MECHANICAL ENGINEERING I PHYSICS I PRESERVATION OF THE ARCHITECTURAL HERITAGE I SPATIAL PLANNING AND URBAN DEVELOPMENT I STRUCTURAL SEISMIC AND GEOTECHNICAL ENGINEERING I TECHNOLOGY AND DESIGN FOR ENVIRONMENT AND BUILDING I TERRITORIAL DESIGN AND GOVERNMENT I URBAN PLANNING, DESIGN AND POLICY I AEROSPACE ENGINEERING I ARCHITECTURAL AND URBAN DESIGN I ARCHITECTURAL COMPOSITION I ARCHITECTURE, BUILT ENVIRONMENT AND CONSTRUCTION ENGINEERING I ARCHITECTURE, URBAN DESIGN, CONSERVATION OF HOUSING AND LANDSCAPE I BIOENGINEERING I DESIGN I ELECTRICAL ENGINEERING I ENERGY AND NUCLEAR SCIENCE AND TECHNOLOGY I ENVIRONMENTAL AND INFRASTRUCTURE ENGINEERING I INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING I INFORMATION TECHNOLOGY I INTERIOR ARCHITECTURE AND DESIGN I MANAGEMENT ENGINEERING I MATERIALS ENGINEERING I MATHEMATICAL MODELS AND METHODS IN ENGINEERING

PhD Yearbook | 2017

# 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:

| ENERGY AND NUCLEAR SCIENCE AND TECHNOLOGY – 29TH CYCLE | |
|---|---|
| Cattarin Giulio | On the calorimetric measurement of the solar factor of transparent building components in outdoor test cell facilities |
| Cerini Marta | Fuel-coolant chemical interaction for Lead-cooled Fast Reactors by a computational approach |
| Cialfi Lorenzo | Experimental and theoretical studies on target normal sheath acceleration with solid and advanced nanostructured targets |
| Frein Antoine | Modeling, optimization and experimental evaluation of solar direct steam generation for integration into industrial heating processes |
| Iadicicco Daniele | High performance ceramic coating for demo breeding blanket |
| Maghbouli Amin | Development of an advanced multi-dimensional cfd framework for modeling low temperature combustion in direct injection compression ignition engines |
| Mazzola Simone | Operation and design optimization for off-grid hybrid microgrids with high res penetration |
| Pezzoli Andrea | Tungsten-based coatings for magnetic fusion research: damage and hydrogen retention |
| Pini Alessandro | Analytical and numerical investigation of natural circulation dynamics in presence of distributed heat sources |
| Rigamonti Marco Michael | Advanced model-based and data-driven methods for prognostics and health management of industrial systems |
| Sharma Rohit | Experimental study of unconfined and confined isothermal swirling jets |
| Tahmasebi Ehsanallah | Simulation of internal flow in fuel injection process |
| Tumino Francesco | Scanning tunneling microscopy and spectroscopy of two-dimensional oxide nanostructures |
| Wu Yan | Numerical Study of Coherent Structures of in-Cylinder Flow by a Hybrid RANS/LES Model |

| ENERGY AND NUCLEAR SCIENCE AND TECHNOLOGY – 28TH CYCLE | |
|---|---|
| Jerome Ndam Mungwe | Improving access to modern energy services in rural areas of developing countries. Towards a comprehensive access strategy |
| Moghadasi Leili | Characterization of multi-phase relative permeabilities in porous media: experiments and modeling |

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

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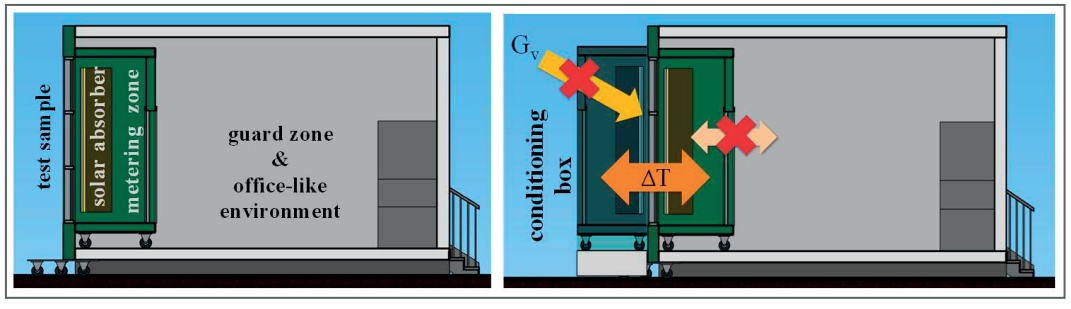
# ON THE CALORIMETRIC MEASUREMENT OF THE SOLAR FACTOR OF TRANSPARENT BUILDING COMPONENTS IN OUTDOOR TEST CELL FACILITIES

**Cattarin Giulio** – Advisors: Prof. Lorenzo Pagliano, Prof. Francesco Causone, Prof. Andrea Kindinis

This thesis deals with the calorimetric determination of the solar factor of transparent envelope components in outdoor test cell facilities and under dynamic conditions.
This type of tests may be used to provide a performance assessment of building components for use in the building industry, in particular in the phase of research and development, and to validate thermo-optical models developed by researchers. Both uses require a rigorous estimation of the measurement uncertainty and care to minimize uncertainty sources under dynamic conditions.
Calorimetric methods for the performance assessment of building components have been largely applied in indoor laboratories and under steady-state conditions. While effects of one or more outdoor weather conditions are sometimes mimicked by means of dynamic schedules, they never fully reproduce the complex interactions of the stochastic processes typical of real climate. Furthermore some outdoor conditions are difficult to mimic, such as radiation diffused by the sky and radiation reflected by the ground. Test cells may fill the gap between laboratories and full-scale buildings, since they maintain the indoor conditions under control, while exposing the test sample to actual outdoor conditions.
Within the present work we conducted an extensive literature review, proposing a classification of outdoor test cells based on the underlying experimental approach (performance assessment in absolute or relative terms) and the construction approach used to minimize heat exchanges through the cell envelope.
The review also summarises previous experimental campaigns conducted in test cell facilities in the last decades and discusses critical issues regarding the measurement of performance indices of advanced (dynamic) building components. The review also presents considerations on the potentialities and limits of test cell facilities and highlights a general scarcity of detailed information on the test cell characteristics and operation, which reduces the replicability and the ease of interpretation of the tests' results. In particular, we found a potential for improvement in the calorimetric determination of the solar factor under dynamic conditions.
The present work investigates the issue of the calorimetric determination of the solar factor under dynamic conditions. In particular, we will address the following questions:

- What is the correct operational definition of the solar factor when determined by means of calorimetric measurements under dynamic test conditions?
- What are the main uncertainty contributions to the overall uncertainty on the measured solar factor?
- When performing calorimetric tests in traditional test cell facilities, what is the impact of the thermal behaviour of the test cell's envelope on the precision and accuracy of the measured solar factor?
- Is it possible to reduce the impact of the above uncertainty contributions? What alternative design configurations and/or control strategies would improve the calorimetric measurements?
- What is the impact of the weather conditions on the accuracy and precision of test results? Is it possible to obtain reliable results when operating the test cell under partially-cloudy sky conditions?

The present work introduces an improved measurement procedure to determine the solar factor under dynamic conditions, applicable to outdoor test cell experiments and taking into account the variation of internal energy in the control volume. The magnitude of the variation of the internal energy depends on the test cell configuration, the operating mode and the test conditions.
An in-depth uncertainty analysis has been conducted in order to highlight the most relevant uncertainty sources and suggest improvements in the measurement techniques, taking into account inter alia the evolution of the meteorological variables during the test.
Based on the indications of the uncertainty analysis, we developed two new strategies to extract and measure the solar load entering through a test sample and a new design concept of test cell facility, which allows adapting the configuration according to the objectives of the specific test (Indoor Environmental Quality tests or calorimetric tests). The calorimetric configuration is represented in **Figure 1**.
In dynamic testing conditions it is or primary importance to take into account the thermal behaviour of the test facility. For this reason, the two proposed strategies and a reference, traditional one have been simulated by means of linear lumpedparameter models and compared from the point of view of the accuracy and precision of the calorimetric solar factor.
The simulation results suggest that, compared to traditional solution, the two proposed solutions offer a higher measurement accuracy and measurement precision in the determination of the solar factor. In addition, the results indicate that partially-covered sky conditions are highly detrimental on the accuracy level of the solar factor measurement; therefore tests should be carried out under fully clear sky conditions.
In order to gain confidence on the ability of our thermal model to predict the thermal behaviour of a test cell, we carried out two experimental validations and an intermodel comparison with the building energy simulation tool TRNSYS. The results of the experimental validations show that the model is able to predict the evolution of the internal air temperature and the envelope's internal surface temperature with residuals lying always within a range of ± 1 °C and lying most of the time within the measurement uncertainty bands. As expected, the residuals are significantly lower for the intermodel comparison (± 0.5 °C) than for the experimental validation, since, when comparing TRNSYS and our Matlab code, input values are not affected by uncertainty, and similar assumptions and simplifications are adopted by both codes.
The simulation work and the exchange with research groups involved in test cell experimental campaigns has led to the development of guidelines for determining the solar factor of transparent components under dynamic conditions, which include indications on the structure of the facility, the typology and accuracy of the sensors, the test procedure, the calculation procedure and the uncertainty analysis.




**1. Left: configuration "Outdoor calorimeter": the test sample is applied on the aperture of the metering box, while the guard zone and the metering box are kept at the same air temperature.
Right: with the configuration "Hot box", it is possible to create stationary or periodically-varying conditions while shielding the test sample against impinging solar radiation.**

# FUEL-COOLANT CHEMICAL INTERACTION FOR LEAD-COOLED FAST REACTORS BY A COMPUTATIONAL APPROACH

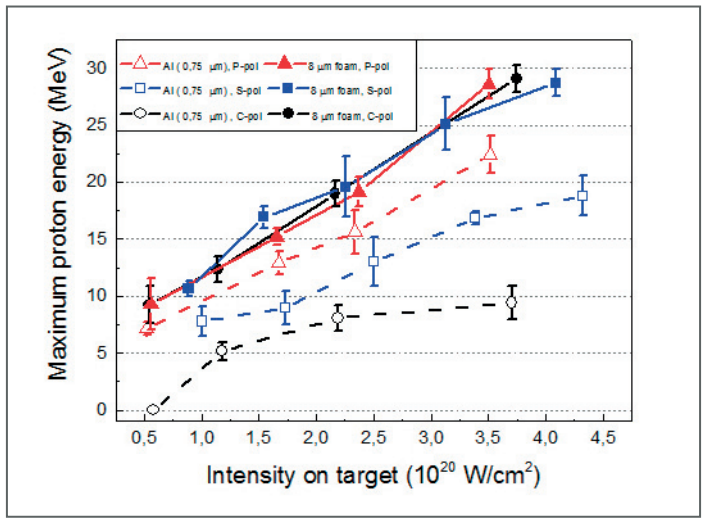
**Cerini Marta** – Advisor: Dr. Elena Macerata

