ecology*. Specifically, it deepen the topics of *Thermoeconomic Analyses*, *Life Cycle Assessment* (LCA) and *Input-Output Analysis* (IOA).

Structure of the thesis

In the first chapter, a brief overview about the concept of *natural resources* and their role in the economic process is provided. Moreover, a focus on *non-renewable fossil fuels* is made and, finally, the following issues are highlighted: (1) unambiguous definition of primary resources cost accounting technique is required; (2) a unique thermodynamic based metric for the quantification of energy-resources consumption need to be established; (3) the role of working hours in the evaluation of primary resource cost of products need to be clarified. Second chapter presents the state of the art of the cost accounting techniques: mathematical structure of *Input – Output analysis* (IOA) and *Process Analysis* (PA) are formalized for a generic productive system, compared and finally discussed. What emerges from this chapter is that any cost accounting problem may be described in a more efficient, simple and standardized way through IOA rather than using PA. Chapter three performs a critical literature review about the *Thermodynamic based methods for system analysis*. *Energy*, *Entropy* and *Exergy* based Life Cycle methods are comparatively analyzed and one taxonomy is proposed. Finally, the use of such metrics for energy-resources characterization is discussed. What emerges from this chapter is that: (1) exergy is widely considered as the most suited metric to account for energy-resources consumption; (2) exergy based LC methods require further methodological improvements. Chapter four is the core of the research activity: it merges the cost accounting technique of IOA with the concept of exergy, formalizing the *Exergy based Input Output analysis* (ExIO). This method allows to evaluate the primary exergy cost of goods and services produced within a specific national economy. The method uses *Monetary Input – Output Tables* (MIOTs) of national economies as standardized data source. The main methodological achievements of this chapter can be summarized as follows:

- Complete formalization of ExIO method is proposed. Specifically, three different techniques are proposed to account for imported products in national MIOTs;
- The Hybrid ExIO approach is proposed and formalized in order to increase the accuracy of results obtained through the use of standard ExIO analysis and to perform Life Cycle Assessment of detailed products;
- Hybrid ExIO approach is used to perform Thermoeconomic analysis and Design Evaluation of energy conversion systems.

In the fifth chapter, the *Bioeconomic ExIO model* is proposed and formalized to account for the effects that working hours consumption has on the primary exergy cost of goods and services. In the last chapter, the ExIO framework is applied to different case studies: (1) evaluation of primary exergy cost of goods and services produced by different national economies; (2) application of Hybrid ExIO approach for the Thermoeconomic analysis and Design Evaluation of an Italian *Waste to Energy power plant* in a Life Cycle perspective; (3) comparison between primary exergy costs of *manual dishwashing and dishwasher*. Finally, conclusions of the thesis remark its main achievements and also give a perspective about the future possible research paths.

REDUCED ORDER METHODS: APPLICATIONS TO NUCLEAR REACTOR CORE SPATIAL DYNAMICS

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In the analysis of the nuclear reactor dynamics, which is governed by the neutronics, the most spread approach is constituted by the *point-kinetics* equations. This description of the neutronics is based on a set of coupled non-linear ordinary differential equations that describe both the time-dependence of the neutron population in the reactor and the decay of the delayed neutron precursors, allowing for the main feedback reactivity effects. Among the several assumptions entered in the derivation of these equations, the strongest approximation concerns the shape of the neutron flux, which is assumed to be represented by a single, time-independent spatial mode. Nuclear reactors are generally characterized by complex geometries and may feature asymmetric core configurations. Therefore, more accurate modelling approaches might be needed to provide more detailed insights concerning the reactor behaviour during operational transients. It is worth mentioning that the innovative reactor concepts, for instance Generation IV reactors, feature power density and temperature ranges, experienced by structural materials, such that the corresponding spatial dependence cannot be neglected. Moreover, in order to develop suitable control strategies for such reactors, the spatial effects induced by the movement of the control rods have to be taken into account as well.

From the modelling viewpoint, the highest fidelity approach is the so called Multi-Physics (MP) approach, where all the partial differential equations, which describe the involved physics, are solved within the same computational environment. The main drawback of the MP is that the computational burden is quite high, and simulating the entire core turns out to be very demanding in terms of computational costs and times. In addition, it is quite difficult to get the dynamics of the governing system and then set up a simulation tool that may assess and represent the dynamic response of the overall system at different operating conditions.

