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DOCTORAL PROGRAM IN ENERGY AND NUCLEAR SCIENCE AND TECHNOLOGY

Chair:
Prof. Vincenzo Dossena

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

- Production, conversion and transmission of energy
- Rational use of energy
- Nuclear systems, nuclear fuel cycle, radioprotection
- Application of ionizing radiations
- Methods for safety and reliability analysis
- Development of innovative materials for energy applications

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SUPERCRITICAL CO_2 CYCLES FOR FLEXIBLE POWER GENERATION: TECHNO-ECONOMIC OPTIMIZATION AND PART-LOAD OPERATIONAL STRATEGIES

Dario Alfani – Supervisor: Prof. Paolo Silva – Co-Supervisors: Prof. Marco Astolfi, Prof. Marco Binotti

Introduction and objectives of the thesis work

In the imminent future, due to the increase of penetration of non-dispatchable renewable energy sources, the electricity generation sector is required to undergo significant changes and conventional power plants will have to gradually shift their role from base-load operation to cover peak demand. In this context, supercritical CO_2 power cycles represent an interesting solution to enhance the efficiency and flexibility of traditional power plants.
The Thesis focuses on the evaluation of the potential of these innovative power cycles and the development of ad-hoc numerical codes able to predict their techno-economic performances.

Methodology and numerical code structure

The numerical tool developed within the research is composed by three main sections: (i) the steady-state on-design simulation numerical code, (ii) the plant components sizing tool and (iii) the numerical code for part load and off-design simulations.
The *nominal design numerical code*, developed in MATLAB, includes different turbomachinery and heat exchangers models allowing to investigate several cycle configurations. Different sets of components cost correlations are integrated in the code to establish a trade-off between system efficiency and investment cost, to select the nominal design which minimizes the specific investment cost or LCOE.
The *components sizing tool*, where a tailored methodology for the calculation of heat exchangers surfaces, volumes and masses is integrated to size the recuperators, heat rejection unit (HRU) and primary heater.
The *part load and off-design simulation tool*, which is employed to assess sCO_2 power cycles operational flexibility by studying different operating strategies with the aim of maximizing the performances at reduced load and variable cold sink conditions, respecting the constraints imposed by the plant equipment or by the selected dispatch strategy.

Applications

The developed numerical code has been then employed to investigate the techno-economic performances of innovative small modular coal-fired power plants, waste heat recovery systems from several industrial sectors and high-temperature CSP power plants.

The sCO_2-Flex project: small modular and flexible coal power plants

The core of the Thesis work presents the outcomes of the H2020-funded sCO_2-Flex project, at which Politecnico di Milano has largely contributed. Its main objective was the design of a $25MW_{el}$ highly flexible and efficient sCO_2 cycle coupled to a coal-fired boiler, as a first step towards demonstration projects for a full-scale plant. This solution aims at increasing the flexibility and responsiveness of coal power plants thanks to a smaller power block weight and volume, lower heat exchangers thermal inertias and a less complex cycle configuration.
The sCO_2-Flex plant nominal and part-load performances have been assessed and optimized by considering realistic components modelling and different operating strategies, also thanks to the consortium partners inputs.
As dry-cooling is considered to reject heat to the environment, the plant actual performance strongly depends on its location. Thus, the simulation of a reference year of operation has been performed for Prague and Sevilla sites, demonstrating that in the second location the criticalities related to the increase of ambient temperature cannot be neglected and further solutions must be employed.
Results show that wet-and-dry coolers can solve this issue at the expenses of a small increase of the investment and operating costs and with limited water consumption, corresponding to just 6.5% of the specific water consumption of conventional coal power plants.
Finally, LCOE of the designed system has been computed: for a $100MW_{el}$ scale-up of the plant a promising value of 62.5 €/MWh is obtained, comparable with conventional larger size coal-fired power plants.