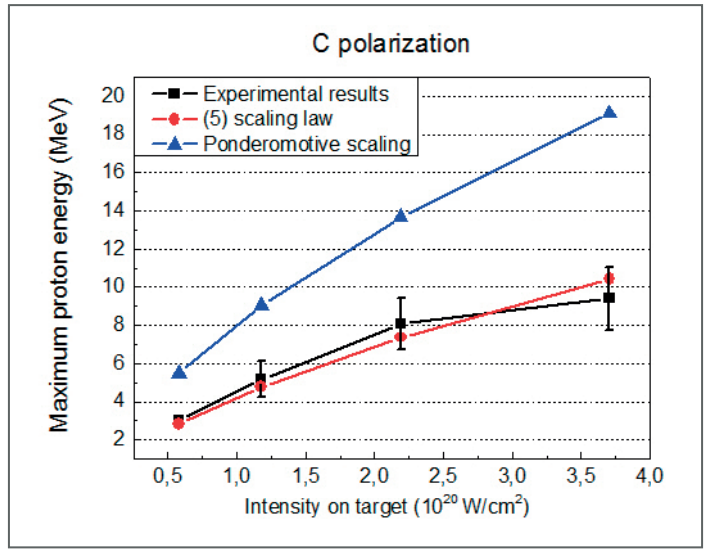
In the last century the population growth has determined an increment of energy demand, revealing the no more negligible problem of the impact of energy generation on the environment. Generation IV nuclear systems, fulfilling high standards in terms of sustainability, economics, safety and reliability, proliferation resistance and physical protection, are now under development, because they could contribute to produce clean energy at reasonable costs. Among the new reactor concepts, Lead-cooled Fast Reactors seem to be promising, even if there are technical challenges that still have to be adequately solved. In particular, the knowledge of the chemical compatibility between the nuclear fuel and liquid lead as coolant is a topic of paramount importance for their development and in particular for assessing their safety. In fact, a cladding failure event could lead fuel in contact with coolant both in nominal and accidental operation conditions and the consequences of such event have to be foreseen in order to plan suitable safety systems.
The present research work deals with the study of fuel-coolant chemical interaction by means of a computational approach. The system originated from the fuel-coolant chemical interaction is a multi-component and multi-phase complex system, whose chemical composition at thermodynamic equilibrium could be studied by minimization of the Gibbs free energy, starting from the database of thermodynamic data of all chemical species involved in the reaction. Due to the lack of experimental thermodynamic data for the majority of compounds of interest and to the difficulties in performing experimental campaigns, an approach based on the Density Functional Theory combined with the Generalized Gradient Approximation (DFT-GGA) was defined. The DFT method was selected because it represents, among the methods of theoretical chemistry, a good compromise between accuracy of the result and computational costs. The validation process clearly showed that the selected method is able to estimate the formation enthalpy, entropy and heat capacity with satisfactory accuracy for intermetallic compounds and oxides, in both gas and condensed phases. Therefore, using well-known computer programs (Gaussian09 and VASP - Vienna Ab–initio Simulation Package codes), the proposed computational method was applied in a semi-systematic way to estimate the missing thermodynamic properties of several species of interest for the case study, on the basis of the binary phase diagrams and other research works available in literature so that the thermochemical database was implemented.
Furthermore, considering few binary systems as case study, it was verified that the SOLGASMIX-PV like code used for the thermodynamic analysis, correctly foresee the chemical composition of the systems on the basis of the estimated thermodynamic data even if affected by a maximum standard deviation of the same order of that found in the validation process.
Moreover, an attempt was made in order to exploit the proposed DFT-GGA approach to gain information about solubility in liquid Pb of the most important fission products and cladding constituents. In particular, the solubility was investigated by applying the infinite dilution model as implemented in the VASP code. The validation process by comparison with a limited number of experimental data highlighted that the model reproduces qualitatively but not quantitatively the experimental solubility.
The computed solubility values were strongly underestimated, however the trends in function of temperature were reproduced as well as the solubility level among the different elements considered.
In conclusion, at the best of the author knowledge, this research activity studies for the first time the chemical interaction between nuclear fuel and liquid lead under reactor operational conditions. Specially, a computational tool able to systematically estimate missing thermodynamic data was proposed, and a thermodynamic database was implemented enabling the evaluation of the chemical composition of simplified fuel-coolant systems at thermodynamic equilibrium.
In general, the research work performed allows to demonstrate that a theoretical approach can be useful to face a problematic such as the chemical compatibility between fuel and coolant in Generation IV nuclear systems, by getting indications that can actively support and better address the experimental activities, which still remain essential to understand all the phenomena that could occur within these new nuclear reactors.

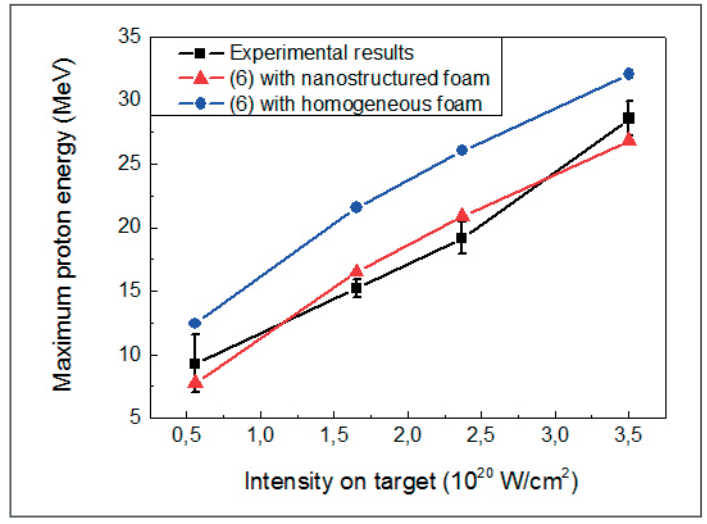
# EXPERIMENTAL AND THEORETICAL STUDIES ON TARGET NORMAL SHEATH ACCELERATION WITH SOLID AND ADVANCED NANOSTRUCTURED TARGETS

**Cialfi Lorenzo** – Advisors: Prof. Matteo Passoni, Dr. Luca Fedeli

Ultra-intense sub-picosecond laser-plasma interaction is a fertile research topic. Laser induced ion acceleration stands out among potential applications for the perspective of providing a compact, cheap (compared to current accelerators) and tuneable ion beam source which can be exploited in: hadron-therapy, neutron/radionuclides production, proton fast ignition and proton imaging. The most experimentally observed mechanism is called Target Normal Sheath Acceleration (TNSA) and can be briefly explained as follows: i) an ultra-intense laser pulse ($I > 10^{18}$ W/cm$^2$) is focused to a target (typically micrometric foils). ii) due to the interaction with the laser pulse it reaches plasma state and an electronic population is heated to high energies (MeVs). iii) these electrons expand through the target and eventually into the vacuum, creating a charge separation responsible for the electrostatic field which accelerates ions on the rear surface up to tens of MeV. Coherently to this description, electron heating plays a crucial role in the acceleration, thus a better control over this process could lead to the development of optimized techniques and, as a consequence, to better performances (e.g. higher maximum energies). The first experimental observations of TNSA were obtained with micrometric solid targets (SLT), in recent years advanced target configurations were proposed. At this purpose, nano-engineered targets have been proven to be ideal candidates. Recent works have shown that using multi-layer targets (MLT), produced by the deposition of a foam layer (~ 10 μm) over the solid one, can increase the laser absorption and ion acceleration capabilities. In the first part of our work we analysed experimental results from two recent campaigns performed in 2014 and 2015 at the PW-class laser facility APRI (GIST, Gwangju, Republic of Korea). As presented in fig. [1], our experimental results demonstrated that under suitable conditions MLTs could outperform SLTs in terms of both maximum energy and total accelerated charge. Fig. [1] also demonstrated that laser polarization strongly influences laser interaction with solid targets while it does not affect MLTs. Besides experimental results, theoretical models proved to be invaluable tools to understand the physics of ion acceleration, providing reliable scaling laws in order to predict experiments and set foundations for future researches. A key parameter in most of the theoretical TNSA models is the electron tem perature. At the state of the art one of the most widely adopted scaling with SLTs is the so called ponderomotive scaling. It provides an estimation of the temperature as a simple function of the laser




intensity, although it doesn't take in account many parameters that are known to influence laser-plasma interaction deeply, such as laser polarization and incidence angle. Moreover, it is not suitable for advanced target designs. In this work we propose a simple law to predict the electron temperature in a wider range of parameters. This model is supported by an extensive 2D and 3D numerical campaign at different incidence angles, intensities and polarization. We then adopted the new scaling law to extend the predicting capability of a known TNSA theoretical model. In fig. [2] we show the comparison between our theoretical predictions and experimental results at different laser intensities in C polarization. A much better agreement with the old ponderomotive scaling is evident.

As anticipated, MLTs could strongly enhance laser-plasma coupling and, as a consequence, laser induce ion acceleration. Electron heating in this scenario is not trivial, since it involves several processes still not completely understood. We have performed an explorative attempt to use a simple scaling law even in this condition. We supported our model with a 2D numerical campaign, adopting two different configurations: a homogeneous near-critical plasma (8 μm) on a bulk thin (0.5 μm) solid target and a more realistic foam with a micrometric mean critical density formed by nanometric sized over-dense nano particles. This investigation proved a strongly enhanced electron heating with respect to simple plain solid targets, also dependent on the foam nanostructure. We finally introduced two simple scaling laws for the uniform and homogeneous foam, respectively. In fig. [3] we present the comparison obtained matching theoretical predictions with our new estimations of the electron temperature and experimental results. We observed a good agreement and better results were achieved with the nanostructured scaling with respect to the homogenous foam one. In conclusion, in this work we investigated with a combined approach TNSA with traditional STLs and MLTs. Our experiments proved that MLT could be a viable solution to achieve better performances. In this PhD we also studied laser induced electron heating, particularly relevant in ion acceleration scenarios. Our results could be combined with TNSA theoretical models to better predict experimental results.

# MODELING, OPTIMIZATION AND EXPERIMENTAL EVALUATION OF SOLAR DIRECT STEAM GENERATION FOR INTEGRATION INTO INDUSTRIAL HEATING PROCESSES

**Frein Antoine** – Advisor: Prof. Mario Motta

## Objectives of thesis work

### *Research theme*

The project scope is to investigate the application of medium temperature [100°C - 250°C] Direct Steam Generation (DSG) from a Linear Fresnel solar reflectors (LFR) into industrial heating processes.

### *Type of study*

The type of study is both numeric and experimental. Detailed numerical models are developed and validated on the Direct Steam Generation Laboratory. Then, they are applied to a real case study, 222 kWth linear Fresnel solar field in Jordan, to characterize the main constraints of this kind of plant. Finally, innovative control strategies and innovative designs are proposed and tested to improve the overall performance and plant stability.

### *Originality*

The industrial sector has been identified as a high-potential and still largely unexplored application for solar thermal. In fact, medium temperatures solar DSG is far from being a mature technology for industrial applications and their market penetration has been slow and difficult. Published performance results from existing installation, both in industrial sector and power generation, are yet scarce. The opportunity to present results from Laboratory test and real case study (RAM, Jordan) is unique and it leads to improve the state of the art of this application. A new methodology for solar field design and flow pattern monitoring is developed and an optimized control strategy and plant layout are proposed

## Research framework

### *Numerical models*

Three numerical models have been developed with three different objectives. A first model is developed to study performance and behavior (pressure drops, steam drum level, flow pattern) of existing solar plants. It is applied to the test laboratory and to the specific case study. It highlights specific transient phenomena that have to be studied more in details under different assumptions. The first phenomena is the effect of the moving evaporation start point within the absorber, done with the dynamic Model 2. The second phenomena is night heat loss of the solar system characterized with the dynamic Model 3.

### *Experimental activity*

A DSG test bench was developed at the department of Energy of Politecnico di Milano (POLIMI), with the objective to validate Model 1 and some of its assumptions:

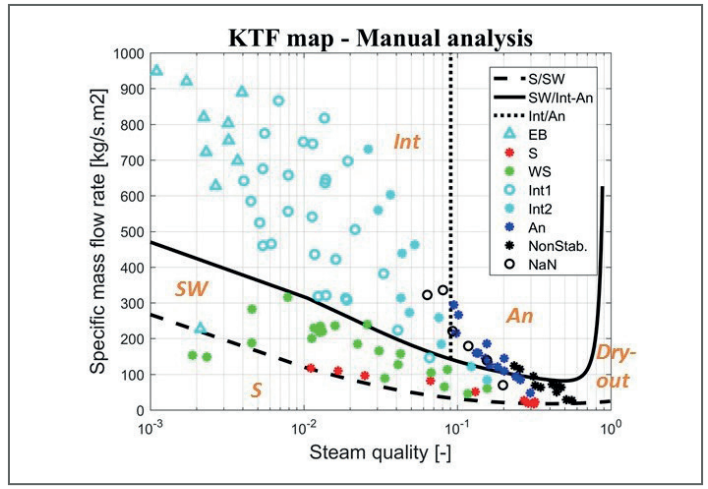
- pressure distribution over the recirculation loop;
- head loss correlations implemented in the numerical model;
- validation of flow pattern map outside of its boundary conditions.

The latter is the most original point as the flow pattern maps used in Model 1 is an extrapolation of Kattan Thome Favrat (KTF) correlations, which have been developed and tuned for refrigerant in small diameter pipe at low pressure. The map is compatible for refrigerants and it is not demonstrated that they are suitable for steam-water systems as its surface tension and density ratio are high with respect to the refrigerant database. In the present study, the KTF correlations have been used outside their boundary conditions for water flow in larger diameter pipes (70 mm compared to 8-20 mm) and higher pressure (3-25 bar compared to 1.1-8.9 bar). The flow pattern transition curves encounter with solar DSG for industrial heating processes delimited the following flow patterns: intermittent, stratified wavy and annular. The experimental activity validates the use of water instead of refrigerant for these specific transition curves. **Figure 1** shows the good agreement between KTF correlations and the experimental tests.