In this context, computational reduced order techniques, such as the Reduced Basis (RB) method, can lead to a simulation tool with real-time calculation, still solving a set of partial differential equations. The goal of a computational reduction technique is to capture the essential features of the input/output behaviour of a system in a rapid and reliable way, i.e.: (i) by improving computational performance, and (ii) by keeping the approximation error between the reduced order solution and the full-order one under control. In particular, the reduced order modelling is aimed at approximating a parametrized partial differential equation (or a set of partial differential equations) solution with a handful of degrees of freedom instead of thousands or millions that would be needed for a full-order approximation. In this way, the full-order problem has to be solved only for few instances of the input parameter (through a demanding Offline computational step), in order to be able to perform many low-cost reduced order simulations (inexpensive Online computational step) for several new instances of the input.

It is worth mentioning that simplification – or approximation – of an equation, or a system of equations, describing a phenomenon is indeed a reduced order technique and it can be phrased as: "Reduce-then-discretize". The herein proposed reduced order methods are complementary and can be described as: "Discretize-then-reduce" and they can still benefit from the former approach.

This PhD work is aimed at tackling the need of nuclear engineering field to have accurate and reliable fast-running simulation tools, which can be tailored to common control systems, able to reproduce spatial effects, in particular those induced by the control rod movement. The present contribution can be considered as a first step toward building a bridge between the "world of design" and the "world of control". The goal is to demonstrate that reduced order modelling is suited to be applied in more complex (and coupled) industrial problems in order to introduce competitive computational performance and allowing, at the same time, a better investigation, thanks to the parametrization of involved phenomena. To this aim, a methodological approach for developing a reduced order model for systems with increasing complexity, up to a preliminary multi-physics analysis of a Lead Fast Reactor (LFR) single channel, has been proposed as proof of concept. The main novel contribution is the application of most recent advances in computational mathematics, namely the reduced order methods, such as the certified reduced basis method, to nuclear engineering field. According to the author's knowledge and to the current state of the art, this is the first time that such techniques have been employed in this context. Therefore, the work focused more on setting up and assessing an innovative methodology, rather than reproduce a real reference reactor.

The capabilities of reduced order methods with respect to the current and/or classical approaches are firstly addressed. In particular, two modelling approaches based on a Modal Method and on the Proper Orthogonal Decomposition technique, for developing a control-oriented model of nuclear reactor spatial kinetics, are compared. The comparison of the outcomes provided by the two approaches focuses on the capability of evaluating the reactivity and the neutron flux shape in different reactor configurations, where different type of perturbations (i.e., homogeneous or localized) are applied.

Subsequently, the modelling of control rods movement is dealt, solving *ad hoc* parametrized multi-group neutron diffusion equations both in the time-dependent and stationary formulations. Several accurate and reliable reduced order models have been developed, which are able to take into account the spatial effects induced by the rods movement still featuring a real-time computational time. A different sampling technique, within the Reduced Basis framework, has been employed, namely, the centroidal Voronoi tessellation, which allows for a hierarchical parameter space exploration, without relying on an *a posteriori* error estimation. In this way, the Offline computational time might be sensibly reduced.

During the doctoral research, attention has also been paid to the multi-physics modelling approach, where all the involved physics are solved within the same computational environment. In fact, a Multi-Physics and time-dependent model for LFR single-channel transient analysis has been developed. The work focused on the coupling among the neutronic, the thermal-elastic and the fluid-dynamic phenomena. A purpose-made six-group neutron diffusion model has been developed, which allows taking into account the local dependency of the neutron macroscopic cross-sections on the temperature and density fields. It is worth mentioning that the majority of LFR analyses available in literature, which employ computational fluid dynamics codes, do not allow for explicit neutronic feedbacks. Relying on this work, a reduced order model of a *parametrized* multi-physics model of a LFR single channel has been proposed as proof of concept. The potentials of such approach have been addressed by choosing both geometrical and physical parameters. Indeed, the outcomes provided by the developed reduced order model have the same accuracy of the full-order multi-physics problem and a fast-running computational time, allowing estimation of a wide set of output of interest in real-time. A particular strategy for handling the nonlinear coupling terms has been proposed in order to allow for an efficient Offline/Online decoupling.