Waste heat recovery (WHR) applications

The thermodynamic potential and commercial appeal of sCO_2 power cycles in WHR applications has been assessed by comparing their techno-economic performance with ORC systems, the reference technology for small-size WHR systems. The comparison is performed for a wide range of heat source temperatures and cooling grades, and sCO_2 power cycles resulted to perform more efficiently, even allowing low condensation pressure for ORCs, for applications with temperature higher than 500°C.
The analysis showed that simple recuperated cycles with recuperator bypass are a promising solution to overcome the problem of the high temperature at the primary heat exchanger inlet, typical of sCO_2 cycles with a high degree of internal recuperation. This configuration has a simple layout and reduced footprint, two particularly interesting aspects for small-size WHR applications.
The part-load operation of both variable and constant inventory sCO_2 power systems have been analyzed: the adoption of an external CO_2 storage allows to vary the working fluid inventory in the system, leading to a positive impact on part-load performances.
However, totally sealed cycles with constant CO_2 inventory can be attractive for WHR thanks to their ease of installation and operation. They can operate with nearly constant efficiency for industrial processes characterized by a high minimum load (>75%) but suffer a significant penalization for lower loads due to the increase of cycle minimum pressure and the marked reduction of cycle pressure ratio.

High-temperature CSP

A final section of the Thesis presents the results of the joint project with the National Renewable Energy Laboratory (NREL) titled "Techno-economic Performance of Supercritical Carbon Dioxide Cycles for Concentrating Solar Systems", assessing the potential of sCO_2 power cycles coupled to high-temperature 3rd generation solar towers.
The potential techno-economic advantages of CSP plants adopting sCO_2 power cycles over conventional steam Rankine cycles have been confirmed as this solution achieves better performance from both efficiency (+3 points of percentage in sun-to-electricity efficiency) and economic (-18% of specific cost) standpoints. The analysis has been then refined through a techno-economic optimization of a solar power tower integrating a sCO_2 power block with a high-temperature central receiver adopting molten salts as HTF.
The results of this study report the trend of the optimization variables along the optimal Pareto front (plant investment cost vs. solar-to-electricity plant efficiency) to give useful insights for the sCO_2 power block design and to suggest reasonable assumptions for the most important cycle variables and components design parameters.

Conclusions

The developed numerical code confirmed the potential of sCO_2 technology for replacing conventional steam Rankine cycles in several power generation applications, and likely playing a relevant role in the future energy scenario.
The research showed that for any power generation application, a different optimal sCO_2 cycle configuration can be selected and must be carefully optimized according to the heat source and cold sink characteristics.
The Thesis also highlighted the importance of adopting a part load control strategy based on CO_2 inventory variation coupled to the adoption of IGV and/or rotational speed control for the compressors. Thanks to this solution, it is possible to flexibly operate sCO_2 power systems down to very low electrical loads (20%) maintaining the main compressor inlet conditions close to the working fluid critical point.
On the other hand, the variation of cold sink conditions is particularly problematic for sCO_2 power cycles, as even CO_2 temperature increases of few degrees at compressor inlet lead to significant changes of the volumetric flow rate, causing operability issues in the main compressor of the cycle. A set of possible actions and equipment to install able to mitigate this issue is proposed in the Thesis, and their potential is numerically assessed for the sCO_2-Flex case-study.

DETAILED MODELING OF FALLING FILM HEAT EXCHANGERS FOR ABSORPTION HEAT PUMPS (AHP)

Mehdi Aminyavari - Supervisor: Prof. Mario Motta

Design of the heat exchangers has always been one of the most critical part of designing any thermally driven thermodynamic systems. The current project, aiming the design of falling film heat exchangers, will be very useful in modelling of thermodynamic cycles and designing of Absorption Heat Transformers (AHT) and small scale Absorption Heat Pumps (AHP) that can be used in various applications, e.g. District Heating (DH) integrated with Absorption Heat Exchangers (AHE), Solar cooling systems and gas driven absorption heat pumps. The schematic of the two types of absorber is demonstrated in Fig.1.