### *Analysis and case study (RAM)*

A system operation with biphasic flow requires a specific optimization to limit the pressure losses, maximize the heat transfer rates and avoid the harmful flow patterns. Requirement as pump cavitation protection , flashing effect minimization and pressure stability should be satisfied for each plant condition.

This analysis is applied to a real case study (RAM plant installed by Industrial Solar) for two distinct periods one in winter (two weeks) and one in summer (two weeks). It is based on the comparison between a validate numerical model 1 and monitored data. The first step consists on a daily analysis of the mass and energy balance for the two specific periods, called global analysis. Then a detailed analysis is applied to one sunny day in winter and one in summer. It consists in the analysis of recirculation pump head loss, liquid level variation of steam drum and daily flow pattern analysis.




**1. Flow pattern maps validation for water as medium**

**2. Linear Fresnel Reflectors at RAM plant in Jordan (source: Industrial Solar)**

### *System optimization*

The system optimization consists in applying the validated numerical models to improve the solar DSG design and control strategy for the specific application of industrial process heat. Different levels of optimization are investigated. The first one is focusing on the methodology to design the solar field layout (parallel vs series, optimal mass flow rate) for a MW plant based on Model 1. The second and third optimizations are focusing on unexpected behavior highlights in the case study. The second one analyzes the effect of fast moving evaporation start point impact with the numerical Model 2 and third one analyzes how night heat loss could be reduced with an improved control strategy. The improvement quantification is done with Model 3.

| ABBREVIATIONS | |
|---|---|
| DSG: | Direct Steam Generation |
| LFR: | Linear Fresnel Reflectors |
| CSP: | Concentrated Solar Powear |
| EB: | Elongated Bubble |
| S: | Stratified |
| SW: | Stratified Wavy |
| Int: | Intermittent |
| An: | Annular |

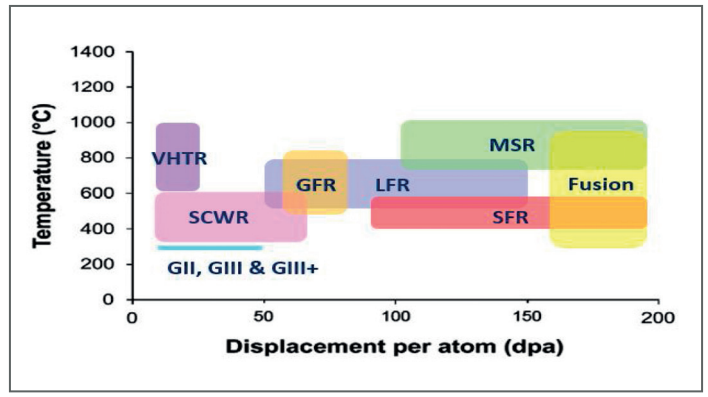
# HIGH PERFORMANCE CERAMIC COATING FOR DEMO BREEDING BLANKET

**Iadicicco Daniele** – Advisors: Prof. Marco Beghi, Dr. Fabio Di Fonzo

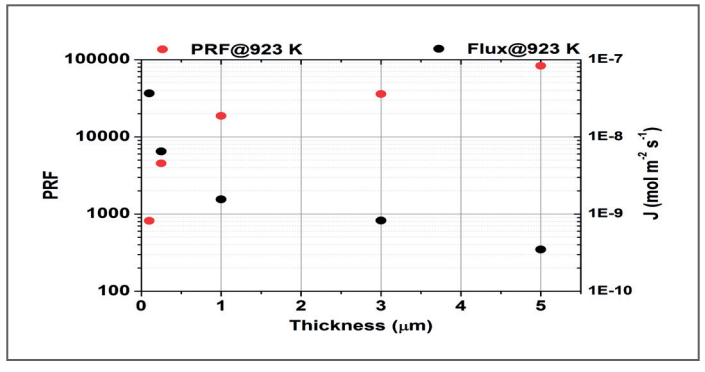
The access to reliable and affordable energy is thought of as crucial to worldwide economic prosperity and stability. Today, nuclear power is totally provided by fission reactors providing about 11% of the global demand of electricity.
According to the **2015 United Nation Climate Change Conference - COP 21 or CMP 21**, held from 30th November 2015 to 12th December 2015 in Paris, nuclear power will play a central role in green house reducing and future energy sustainability.
**Nuclear fusion systems** offer the possibility of an inexhaustible energy source. It has many potential advantages as compared to nuclear fission system, such as:

- **Higher efficiency:** the basic fusion reactions are more energetic than the fission reactions and light nuclei are plentiful and easy to obtain.
- **Safe and controllable:** in case of accident (e.g. LOCA) reaction can be stopped without fuel melting risks.
- **More environmental acceptable:** fusion products are usually light, stable nuclei rather than heavy radioactive ones.

Today, the **tokamak** configuration (as ITER under construction in France), where a **deuterium-tritium** fusion reaction will occur, is considered the most promising design for the future commercial fusion power plants (e.g. **DEMO**). Energy will be extracted from the 14.1 MeV kinetic energy of neutrons producing in the fusion reaction. This energy will be adsorbed, efficiently channelled inside the **breeding blanket (BB). BB** will provide the production of tritium to self-sustain the fusion reaction, and covert the kinetic energy adsorbed into electricity by conventional scheme of a thermal power plant. The main breeder candidate in European project is the **eutectic Pb-16Li**. The general environment framework for the future fusion reactors, in terms of operating temperatures and radiation damage (Displacement per Atom or **dpa**) of the structural materials in shown in **figure 1**.
The choice of suitable structural materials for the BB environment remains however the main technological issue to be solved to DEMO deployment. In addition to high power density, high temperatures, high dose by energetic neutron spectrum **corrosion aggressiveness** and **tritium permeation** impose several and special requirements to structural materials.
Dimensional stability (in terms of void swelling, thermal and irradiation creep), adequate thermal, mechanical, and chemical properties, as well as corrosion, tritium retention and liquid metal embrittlement resistance should be guaranteed under all operating conditions.
To tackle tritium permeation and corrosion attack by heavy liquid metal, an adequate protective barrier is required. Advanced ceramic coatings, in particular **alumina** ($Al_2O_3$), are suitable towards this task thanks to its chemical inertia, high density and amorphous character.
In this framework, this **Ph.D.** thesis deals with the characterization and the testing under **DEMO**-relevant conditions of a corrosion resistant hydrogen permeation coating. To meet these requirements, custom processes, namely **Pulsed Laser Deposition (PLD) and Atomic Layer Deposition (ALD)**, is proposed according to a bottom-up approach. The main advantages of **PLD** is that it allows tailoring the structural features and mechanical properties of the coatings through **nano-scale engineering**. Previous characterization, underline an unusual ensemble of **metal-like** mechanical properties which can be explained in terms of structural features.
The characterization of the coating as hydrogen permeation barrier is performed in collaboration with C.R. ENEA (Brasimone (BO) – Italy) by means the PERI II facility. As a general statement, PLD-grown alumina (onto eurofer 97 disks of 52mm of diameter) performs effectively as permeation barrier in gaseous condition, in tests performed up to 650°C and 100mBar of hydrogen partial pressure. An unprecedented **Permeation Reduction Factor (PRF)** value near to $10^5$ are obtain, with a dramatically decreasing of **Permeated flux (J)** of hydrogen, as shown in figure 2. By means the **diffusion-limited model** of permeation, some physical quantities such as **permeability** and **activation energy** are defined. The analyses reveal as alumina act as barrier permeation increasing, up to five time, the activation energy of couple coating-substrate (56,59 kJ mol$^{-1}$) respect to the bare sample (11,4 kJ mol$^{-1}$). The effectiveness of the permeation coating is evaluated in **DEMO**-relevant corrosion environment. Eurofer 97 plates are both sides covered with 1μm of PLD-grown alumina. Short test (1000h) at 550°C in saturated condition of Pb-16Li are performed at C.R. ENEA, performs effectively as a corrosion barrier. Thus, **PLD**-grown $Al_2O_3$ is a suitable and promising coating materials, as barrier, for **Nuclear Fusion** breeding blanket.
Finally, to improve the coverage of PLD-grown coating in complex geometries like **BB** and **ALD** facility is developed. In particular, ALD is developed in stop flow and optimized to grown coating onto stainless steel substrates, such as eurofer 97 samples. A first of kind thin films of the most common metal oxides namely $TiO_2$ and $Al_2O_3$ are produced with a good adhesion and conformality in a defects and pinhole free coating.




**1. Temperature and DPA requirement for structural materials for future concept nuclear reactors. The dimensions of the rectangles define the ranges of temperature and dpa for each reactor design.**




**2. PRF and J for samples coated with different thickness of alumina coating tested in PERI II at 923K**

# IMPROVING ACCESS TO MODERN ENERGY SERVICES IN RURAL AREAS OF DEVELOPING COUNTRIES. TOWARDS A COMPREHENSIVE ACCESS STRATEGY

**Jerome Ndam Mungwe** – Advisor: Prof. Emanuela Colombo

This thesis was realized as part of the research activities of the UNESCO Chair in Energy for Sustainable Development, Department of Energy and in collaboration with the University of Milan and the Catholic University of Cameroon, Bamenda. It contributes to the development of a *"comprehensive energy access strategy"* to improve access to modern energy services for cooking within the context of households in rural areas of SSA.

It is projected that more than 650 million people in the region will continue to rely on the traditional use of biomass beyond 2040. Increasing access to energy in DC may entails innovative business models, increase investment, policies and a comprehensive access strategy, etc. In particular, a "comprehensive energy access strategy" is envisaged in order to intensify research, development and dissemination of small scale technologies to improve energy access.

Existing Rural Energy Planning (REP) procedures do not consider the sustainability of rural energy systems; do not take into account the existing rural energy supply system and the energy services supply network (ESSN) do not allow for a cost-effective way to identify appropriate end-use devices to meet the energy services demanded.

The selection, research and development of small scale technologies like biogas digester within the intended application context could be a sustainable solution to the issue.

The thesis had three specific objectives, namely:

1. To propose a comprehensive procedure for the SE of rural areas of DC.
2. To develop and apply a Decision Support Tool for the selection of an appropriate small scale technology to improve access to energy in rural areas.
3. To elaborate a procedure for the optimization of the performance of the selected technology within the local context.

The methodology to achieve these objectives included review of literature, desk studies, field case study, experimentation, and laboratory investigations with application of numerical techniques.

## Results

1. **Improved Rural Energy Planning Procedure:** The Nissing et al six-step planning procedure was adopted and modified in two ways: (i) it was extended to account for the existing energy situation. This allowed for the creation of a systematic database and quantification of energy consumptions to levels required for a realistic energy system modelling (ii) energy drivers were integrated in the ESSN model. This allowed for a more cost-effective way to identify appropriate end-use devices to meet the energy services demanded and resolved the issue of "technology stacking" in households. The validity of the modified procedure was demonstrated in a rural context through a case study in Cameroon. The results showed an improved, reliable, affordable and diversified primary energy supply based on local energy resources; 85% increase in final energy consumption by the rural community and a 50% improvement in energy efficiency. Alternative and more sustainable energy sources, such as biogas, hydropower and solar featured in the new energy mix of the community. Some of these sources, especially biogas could be exploited to improve access to modern energy carriers for cooking.
2. **Technology selection process:** The Analytic Hierarchical Process was elaborated and applied in the selection of an appropriate technology. The selection of an appropriate digester design for dissemination in Cameroon was used to demonstrate the application of the selection strategy. Technical, economic, social and environmental criteria were used together with appropriate indicators following the approach of the Energy Indicators for Sustainable Development. Amongst the five identified candidate digesters, the Nepali GGC2047 design emerged as the appropriate design for the context of Cameroon.
3. **Technology optimization:** this was carried out in three steps. This first step was the field experimentation of a full scale unit of the Nepali GGC2047 digester installed and operated within the socio-economic and environmental context of rural Cameroon in order to identify issues which may relate to the performance of the technology in its operational milieu. Two crucial issues affected the performance of the design within the local context, namely: water scarcity, which led to the digester being operated at 16 %TS higher than the designed 10 %TS concentration in the influent. The average operating temperature inside the digester was 26 °C, which was below the 30-35 °C optimal range for mesophilic digestion. The digester design operated between upper psychrophilic and lower mesophilic range of temperature, away from its design mesophilic operation. The biogas production rate was 0.16 $m^3_{biogas}/m^3_{digester}$ per day and productivity was 0.18 $m^3_{biogas}$/kgVS. These values were lower than the expected values of 0.34 $m^3_{biogas}/m^3_{digester}$ per day and 0.25 $m^3$/kgVS respectively. The energy recovery efficiency was only 20%. The low technical performance of the design could be related to poor mixing of the digester content and low temperatures. This thesis focused on improving mixing of the digester content.