NOVEL APPROACHES FOR CFD MODELING OF DIESEL ENGINES

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The thesis focuses on the development, implementation, testing and validation of computational tools for Diesel Engines modeling. Different aspects were investigated with a special attention on the Eulerian-Lagrangian description of the injection process and on the interaction of the injected liquid fuel with Cartesian mesh structures. Critical aspects were pointed out, mainly concerning the dependency of energy and momentum exchange between the phases on the spray-grid mutual orientation.
The first half of the thesis deals particularly with the effect that the adoption of Cartesian grid structures can have if evaluated on varying the injector nozzle position with respect to the cell hosting it. To this end, an implementation and evaluation of a novel approach for describing exchange of mass, momentum and energy in Diesel spray CFD simulations based on the Discrete Droplet Modeling (DDM) is presented. During the calculation, each parcel in the domain is surrounded by a spherical volume of ambient gas and interacts first with it instead of interacting directly with the cell volume hosting the parcel. In this way, the interaction volume is independent of the mesh and can be located in more than one cell. This model was implemented using the OpenFOAM® CFD opensource C++ library. It was developed with the aim to reduce grid dependencies related to spray-grid mutual orientation and to the choice of the injector nozzle position with respect to the cell hosting it.
All the sub-models constants were set to match experimental data of a chosen baseline case in non-reactant vaporizing conditions. Then the new approach predictions were firstly compared with standard DDM, initially by moving the injector position within the hosting cell and later by varying ambient density and injection pressure of fuel. In addition, a study of the dependency of the results on the spray-grid mutual orientation was carried out. High-speed imaging and Rayleigh-scattering measurements taken from the Engine Combustion Network (ECN) web database were used to assess numerical results: a good accuracy in the predictions of liquid and vapor spray penetration as well as axial and radial mixture fraction profiles, can be simultaneously achieved on varying thermo-physical and geometrical settings. If applied to engine calculations, the reduced dependency on the nozzle position becomes appreciable when injectors with multiple nozzles are used.
The second part of the thesis focuses on the development of an automated procedure for Cartesian grid generation. The definition of a robust methodology to perform a full-cycle CFD simulation of IC engines requires as first step the availability of a reliable grid generation tool, which does not have to guarantee only a high quality mesh but has to prove also to be efficient in terms of required time. In this part a novel approach entirely based on the OpenFOAM technology is presented. The available 3D grid generator was employed to automatically create meshes containing hexahedra and split-hexahedra from triangulated surface geometries in Stereolithography format. The possibility to introduce local refinements and boundary layers makes this tool suitable for IC engine simulations. Grids are sequentially generated at target crank angles, which are automatically determined depending on user specified settings such as maximum mesh validity interval and quality parameters like non-orthogonality, skewness and aspect ratio. This ensures high quality grids for the entire cycle and requires a reduced amount of user time. Experimental validation was carried out by simulating the full cycle in the so-called TCC (Transparent Combustion Chamber) engine, whose experimental data are available through the ECN database. In particular, a detailed comparison between computed and experimental in-cylinder pressure, turbulence intensity distribution and velocity field was performed so that it was possible to assess the requirements in terms of minimum mesh size and numerical method accuracy to be employed with the proposed methodology.
The final part shows the extension of the automatic Cartesian mesh generation process to sector grids for simulating full-cycle simulations involving injection of fuel and combustion. The choice to use sector meshes implies the hypothesis of axial symmetry, which is commonly accepted when the injector is located at the center of the cylinder head (typical of Diesel applications). The adoption of sector meshes requires the application of cyclic boundary conditions and consequently the perfect correspondence between points and faces on the two sides of the sector. Many features were added to the original approach so that Cartesian sector grids could be generated in OpenFOAM. The grids were generated starting from a real heavy-duty engine geometry and then tested and validated qualitatively and quantitatively on varying minimum mesh size.
Detailed chemistry modeling coupled with Multizone discretization and In Situ Online Tabulation was adopted to describe the combustion process.
Good agreement and limited mesh dependency were found showing that this approach could be generally suitable for engine simulations and hence for application to industrial cases.
All the models, solvers and utilities used in this work were implemented within the OpenFOAM framework, as a contribution to the library "Lib-ICE", developed by the Internal Combustion Engine group of the Energy Department at Politecnico di Milano.