The second step involved laboratory investigations using CFD techniques carried out on eight candidate inlet configurations which were suspected to improve mixing of the digester content. The funnel-shaped inlet configuration which opens into the digester seemed to improve mixing of the digester content. The effect of this inlet configuration on the performance of the digester was further investigated through a field experimentation.

The third step was a field experimentation to validate the effect of the modified inlet configuration on the performance of the selected Nepali GGC2047 design. A first experimentation was between August 2015 and January 2016 during which it was realized that the modified inlet was poorly produced due to insufficient local manufacturing know-how. A second experimentation was carried out between January and September 2016. The modified digester and the control digester in both campaigns were operated under the same essential operating conditions. During the first campaign, the mean biogas production from the modified digester was 0.159 ± 0.098 $m^3$ while the control digester had a mean production of 0.267 ± 0.171 $m^3$. A t-test of the hypothesis produced a p value of 3E-05. During the second experimentation, the mean biogas production from the modified digester was 0.239 ± 0.134 $m^3$ while the control digester had a mean production of 0.296 ± 0.067 $m^3$. A t-test of the hypothesis produced a p value of 0.005. Thus the modified inlet seemed to demonstrate an improved mixing of the digester content. The second version of the modified digester produced better results than the first. This showed that, translating, high-tech laboratory results into locally produced technology is a challenge in the context of DC where the development of small scale energy technologies is still in the embryonic stages. Thus the optimization of small scale technologies to improve access to energy would necessitate coupling laboratory analysis with local capacity building in manufacturing know-how.

## Conclusions

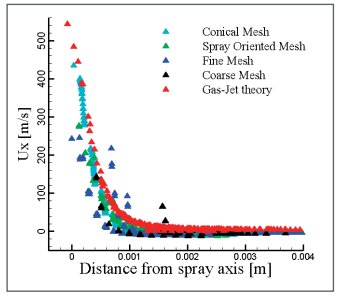
Improving access to modern energy services for cooking in DC would require the integration of the concept of SE within a "comprehensive energy access strategy". This study fulfilled the set specific objectives, namely: an improved REP Procedure is proposed, the AHP was developed and applied in the selection of an appropriate small scale technology to improve access to cooking in the context of DC, a three step procedure for selected technology optimization was developed.

The outcomes of this thesis were consolidated into a three-stage energy access strategy (Figure) named *"Towards a comprehensive energy access strategy for DC"*, thus making a contribution to the search for a comprehensive energy access strategy to improve access to energy in rural areas of DC, as highlighted in the REN21 Global Status Report 2016.

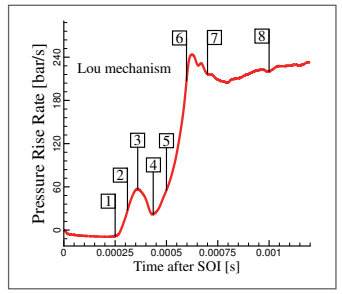
# DEVELOPMENT OF AN ADVANCED MULTI-DIMENSIONAL CFD FRAMEWORK FOR MODELING LOW TEMPERATURE COMBUSTION IN DIRECT INJECTION COMPRESSION IGNITION ENGINES

**Maghbouli Amin** – Advisors: Prof. Gianluca D'Errico, Prof. Tommaso Lucchini

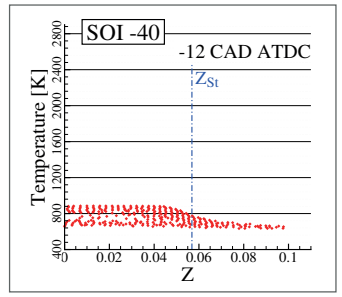
The main objective of this work is to study combustion characteristics of the reacting high pressure liquid sprays and compression ignition Diesel engines under conventional and low temperature operating modes by development of a robust computational framework. All the computational efforts in this work 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 of Politecnico di Milano. Reactive spray modeling has been done under RANS turbulence modeling methodology and Lagrangian Droplet Eulerian Flow formulations of multi-dimensional computational fluid dynamics modeling perspective.
Initially, Conical and Spray-Oriented grids were introduced for non-reacting liquid spray simulations and noticeable enhancement of air-fuel mixing process and better representation of the scalar dissipation rates were depicted. Figure below shows comparison of different mesh types, Cartesian and Spray-Oriented and Conical for velocity distribution compared to the gasjet analytical theory results.
It was shown that a reliable non-reacting simulation is the perquisite of accurate results for reacting liquid spray simulations. In this regard, uncertainties from the liquid spray simulations should be minimized. For instance, it was shown that occurrence of cavitation while injecting of the liquid fuel can highly alter the spray properties, breakup, evaporation, air-fuel mixing, and subsequent combustion. It was discussed that for the fuels that are more prone to cavitation care must be taken both in experimental observation and measurements and numerical model selection and application.
Attention then was given to the reactive simulations of the Engine Combustion Network Spray A and Spray B configurations. Two well-known combustion closures, models based on well-mixed assumption and flamelet concept, with enhanced applicability were selected. After extensive validations over wide range of operating conditions in case of ambient temperature, density, oxidizer level, and injection pressures, a detailed combustion phasing analysis and mathematical reasoning of observed model-to-model differences were made. As depicted by figure below Pressure Rise Rate was introduced as an effective parameter to distinguish different phases of the Diesel combustion.
Pressure rise rate of baseline Spray A case for multi-zone well-mixed combustion model using Lou n-dodecane chemical mechanism.
Ignition Delay and length of flame lift-off are characteristics of Premixed Combustion and Diffusive Combustion phases, respectively. As the figure above shows, pressure rise rate can be used as a global parameter both in the experiments and in the numerical simulation to identify ignition and separate phases of the Diesel combustion. This will help to comprehensively explain transient Diesel spray flame from the sequence of start of liquid fuel injection till the time for established diffusive flame.
It was concluded that there is a shift of reaction zone from leaner mixture fractions ($Z_{MR}$, so-called Most Reactive mixture fraction) of the baseline Spray A conditions in the Diesel spray periphery to the rich mixture fractions in the tip of the spray. This will generate initial rise in the pressure rise rate diagram. Pressure rise rate then reduces as reaction zone burns the premixed fuel which is prepared during the ignition delay time but then again increases as combustion phases from the premixed combustion to the diffusive combustion. It will then plateaus once the diffusive flame is fully established and progress of the combustion is then depends on mixing of fuel and oxidizer. As $Z_{St}$, Stoichiometric mixture fraction is already ignited, combustion then proceeds in high temperature diffusive combustion manner provided by the governing time and length scales of the sub-grid scale mixing.
This is the place Turbulence Chemistry Interactions (TCI) plays a significant role and the models that neglect TCI, are generally unable to have acceptable predictions for the heat release rate and flame structure and lift-off.
Lastly, study was focused on modeling of Partially Premixed Compression Ignition (PPCI) engines as an advanced Low Temperature Combustion (LTC) mode. It was discussed that how air-fuel mixture stratification levels can modify the history of pressure and heat release rate. Air-fuel mixture stratification which was introduced by partial premixing, creates mixture with different reactivity levels. This can be seen for two case of start of injection at -80 as low and -40 as high air-fuel stratification cases in figure below at the time of first stage ignition:
Z-T diagram of flame structure for the low and high mixture stratification at their first stage ignition. $Z_{St}$=0.0558.
This difference in mixture reactivity range was reduced the time delay between first and second stage combustion providing better controllability on timing of the main heat release stage. This practical advantage can be effectively used by engine designers to gain optimum engine output while maintaining pollutant emissions in desired levels.




**Velocity distributions on the injection axis for four mesh types compared to the analytical gas-jet theory results.**




**Pressure rise rate of baseline Spray A case for multi-zone well-mixed combustion model using Lou n-dodecane chemical mechanism.**




**Z-T diagram of flame structure for the low and high mixture s tratification at their first stage ignition. $Z_{St}$=0.0558**

# OPERATION AND DESIGN OPTIMIZATION FOR OFF-GRID HYBRID MICROGRIDS WITH HIGH RES PENETRATION

**Mazzola Simone** – Advisor: Prof. Ennio Macchi

## Background

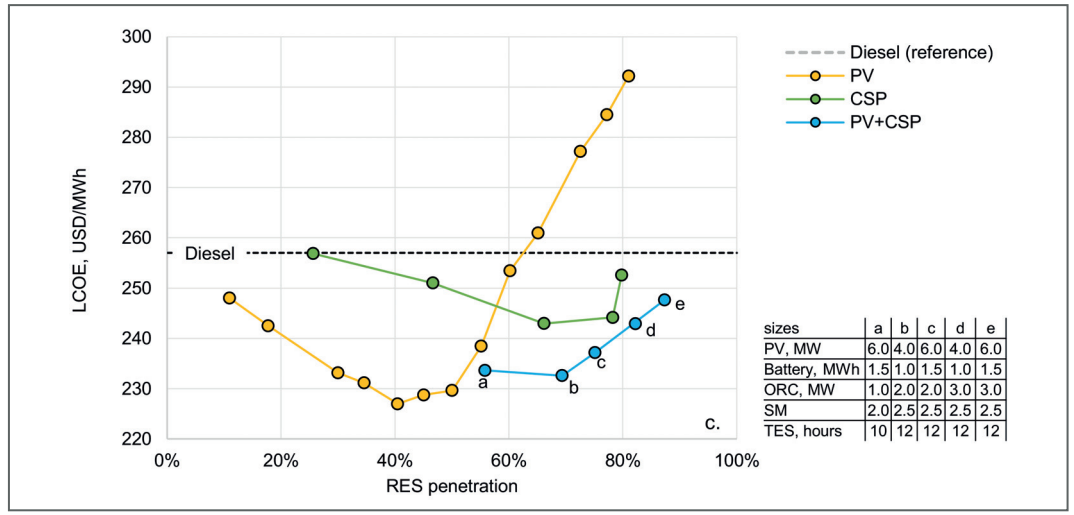
Nowadays, electricity production in off-grid contexts is mainly based on fossil fuels, especially diesel. Considering that diesel oil cost is considerably higher than on mainland, this entails very high electricity costs together with other drawbacks, as the energy dependence from the outside and possible environmental concerns. Renewable energy sources (RES) have proven to be effective to reduce the overall electricity costs in remote contexts and to ensure a sustainable energy access, characterized by low emissions of pollutants and carbon dioxide. For these reasons, we are witnessing at numerous projects worldwide aiming at 100% production from renewables. Unfortunately, this goal is not feasible in a cost-effective way relying only traditional RES as sun and wind, which are characterized by a strong intermittency and it would require huge energy storages.

## Methodology

The thesis starts from this background and investigates two possible approaches to increase RES penetration without incurring in a sharp increase of electricity cost. The core objectives are two. The first one was to develop innovative mathematical tools to efficiently operate and simulate off-grid microgrids operation. The most important capabilities and features are the following:

- units scheduling based on forecast-based optimization
- detailed representation of components behavior (e.g. startups, battery wear)
- capability to handle advanced microgrids architectures, with multiple valuable goods
- limited computation time, compatible for real time operation and long-term simulation

The state of the art analysis showed that such a tool was not present in literature and it has been developed from scratch using AMPL optimization language. The final model is capable to operate and simulate advanced microgrid architectures considering not only electricity request, but also other valuable goods as heating and potable water. This capability is obtained resorting to a rolling horizon approach, which allows to simulate the behavior of complex microgrids using an optimization model for scheduling with a limited time horizon for forecasts.
State of the art models describing the wear and the kinetics of the battery energy storage, which is one of the key component of an off-grid energy system, have been embedded in the optimization problem, as well as start-up constraints and costs for components as diesel generators and biomass boilers. Despite of the increasing complexity of the optimization problem, computation time are sufficiently low for real-time operation and, using expedients as variable time steps unit commitment, the model can be effectively used to perform long-term simulations and system design.
The potential cost savings in operation related to the developed model in comparison with standard non-predictive approaches was evaluated. Results show that considerable cost savings on microgrid operation (4-8%) are achievable, especially in microgrids with a high share of renewable energy sources (RESs). On the other hand, the study highlights that these savings are strictly related to the forecast accuracy and the potential advantage could vanish in the case of low quality forecasts. Another important point emerged from the simulations is that the dispatch strategy used for simulations has an impact of the optimal sizing of the microgrid. In fact, using standard non-predictive approaches lead to conservative sub-optimal solutions, in which the share of RES is limited.
Note that these results have been obtained temporally removing some key features of the models only to make it comparable with state of the art models. The advantages obtainable in advanced multigood microgrids are expected to be higher, as shown in the two final test cases of the thesis.




**1. LCOE as a function of RES penetration obtained with PV, CSP and a hybrid system in comparison with traditional diesel oil generation (dotted line) in a remote island.**

## Simulation results

The second main objective was to investigate the possibility to increase RES penetration in remote contexts in a cost-effective way, exploring the two following alternatives:

- load scheduling to cope with the intermittency of RES as PV
- feasibility of dispatchable RES generators, considering biomass-based systems and CSP

Both possibilities were studied applying the developed mathematical model on two test-cases, a rural village in a developing country and a community in an island. Despite of the considerable differences between the two test-cases, the insights coming from the results are the same. First, the studies show that advanced models used for microgrid operation allows to handle efficiently a large amount of intermittent RES, as PV. In fact, the possibility to shift in time a part of the loads helps to match the RES production, reducing the curtailment and the battery usage. In the case of the rural village this possibility is given mostly by the irrigation needs; thanks to a relatively inexpensive water tank, it is possible to shift in time the energy consumption by the pumps without changing the water supply schedule. In the case of the island, same synergy can be found with desalination units, which are responsible of a good share of total electricity consumption (10-20%) and can be shifted in time using a potable water storage. However, even using this possibility, the RES share reachable using only PV is limited (<50%) because a massive usage of battery storage, with the consequent expenses, is requested to increase the RES penetration.
The other possibility investigated is the use of programmable RES generators. The implementation of wood biomass generators was considered for the rural village while the use of Concentrating solar power technology (provided with a thermal energy storage) was considered for the island community. In both cases, the dispatchable generators cam reach considerably higher RES share (>60%) offering a considerable cost reduction compared to the only-diesel case. Despite these technologies have a higher LCOE than PV if connected to a grid with infinite capacity, their capability to produce energy when it is needed represents an important advantage in off-grid contexts.
Finally, test-cases show that the most cost-effective configurations to reach high RES penetration are hybrid ones (see Figure 1). A proper balance of intermittent and dispatchable RESs is the best option, benefiting of low energy cost of the former and the dispatchability of the latter to cover most of the electricity requests.

# CHARACTERIZATION OF MULTI-PHASE RELATIVE PERMEABILITIES IN POROUS MEDIA: EXPERIMENTS AND MODELING.

**Moghadasi Leili** – Advisor: Prof. Fabio Inzoli

Flows of two or more phases through porous media are common in a diverse range of geological processes and industrial areas, such as petroleum reservoirs. The analysis and understanding of multiphase flow is of paramount importance if processes involving multiphase flows are to be optimally and safely designed and controlled.
We present experimental investigations of multi-phase (two-phase (oil/water, oil/gas) and three-phase (oil/ water/ gas)) relative permeabilities performed at eni laboratory (LAIP).
The tasks undertaken during this research include the following three main steps: (*a*) laboratory measurements of multi-phase relative permeability and corresponding saturations on diverse rock samples, (*b*) assessment of a set of alternative two-phase models by estimating model parameters within a Maximum Likelihood (ML) framework in the context of the interpretation of laboratory scale experiments and (*c*) feasibility of direct numerical multi-phase flow modeling through porous media directly at the pore-scale.
The first part of this study falls into two main categories of (*i*) two-phase relative permeabilities conducted on different core samples a (Sand-Pack, Berea sandstone and a Portland limestone) by way of a Steady-State (SS) technique and (*ii*) SS three-phase experiments performed by following an IDI (Increasing-Decreasing-Increasing) saturation path on Sand-Pack. Spatial and temporal dynamics of in-situ saturations along core samples are directly measured through an X-Ray absorption technology. The latter yields detailed distributions of (section-averaged) fluid flow phases through the medium, which can then be employed for the characterization of relative permeabilities.
In the two-phase setting, we perform SS imbibition and drainage relative permeability measurements. The two-phase experiments are motivated by the observation that appropriate modeling of two fluid displacement in porous media requires to be firmly grounded on accurate and representative core flood experiments and appropriate interpretation of laboratory evidences. As a result, experimental curves embed key information relating relative permeability to these observables and are explicit representations of the nature of multiphase flow taking place in natural media.
For the oil/water settings we consider low and high viscose oil, our findings supporting the observation that relative permeability to oil and water is sensitive to oil viscosity. The comparison of different preamble samples high displacement efficiency and recovery factor corresponds to the high permeable and well-connected pores.
In the three-phase experiments, water and gas relative permeabilities display an approximately linear dependence on the logarithm of their own saturation. Consistent with the observation that oil behaves as an intermediate phase in our system , three-phase oil relative permeabilities lie in between those of their two-phase counterparts.
The complete experimental data-base is here illustrated and juxtaposed to results obtained by the implementation of commonly employed two- and three-phase relative permeability models.
Our data-set stands as a reliable reference for further model development and testing, as only a limited quantity of three-phase data are currently available. In this study, we also illustrate the benefit of employing direct X-Ray measurements of fluid saturation through a set of laboratory experiments targeted to the estimate of multi-phase relative permeabilities of homogeneous samples.
In the task (b), we consider a set of empirical two-phase relative permeability models which are typically employed in industrial applications requiring water/oil relative permeability quantifications. We illustrate the way formal model identification criteria can be employed to rank and evaluate a set of alternative models in the context of the interpretation of laboratory scale experiments yielding two-phase relative permeability curves. The parameters of each model are estimated within a Maximum Likelihood framework. Model uncertainty is quantified through the use of a set of model weights which are rendered by model posterior probabilities conditional on observations. These weights are then employed to (i) rank the models according to their relative skill to interpret the observations and (ii) obtain model averaged results which allow accommodating within a unified theoretical framework uncertainties arising from differences amongst model structures. Posterior probabilities reveal that in several cases, most notably for the assessment of oil relative permeabilities, the weights associated with the simplest models is not negligible. This suggests that in these cases uncertainty quantification might benefit from a multi-model analysis, including both low- and high-complexity models. In most of the cases analyzed we find that model averaging leads to interpretations of the available data which are characterized by a higher degree of fidelity than that provided by the most skillful model.
In the latter part of the thesis (task (c)), we provide evidence of the feasibility to employ Computational Fluid Dynamic (CFD) for fluid flow modeling through a porous media so core samples experiments may be optimized. Through this modeling, the relative permeability curves for two-phase (oil /water) in a porous medium can be estimated.

# TUNGSTEN-BASED COATINGS FOR MAGNETIC FUSION RESEARCH: DAMAGE AND HYDROGEN RETENTION

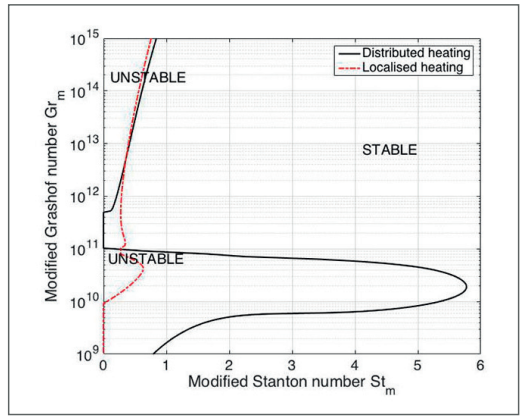
**Pezzoli Andrea** – Advisors: Prof. Matteo Passoni, Dr. David Dellasega

The main objective of my Ph.D. thesis was to study the properties of non-conventional tungsten-based layers and their behaviors when faced to fusion relevant plasma.
One of the most studied design solutions for a fusion power plant uses suitable magnetic fields to confine a hot (temperatures of about $10^8$ K) deuterium-tritium plasma in a torus shape, in devices called tokamaks. The most advanced experiment focused on controlled nuclear fusion is the ITER project, which is scheduled to start its operations in 2025 with the ambitious goal of proving the scientific feasibility of fusion energy production. Nowadays, nuclear fusion is an attractive option for satisfying energy demands because it makes it possible to produce energy on a large scale by using cheap and abundant fuels with negligible levels of greenhouse emissions.
During plasma discharges, Plasma Facing Materials (PFMs) must withstand extreme conditions, such as very energetic neutrons (14.1 MeV neutrons able to generate radiation fields of about $10^3$ Gy $s^{-1}$) and high particle fluxes (up to $10^{24}$ $m^{-2}$ $s^{-1}$), as well as extreme heat loads (20 MW $m^{-2}$ during steady-state operations and 10 GW $m^{-2}$ during off-normal events). These phenomena induce severe modifications on PFMs, which can lead to erosion and sputtering processes. The eroded materials can migrate and re/co-deposit in other regions of the first wall, depending on tokamak geometry and design. In order to minimize these effects, different materials have been studied as PFMs: tungsten (W) has shown a good capability of facing thermonuclear plasmas because of its properties (high melt temperature, high thermal conductivity, low sputtering yield and low hydrogen isotope permeability and solubility).
Even though the operative conditions of present-day tokamaks are not comparable with those foreseen for ITER and future reactors, their harsh environments make it possible to obtain first insights about material damage, material erosion, migration, mixing and re/co-deposition phenomena. These W-based re/co-deposited layers show complex morphologies, structures, elemental compositions and stoichiometries. Due to their peculiar features, re/co-deposited layers can retain extremely high amounts of hydrogen isotopes. Since the availability of layers made in tokamak environments is limited, it is essential to develop a material science approach which consists of depositing, via a suitable technique, coatings with desired and fusion-relevant properties and of testing these materials in dedicated linear devices which make it possible to simulate tokamak-like plasma.
The goals of this thesis were to produce W-based coatings, to characterize these systems via suitable analysis techniques and to expose these tailored films to relevant plasmas and address the relationship between film properties, hydrogen isotope retention and modifications induced by plasma itself.
The Pulsed Laser Deposition (PLD) technique was used to produce different W-based films. In addition, thermal annealing treatments were used both to study modifications induced by ITER-relevant temperatures and to have an extra degree of freedom to control film properties. Finally, selected W-based films were exposed to ITER-relevant plasmas which were produced by the PILOT-PSI, Magnum-PSI and PSI-2 linear devices. These machines can work either in a pulsed or steady-state regime: the former can produce high flux plasma shots, while the latter can generate low flux continuous plasma.
The production of relevant W-based films has been focused on depositing films with controlled properties in order to produce coatings that are relevant for magnetic fusion research. In particular, it was possible to deposit metallic W, W-O and W-N films with compact, porous and multilayered morphologies.
The deposition conditions were carefully optimized. In particular, helium, argon, oxygen, nitrogen and mixed atmospheres were explored. These investigations focused on the possibility of controlling film morphology and structure by selecting deposition pressure and the gas type: low pressures make it possible to obtain compact films, while high pressures induce porous morphology formations. Moreover, it was highlighted that porous film morphology naturally induces gas inclusion within the films.
Coatings, which were deposited in a reactive atmosphere (i.e. oxygen and nitrogen), exhibit a threshold deposition pressure above which oxide or nitride formation occurs and below which metallic films with a high gas inclusion were made.
Thermal annealing treatments made it possible to control both film structure and gas content: it was highlighted that the crystallization temperature in these metastable systems is lower than that of bulk W. Moreover, electrical resistivity measurements of annealed films, which were done in order to evaluate the overall system status, made it possible to show the variation of defects and impurities in films with regard to annealing temperature and to qualitatively quantify the recovery processes with regard to annealing temperature. Moreover, these temperature investigations highlighted a collateral aspect that is of particular interest: W-oxide nanowire nucleation and growth was possible in a very interesting regime by opportunely calibrating oxygen content in films and annealing temperatures.
Some selected W-based films were exposed to deuterium (D) tokamak-relevant plasmas to study their retention behavior and morphological modifications with regard to their as-deposited properties. The exposed samples can be divided into metallic W samples and W-O samples.
In particular, in the case of metallic-W films, it was highlighted that both high-flux plasma ($10^{24}$ $m^{-2}$ $s^{-1}$) and low-flux plasma $10^{21}$ $m^{-2}$ $s^{-1}$) induced morphological modifications and D retention values that are comparable in the same film types. The D retention and morphological modifications strongly depend on the defect density of coatings. In particular, high defect densities induce large D retention values, up to 20 times higher compared with bulk W, and intense morphological modifications. Interestingly, it was highlighted that a linear dependence seems to exist between D retention and film mean crystallite sizes, while a non-obvious dependence appears between D retention and film oxygen content, on the other hand. In particular, it was demonstrated that films with a similar morphology and different oxygen contents (from 15 up to 70 at. %) retain comparable amounts of D. Oxide-W films were exposed to high flux D plasma and the results showed that oxide-W films change their properties after plasma exposures. This leads to oxygen loss, morphological modifications and oxide amorphisation: all these phenomena depend strongly on exposure temperature. Due to the modifications induced by different temperature exposures, the D retention values are different. It was highlighted that D plasma exposures induce the formation of an oxygen-depleted layer. In the case of low temperatures, this layer is superficial, and vice versa for high temperatures. Moreover, it is known that the mobility of D in W is higher in higher temperature regimes. For all these reasons, the D retention values found in similar films but exposed in different temperature regimes (low temperature regime 300°C and high temperature regime 600°C) are different.
In addition, the multilayer systems, made of a thick metallic-W film and a thin oxide-W film, were exposed to D plasma. The results showed that the presence of this thin oxide-W layer deeply modifies D retention behavior by acting like a passivation layer.
At the end, preliminary exposure to a mixed helium-deuterium plasma of some W-based samples was also performed, highlighting nanostructuration phenomena.
The detailed study of this relevant topic is the natural continuation of this thesis, as well as the achievement of a better film property control.

# ANALYTICAL AND NUMERICAL INVESTIGATION OF NATURAL CIRCULATION DYNAMICS IN PRESENCE OF DISTRIBUTED HEAT SOURCES

**Pini Alessandro** – Advisors: Prof. Antonio Cammi, Prof. Lelio Luzzi

In case of density gradients induced by temperature differences, convective motions can arise in a fluid due to the action of the buoyancy force. Thermal-hydraulic machineries that are able to adopt this kind of flows in order to transfer heat from a hot source to a cold sink are known as natural circulation systems. Although forced convection represents a more efficient cooling strategy, natural convection does not require any active component and thus it can be used for high-reliability engineering applications. In this regard, the high-level safety requirements (which are being even more stringent after the Fukushima accident) needed in the nuclear industry have demanded research on emergency components relying on natural convection.
However, natural circulation systems can be affected by functionality-compromising dynamic oscillations of velocity, pressure and temperature fields that have to be avoided by adopting an accurate design-by-analysis approach. The onset of these instabilities can be influenced by several factors, among which the presence of distributed heat sources has not been deeply investigated in literature. Actually, this research topic is of interest not only from a scientific point of view but also for the practical instances that are characterized by distributed heating systems or involve peculiar fluids (such as exothermic reagents or nuclear liquid fuels). As for the nuclear engineering field, an example is given by the Generation IV (GEN-IV) Molten Salt Fast Reactor (MSFR), in which a molten salt simultaneously acts as fuel and coolant. In the MSFR, the heat production inside the fluid takes place through fission reactions in the reactor core and through nuclear decays of the fission products in the whole primary circuit. Such decay heat distributed along the primary circuit may modify the dynamics of a natural circulation system for the reactor cooling after the shutdown, and may lead to an undesired behaviour of the nuclear power plant, which is an occurrence that needs to be prevented. Therefore, the study of the dynamic behaviour of natural circulation with distributed heat sources, one of the key points of the EURATOM SAMOFAR Project (http://samofar.eu), is important in order to achieve high levels of passive safety, as envisaged by the guidelines of the GEN-IV Project.
In the thesis, the dynamics of natural circulation with distributed heat sources is thoroughly analysed by means of different strategies in order to highlight the several aspects that characterise this complex phenomenon. As reference natural circulation systems, single-phase Natural Circulation Loops (NCLs) are chosen. NCLs are either rectangular or toroidal loops characterised by the presence of one or more power sources, a heat sink and the pipes connecting them in such a way that they form a continuous circulation path filled with a working fluid.
In the analysis of the dynamic behaviour of NCLs with distributed heat sources, throughout the thesis, attention is paid to the influence of the following factors: the NCL configuration; the system heat exchange features; the presence of piping-wall materials.
As for the different investigation strategies that have been followed, from the linear-stability point of view, the modal analysis has been applied to evaluate the asymptotic behaviour of natural circulation systems by considering an infinite time horizon. The results of the modal approach are mainly expressed in terms of dimensionless stability maps, which are diagrams in the space of usually two parameters or dimensionless numbers, where a transition curve separates the asymptotically stable equilibria




1. Stability map of the DYNASTY facility. Unstable equilibrium points lie on the left of the transition line

of the system from the unstable ones (**Fig. 1**).
Differently, to take into account processes that occur on a finite-time scale, the non-modal approach has been adopted and has allowed highlighting the occurrence of the so-called "transient energy growth" also in NCLs.
Anyway, since the mentioned methods rely on the linearization process of the governing equations and give information only on the perturbation of the fluid variables, nonlinear simulations (e.g., by means of CFD) have been used as complementary approaches in order to study the actual time-dependent behaviour of the velocity, pressure and temperature inside the system.
In this regard, in order to discriminate between stable and unstable operating conditions in case of numerical (but also experimental data), a stability analysis based on the information entropy approach has been developed during the Ph.D. work.
Last, but not least, an experimental facility (named DYNASTY - ***DYnamics of NAtural circulation for molten SalT internallY heated***) has been designed and realised during the Ph.D. work to complete the assessment of the theoretical approaches, already validated in the case of natural circulation with localised heat sources thanks to the experimental data of the L2 loop installed at the University of Genoa.
DYNASTY is a vertical square hydraulic loop (**Fig. 2**), made of stainless steel components, and designed in a modular way to allow future modifications and extensions. In the top part of the system, the heat sink is a finned pipe that can operate either in passive mode or coupled with an axial fan. The bottom part of the loop is branched, with each branch devised for specific experiment types. In the top one, a centrifugal pump is present in order to initialize the mass flow at system start-up, and to conduct experiments also in forced flow conditions. The bottom branch presents a flow-meter. Fiberglass electrical resistances are employed to provide the distributed external heating and can supply to the system a power from 0.5 to 10 kW. The power lines are divided into four groups, each with its own regulating system to allow for several heating set-ups. Several thermocouples are present to measure the temperature in the loop, which is thermally insulated with mineral wool material. The loop contains a molten salt as circulating fluid. The DYNASTY salt is a mixture commercially known as Hitec®, composed of $NaNO_3$ (7wt%), $NaNO_2$ (40wt%), and $KNO_3$ (53wt%). A tank placed at the top of the loop, which serves also as expansion volume, is used to fill the system. A second tank at the bottom is used as salt storage during the draining procedure. As for the dimensions of the system, the height and the width of the loop are equal to 3.0 m. The inner diameter of the pipe is 38.2 mm (with a thickness of 2 mm).

2. The DYNASTY facility at the Energy Labs of Politecnico of Milano

# ADVANCED MODEL-BASED AND DATA-DRIVEN METHODS FOR PROGNOSTICS AND HEALTH MANAGEMENT OF INDUSTRIAL SYSTEMS

**Rigamonti Marco Michael** – Advisors: Prof. Piero Baraldi, Prof. Enrico Zio

Prognostics and Health Management (PHM) is a field of research and application aiming at detecting the degradation onset of industrial equipment, diagnosing its malfunctioning and predicting its failure time in order to increase the whole system reliability and safety and reduce its maintenance costs. PHM relies on diverse sources of information such as physics knowledge of the degradation process, statistical data on failure times of similar components and data collected through sensors placed on the monitored component which measure signals related to the component behavior and its working and environmental conditions. The available information is used for evaluating the equipment degradation state and predicting its Remaining Useful Life (RUL), thus enhancing the decision making process for the optimal setting of the maintenance strategy. Typically, different industrial applications are characterized by the availability of different sources of information, thus needing to be tackled with suited PHM approaches. Furthermore, modern industrial systems work under variable operating conditions, which are expected to severely affect the component degradation process and to modify the variation ranges of the monitored signals, thus masking the degradation trends and severely complicating the development of accurate PHM methods. According to this, the main challenge addressed by this Ph.D. thesis regards the development of PHM methods for industrial systems under variable operating conditions, taking into account the specific setting of available information and constraints. Three different general cases of information available for the PHM model development in practical industrial contexts are considered in this Ph.D. research: *i*) large knowledge of the system behavior in the form of a physics-based model of the degradation process, an estimate of the future operating conditions profile and of their effects on the degradation process, and few available data from historical run-to-failure component degradation trajectories; *ii*) low knowledge of the system behavior, estimation of the future operating conditions profile not available and few available run-to-failure trajectories; *iii*) low knowledge of the system behavior, available estimate of the future operating conditions profile and of their effects on the degradation process, and large amount of data from run-to-failure trajectories.

With respect to case *i*), we resort to a model-based prognostic approach for components working under variable operating conditions. The available physics-based degradation model of the component is embedded into a Particle Filter (PF) framework for the estimate of the component degradation state and into a Monte Carlo approach for the prediction of its RUL and the quantification of the associated uncertainty. In this case, the novelty introduced in this Ph.D. thesis is the definition of a novel component degradation indicator which is independent from the operating conditions. The performance of the developed approach is evaluated with respect to an experimental case study regarding the RUL prediction of electrolytic capacitors working under variable operating conditions in Fully Electric Vehicles (FEVs), which are responsible for almost 30% of the total number of failures in motor powertrain.
With respect to case ii), we develop a data-driven degradation classifier for components working under variable operating conditions. The developed classification model is based on the use of an ensemble of Self-Organizing Maps (SOMs), which allows handling typical industrial signals characterized by large noise and by the presence of outliers. In this case, the novelty introduced in this Ph.D. thesis is the creation of an ensemble formed by component-based degradation classifiers, which are based on SOMs trained using only healthy data collected from the component under test and are therefore specially tailored on it and on its operational and environmental conditions, and population-based degradation classifiers, which are based on SOMs trained using healthy data collected from components similar to that under test and are therefore representative of the healthy behavior of a general component. The performance of the developed approach is evaluated with respect to an experimental case study regarding the assessment of the health state of Insulated Gate Bipolar Transistors (IGBTs) working in FEVs under variable operating conditions, which are among the most critical and extensively exploited components in electrical systems.
With respect to case iii), in this Ph.D. thesis we develop a data-driven Artificial Intelligence (AI)-based prognostic approach for components working under variable operating conditions. The proposed approach resorts to Echo State Networks (ESNs), a relatively new approach for training Recurrent Neural Networks (RNNs). Thanks to the RNN intrinsic memory properties provided by the internal cyclic connections among neurons, ESNs allow taking into account the whole specific degradation history of the monitored component, thus providing more accurate predictions of the component RUL. In this case, the novelty introduced in this Ph.D. research is the creation of a local ensemble of ESN models, optimized by using a Multi-Objective Differential Evolution (MO-DE) algorithm for enhancing the individual models diversity, which aims at predicting the component RUL and the associated uncertainty by exploiting the individual models memory properties for the aggregation of their outcomes. The performance of the developed approach is evaluated with respect to an experimental case study regarding the RUL prediction and uncertainty quantification of a fleet of turbofan engines working under variable operating conditions, which are the most critical aircraft components from both the safety and the availability points of view.
According to the obtained results, the PHM approaches developed in this Ph.D. thesis are shown able to improve the accuracy and the confidence of the degradation assessments and RUL predictions with respect to conventional PHM approaches. The outcomes of this Ph.D. are expected to reduce the gap between the PHM methodological research and the practical implementation of PHM techniques in industrial applications, providing useful guidelines for the strategy to adopt for tackling specific cases characterized by different available information.

# EXPERIMENTAL STUDY OF UNCONFINED AND CONFINED ISOTHERMAL SWIRLING JETS

**Sharma Rohit** – Advisor: Prof. Fabio Cozzi

## Introduction

Basically, swirling jets are characterized by having a velocity component in the azimuthal direction (swirl). They are ubiquitous and can occur either naturally as in tornado, or be artificially produced as in many practical applications such as gas turbine combustors, swirl burner, furnaces, spraying machine, whirlpools, cyclone separators and in vortex shedding from aircraft wings. Two basic phenomena occur in swirling flow when the degree of rotation imposed to a jet is increased above a certain threshold (strong swirling flow): vortex breakdown (VB) and precessing vortex core (PVC). The first phenomenon, i.e. the vortex breakdown, corresponds to an abrupt change in the flow structure evidenced by the appearance of a stagnation point in the jet and of a zone of reverse flow; PVC on the other side usually appears after the onset of the vortex breakdown, it is characterized by the precession of the jet around its geometrical axis. These phenomena can significantly affect the overall performances of any swirl flow based system. For example, in gas turbine combustors VB improves combustion efficiency, pollutant emissions and combustion stability. Unfortunately, such phenomena are really complex to be investigated experimentally, theoretical or even numerically being strongly unsteady and three-dimensional. In the last 10-15 years the uses of advanced flow diagnostics and data analysis techniques have greatly helped in unveiling their structure and their behavior, nevertheless they are still not yet fully understood. Moreover, very few work and experimental data are available in the literature for the entrainment phenomena in swirling flow. Besides that, the effect of confinement in swirling jets and comparison with the unconfined case has not been fully addressed.

## Experimental approach and main results

This thesis provides an experimental investigation of an unconfined and confined turbulent swirling jet in an isothermal condition, for an experimental laboratory swirl burner.The aim of this study is to achieve a better understanding of the dynamics of isothermal swirling jets undergoing VB and PVC and to characterize the jet entrainment phenomena.
An axial plus tangential entry type swirl burner is used in this study. It allows a fine control of the swirl level of the jet by independently controlling the amount of air injected in the axial and in the tangential directions. The Stereoscopic Particle Image Velocimetry (S-PIV) technique is used to measure the 3 velocity component of the flow field. The measurements are performed in two transverse and longitudinal planes for the unconfined flow and only in a longitudinal section through the combustion chamber for the confined case.
Firstly, this work describes the measured time-average flow fields and their associated velocity fluctuations for both the unconfined and confined cases. By this way, the macroscopic behavior of the flow, for a wide range of swirl intensity, is highlighted and the critical and unstable conditions, as regards the formation of vortex breakdown, recirculation bubble and PVC are identified.
The instantaneous velocity field reveals that by increasing the swirl number the jet first passes through different highly unsteady conditions where vortex breakdown appears randomly and intermittently in time but no reverse flow or stagnation point is revealed by the time mean flow field. When the swirl intensity reaches a critical value the VB clearly show up in the time-averaged flow field. A smaller geometrical critical swirl number, $S_{g,critical}$, is observed in confined flow ($S_{g,critical}$=1.8) as respect to the unconfined ones ($S_{g,critical}$=2.6). For both confined and unconfined cases the velocity profiles show a non-axial-symmetric shape up to the critical swirl number, an almost axial-symmetric flow is obtained once the onset of VB has occurred. Velocity maps show the recirculation zone is significantly enlarged by the confinement. Secondly, acoustic and Laser Doppler Velocimetry (LDV) techniques were employed to investigate the effect of swirl intensity on the formation of the PVC. The spectra of pressure and velocity fluctuations measured by a capacitive microphone and LDV clearly indicate the presence of periodic oscillation related to the existence of the PVC. A POD applied to the instantaneous velocity vector fields allows to identify the dominant flow structure associated to the PVC. The time coefficients of the first two most energetic POD modes were used to reconstruct the phase-averaged velocity field of the oscillatory motion in the swirling flow. The instantaneous minima of negative swirl strength values calculated from the instantaneous velocity field revealed the presence of two helical structures located in the inner and outer shear layers. By phase averaging the instantaneous swirling strength maps, the 3D helical vortex structure was reconstructed (see Figure.1). Finally, the last part of the work deals with the study of the entrainment phenomenon in the very near region of the jet.Results show that the entrainment rate is significantly affected by the swirl level highlighting a non-linear behavior.

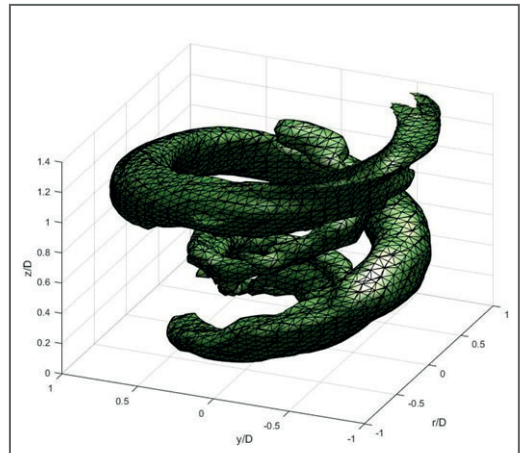


Figure.1 Isosurface of swirl strength for the swirling jet, Sg = 4.6

## Outline of the thesis

In Chapter 2 an introduction into the current state of the art in vortex breakdown and precessing vortex core research is offered and also the choice of the swirl number definition used in the present study is discussed. In Chapter 3 a description of the Proper Orthogonal Decomposition (POD) and of the phase-averaging technique is provided. The visualization of coherent structures by means of the swirl strength parameter is also briefly described. In Chapter 4 we present the literature and theory of entrainment phenomenon by turbulent swirling jet. Chapter 5 mainly describes the swirl burner, the combustion chamber and the equipment used for the S-PIV measurements. Moreover, a background theory on the S-PIV measurement technique along with the description of the jet entrainment evaluation methods are also reported. Chapter 6 is aimed to provide quantitative insights of turbulent unconfined and confined swirling flow focused into the onset of vortex breakdown. Several flow features are presented, starting from a non-swirling jet and ending with a strongly swirling jet. Isothermal swirling jets with different swirl intensity and Reynolds number are characterized by means of S-PIV measurements. Chapter 7 describes the coherent vortex structures emerging in a turbulent swirling jet undergoing vortex breakdown. Microphone recordings and LDV measurements highlight a monotonic increase in the frequency of oscillation of the PVC by either increasing the Reynolds or the swirl number. Results from POD analysis applied to the instantaneous velocity fields is reported. Conditional phase averaging of instantaneous velocity field based on the POD coefficients reveals the pronounced effect of PVC on the flow structure. Eventually, the 3D helical vortex structure of the PVC is reconstructed by phase averaging the instantaneous swirling strength maps. Chapter 8 depicts the influence of vortex breakdown and of PVC on the entrainment phenomena. Two Reynolds numbers, i.e. Re=10900 and Re=21800, and different swirl intensities have been analyzed. The initial region of the swirling jet, i.e. up to about 2.5 times the nozzle diameter in the downstream direction, is investigated. The entrainment rate increases quickly with swirl level up to about the onset of VB, while a small, approximately linear increase in the entrainment rate is observed by further increasing the swirl number. We conclude our study in Chapter 9 by summarizing the main results and conclusions and suggesting future works.

# SIMULATION OF INTERNAL FLOW IN FUEL INJECTION PROCESS

**Tahmasebi Ehsanallah** – Advisors: Prof. Gianluca D'Errico, Prof. Tommaso Lucchini

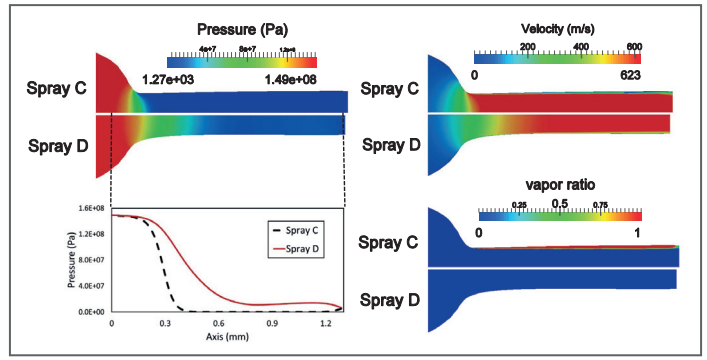
The role of injection system in Diesel and gasoline engines is to deliver a high quality air-fuel mixture in combustion chamber as follows efficient combustion while minimized pollutant and noise emissions. Due to the growing restrictions for emissions and energy consumption, injection process is gaining in importance. Despite the higher uncertainty and technical limitation of experimental investigations in complex systems with difficult physical conditions, numerical modeling provide a reliable results and calculate the temporal behavior of every variable at any place inside the domain.

Finding a reliable methodology for simulation of fuel flow inside Diesel and gasoline injectors is the main objective of this thesis. Considering intensive working conditions in high pressure modern injectors, including tiny dimensions, drastic pressure gradient, huge amount of velocity and turbulence properties inside the nozzle, phase changing and formation of cavitation in specific conditions make this problem more complicated.

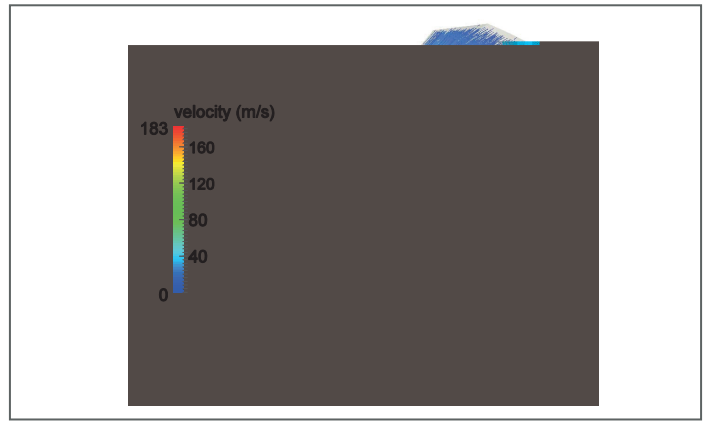
In current research, a Homogeneous Equilibrium Model is selected and implemented for simulation of multiphase flow inside the modern injectors. This model considers phase changing, formation of cavitation and turbulence effects in severe working conditions of real size injectors. After assessment of the approach with different experimental studies, simulation of real size industrial Diesel injectors are performed to understand the effects of working conditions and nozzle geometry on flow properties inside the nozzle and emerging sector (**Figure 1**). These results could be used for improvement of the simulation of spray breakup and atomization process in high-pressure Diesel sprays.

Simulation of multi-hole gasoline direct injection fuel injector (**Figure 2**) is another part of this thesis in which a complete realistic gasoline injector geometry, considering manufacturing tolerances is considered. Presented results for different nozzles emphasize the role of small differences in geometry on flow properties inside the nozzle and at nozzle exit sector of each nozzle (**Figure 3**). This difference in results consequently could affect the spray breakup of each nozzle that is interesting for further studies in future.

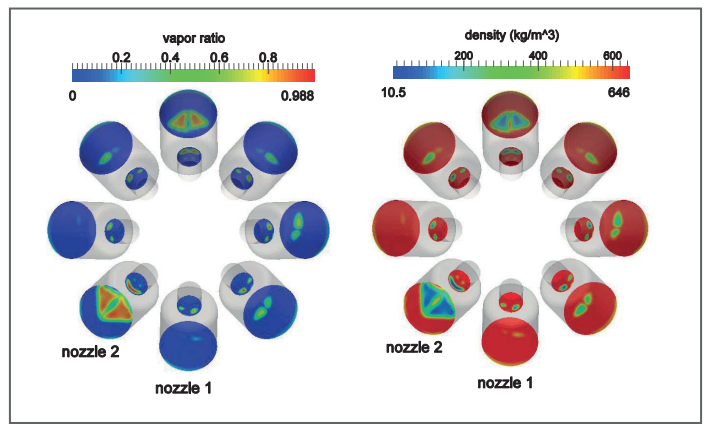
All the models and simulations using in this thesis are performed within the OpenFOAM technology framework and could be continued in supplementary researches in this field, as well as future works in Internal Combustion Engine (ICE) group of Politecnico di Milano.




1. Comparison of the results for two Diesel injectors (spray C and D from ECN database) with different geometry




2. Flow streamlines inside a nozzle from multi-hole gasoline injector (spray G from ECN database)

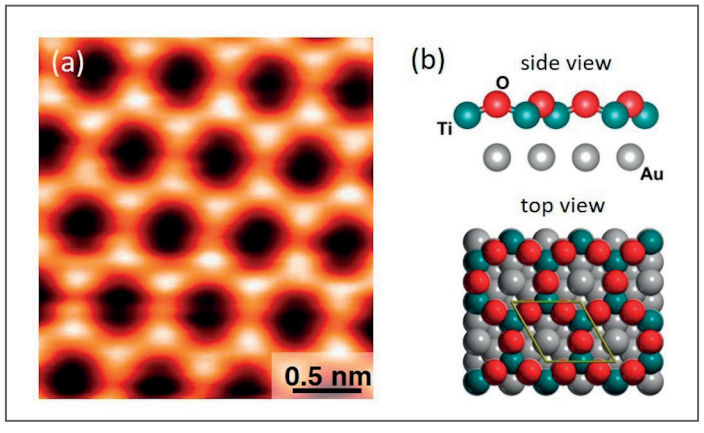



3. Distribution of vapor and density at nozzle exit and bore exit of multi-hole gasoline injector (spray G from ECN database)

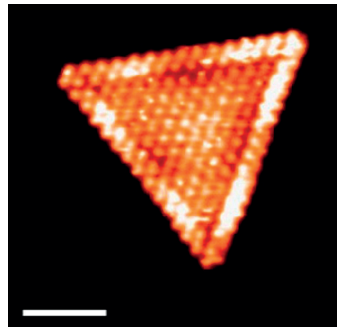
# SCANNING TUNNELING MICROSCOPY AND SPECTROSCOPY OF TWO-DIMENSIONAL OXIDE NANOSTRUCTURES

**Tumino Francesco** – Advisors: Prof. Andrea Li Bassi, Prof. Carlo S. Casari

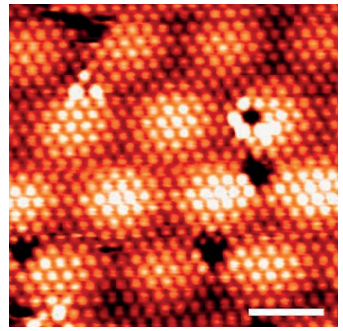
The development of new materials has its historical roots in prehistoric times and has always had a crucial impact on technological progress and human lifestyle. Recent times have seen the emergence of a new perspective in the research for new materials: it has become clear that not only a new chemical compound may form a new material, but also the reduced size and dimensionality can produce unprecedented properties and novel physical and chemical behaviours. Probably the most popular example is provided by graphene, an atomically thin material made by carbon atoms: the discovery of some of its remarkable properties in 2004 prompted the rise of a new class of materials: two–dimensional (2D) materials. Since then, the class of 2D materials has experienced a formidable expansion, with the synthesis and study of novel atomically thin crystals, such as transition metal dichalcogenides ($MoS_2$, $WS_2$ and others) and hexagonal boron nitride. Huge potential is attributed to a particular family of 2D materials: 2D oxides. Oxides are abundant in nature and extensively used in a number of present-day technologies. In the last twenty years, prompted by the experimental research on oxide surfaces and interfaces, novel 2D oxide structures, mainly supported by metal substrates, have been produced and investigated. Differently from 2D materials obtained by exfoliation of van der Waals solids (such as graphite and $MoS_2$), oxides, in general, interact strongly with the substrate, which, thus, may play a fundamental role in the stabilization of novel 2D phases. The study of metal-supported 2D oxides has taken enormous benefit from the important experimental advances in surface science techniques of the last thirty years, most of all embodied by the invention of the scanning tunneling microscope in 1986. Scanning tunneling microscopy (STM) is an imaging technique whose working principle is based on quantum tunneling between a sharp metal tip (the probe) and the sample surface, brought to within a fraction of nanometer each other. The tip apex behaves as a probe of atomic dimension, thus, capable of imaging the investigated surface with extremely high spatial resolution, even down to the atomic scale. This characteristic has made STM an incredibly valuable technique for studying the nano-scale morphological, structural and electronic properties of surfaces, interfaces and nanostructures, contributing to access the comprehension of physical phenomena occurring at the atomic scale. STM also supports a closely related spectroscopic technique, scanning tunneling spectroscopy (STS), which allows to experimentally probe the surface electronic density of states around the Fermi level, thus providing key information on the local electronic properties of the investigated material. STM and STS are ideal tools for studying the fundamental properties of metal-supported oxide nanostructures, which is a key premise to address future applications of these materials, e.g. in the fields of catalysis and optoelectronics. The study of 2D oxides by means of STM and STS is the main subject of this thesis. The activity has been focused in particular on two of the most important transition metal oxides: titanium oxide ($TiO_x$) and zinc oxide (ZnO), with the general aim to produce 2D $TiO_x$ and ZnO nanostructures under ultra-high vacuum conditions and study their growth and nano-scale morphological, structural and electronic properties by means of *in situ* STM and STS measurements. Different fabrication approaches have been explored, based on metal evaporation or Pulsed Laser Deposition (PLD). The latter is a well-established technique for the growth of thin films with different morphologies but has been scarcely applied to the production of 2D materials. The Au(111) surface has been mainly used as supporting substrate, as it is a well-known surface, whose inertness toward oxygen makes it suitable for oxide deposition. This experimental work has led to the observation of novel 2D structures with very different properties in comparison to the well-known $TiO_2$ and ZnO bulk forms. For instance, **figure 1**(a) shows an atomic resolution STM image of a particular 2D TiOx phase, in which Ti and O atoms form a single layer having a peculiar honeycomb arrangement. In contrast with the typical semiconducting behaviour of bulk $TiO_2$, this phase shows a partial metallization, as revealed by STS measurements. The interpretation of experimental data has been supported by theoretical simulation of the electronic structure, leading to the structural model schematically depicted in figure 1(b), which is based on a $Ti_2O_3$ honeycomb structure. As far as ZnO is concerned, a recently predicted graphene-like structure has been experimentally observed. In particular, the PLD technique has made possible the production of graphene-like ZnO nanocrystals of different thicknesses, from 1 to 5 atomic layers. For instance, single- and bi-layer ZnO nanocrystals with a clearly resolved hexagonal atomic lattice are shown by the atomic resolution STM image in **figures 2** and **3**, respectively. Hence, this work allowed to study different 2D titanium oxide phases and the graphene-like 2D zinc oxide structure, revealing novel structural and electronic characteristics not observed in their bulk counterparts and setting the basis for further exploration of 2D oxide systems, both pure and doped, with potentially tunable electronic properties.




**1. (a) Atomic resolution STM image of the 2D $TiO_x$ honeycomb structure. (b) Schematic representation of the corresponding structural model.**



**2. Atomic resolution STM image of a single-layer ZnO nanocrystal. Scale bar: 2 nm.**



**3. Atomic resolution STM image of the surface of a bi-layer ZnO nanocrystal. Scale bar: 2 nm.**

# NUMERICAL STUDY OF COHERENT STRUCTURES OF IN-CYLINDER FLOW BY A HYBRID RANS/LES MODEL

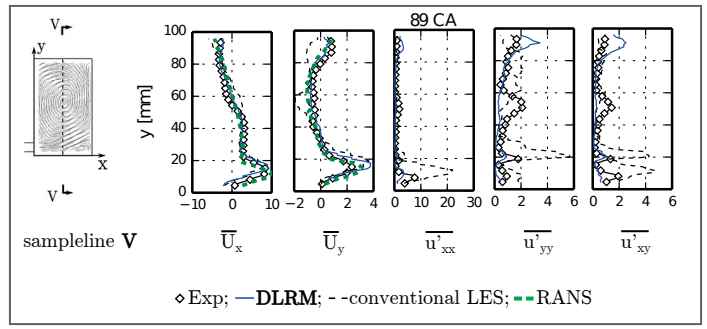
**Wu Yan** – Advisor: Prof. Federico Piscaglia

Investigation into the turbulent unsteadiness of the engine flow requires scale resolving simulation methods that could study the geometrically complex and high-dimensioned dynamic system with sufficient numerical precision and affordable computational cost. The reported thesis work proposes a solution to use a hybrid RANS/LES turbulence model for CFD study of IC engine. Coupled with an enhanced dynamic meshing strategy and proper numerical set-up, the proposed scale resolving model draws a critical balance between the low computational cost of RANS and the resolving capability of LES. Thanks to its cost-effective nature, flow decomposition based on multi-cycle realization could be conducted on high-fidelity experimental measurement and simulation results simultaneously. The proposed hybrid turbulence model is the latest development of dynamic length-scale resolution (DLRM), which adjusts its filtering behaviour dynamically based on the comparison of local resolvable length scale lt and the estimated turbulence integral length scale $L_t$. The renewed definition of lt treats spatial and temporal resolutions separately, the former one is defined as a reference to the lowest resolvable length scale allowed by local grid step size according to Nyquist criterion, while the later one borrows the idea of the concept of ***CFL*** number so that local resolvable time scales could be treated with an corresponding time scale objecbtively. Such definition allows robust damping/filtering behaviour and much better adaptivity to coarse mesh and large time step. Generic implementation of the hybrid model is finished within the environment of the open sourced c++ library OpenFOAM®, and the hybridization between arbitrary RANS and LES filtering shape is straightforward.

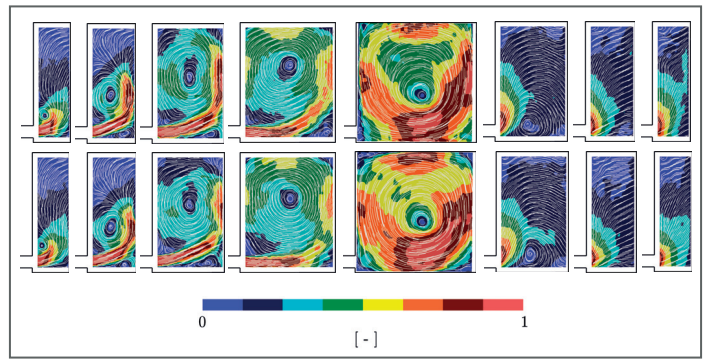
Enhancement of the dynamic mesh strategy of OpenFOAM® is developed with both generic techniques and case-specific method so that the moving boundaries of IC engine are handled automatically with sufficient numerical accuracy. Generic techniques are developed for the motion law of the piston and the run-time mesh topology changes, namely layer addition/removal (A/R) and mesh interfacing. Motion law of the piston/valve are tracked either through curve fitting with user-provided Fourier series coefficient, or a map of the lift profile of sufficient accuracy. Automatic layer A/R tracks the motion of the piston while keeps the mesh resolution (hence the "filter" size in the context of LES) almost unchanged through the entire engine cycle. Mesh interfacing are performed through either sliding interface or arbitrarily coupled mesh interface (ACMI). While ACMI is already available in OpenFOAM® from the fork maintained by OpenFOAM Foundation, the couple/decouple mechanism of the sliding interface has to be optimized so that renumbering of the grid points is avoided during the time steps when the sliders are not coupled or have no relative displacements. All the generic techniques are implemented to be compatible with the polymorphism of the dynamic mesh library so that only the necessary topology changes are constructed run-time as required by the user during simulation.

Case-specific character of the moving boundary problem is treated by run-time boundary condition, so that the polymorphism of the code structure is kept intact and the abstraction overhead from generic programming could be avoided. To keep the compactness and the generic nature of both the solver and the necessary library for dynamic mesh handing, the run-time boundary condition is fulfilled by the function Object techniques of OpenFOAM and its entire behaviour and potential negative side effect are contained within the specific case set-ups.

Validation of the turbulence model and dynamic mesh strategy on an optical test engine confirms the advantage of hybrid turbulence method when simulation is performed on considerably coarse mesh which typically does not satisfy the requirement of conventional "fully resolved" LES, as shown in **Fig. 1**. Besides, grid and time step dependency studies also suggest that the simulation results of the proposed hybrid model benefits from a refined numerical resolution even on the very coarse range of spatial resolution far from "inertial sub-range", which is the main interest of the thesis study. The POD analysis on the flow field being investigated provides a low-dimensioned description to the understanding of turbulent unsteadiness. Along with standard statistics such as the ensemble-averaged mean value or the variance, which are used to validate the performance of the proposed simulation methods, POD helps to identify the most important (energy containing) flow structures with mathematically well-defined criterion. Further development based on the parallelized model reduction library modred (maintained by Belson *et al.*) is carried on so that the modal decomposition directly deals with the vector field and the inner product of the "vector" in the POD domain are more consistent with the kinetic energy of the velocity field in the physical domain. It is realized that for the quasi-engine flow without compression, most of the kinetic energy is contained in the ensemble-mean flow, which essentially corresponds to the leading POD mode, as shown in. Further to that, evidence of the competing effect between the mean flow structures is identified in the higher mode flow structures, which are not self-organized enough to maintain its trace in the mean flow.




**1. Comparison of the phase-average and variance of the resolved velocity field on the vertical sample line**




**2 Normalized eigenvectors of the leading POD mode at (left to right) 34, 56, 89, 121, 185, 276, 306, 327CA, top: experiment, bottom: simulation**