A lumped element model of falling film absorber was developed in this work which takes into account heat and mass transfer in both phases of gas and liquid. In order to validate the capacity and accuracy of the model in predicting the absorption phenomenon, two in-tube vertical falling film absorber with gas and film in co-current and counter-current arrangement, respectively were built and installed in a single-stage cycle absorption heat transformer and a single effect absorption heat pump. It has been shown that the mass and heat transfer coefficients between the liquid film and the interface are higher than the ones between the gas and the interface. Therefore, absorption process is being controlled mainly by heat and mass transfer coefficients between the falling film and the interface, while the biggest resistance to heat and mass transfer is the ones between gas and the interface. Furthermore, it has been demonstrated that the inlet condition of the absorber is different than the condition at the inlet of tubes for both absorbers, as the gas and solution have the possibility to go through and adiabatic mixing before entering the tubes.

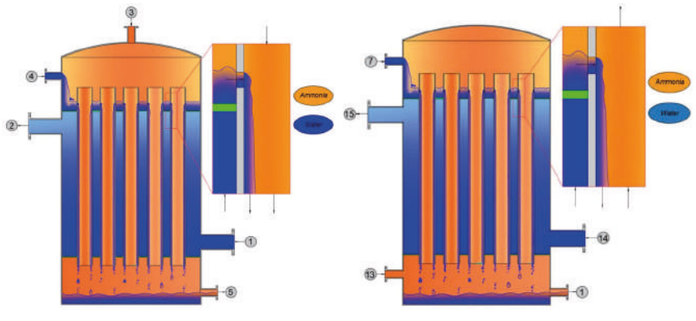

Fig. 1
a) Schematic of the co-current falling-film absorber
b) Schematic of the counter-current falling-film absorber

Table 1 illustrates a sample set of experimental data as well as the corresponding model-calculated ones for the model without consideration of an adiabatic mixing at the gas inlet section of counter-current absorber (point 13 of Fig. 1.b). Comparing this table with Table 2 where the adiabatic model is added, one can perceive the improvement of the accuracy of the model in predicting the absorption phenomenon.

Table1	Test 1		Test 2		Test 3		Test 4		Test 5		Test 6	
	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.
$\dot{m}_s = (kg/h)$	36,42	35,96	37,43	36,92	33,61	33,13	32,99	32,55	36,33	35,74	31,47	30,95
$T_s(°C)$	33,33	31,59	37,76	36,53	41,81	41,01	46,05	45,63	32,77	31,31	36,35	35,8
$Y_s(\%)$	41,12	40,39	40,46	39,69	40,94	40,17	40,77	40,04	40,96	40,05	42,14	41,24
$Q(kW)$	3,66	3,53	3,36	3,19	3,68	3,5	3,28	3,12	3,45	3,25	3,06	2,85
$dT_{sc}(°C)$	0,19	3,19	0,1	2,67	0,1	2,26	0,01	1,81	0	3,05	0	2,1

Table 1
Outlet Conditions of the experimental tests vs the model without adiabatic mixing in the bottom

Table1	Test 1		Test 2		Test 3		Test 4		Test 5		Test 6	
	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.
$\dot{m}_s = (kg/h)$	36,42	36,25	37,43	37,18	33,61	33,34	32,99	32,76	36,33	36,04	31,47	31,14
$T_s(°C)$	33,33	34,01	37,76	38,53	41,81	42,67	46,05	46,83	32,77	33,55	36,35	37,34
$Y_s(\%)$	41,12	40,84	40,46	40,08	40,94	40,51	40,77	40,39	40,96	40,52	42,14	41,57
$Q(kW)$	3,66	3,55	3,36	3,21	3,68	3,53	3,28	3,16	3,45	3,29	3,06	2,88
$dT_{sc}(°C)$	0,19	0	0,12	0	0,11	0	0,01	0	0	0	0	0

Table 2
Outlet Conditions of the experimental tests vs the model with adiabatic mixing in the bottom

It also has been demonstrated that small errors in the rate of absorption can lead to big errors in the design of FFABS and, in order to utilize FFAB models for design purposes, the model needs to evaluate the heat and mass transfer perfectly. Moreover, results have established that the main absorption takes place in the top section of the tubes (entrance of solution film) where the solution film is less rich in ammonia and has highest temperature difference with respect to the coolant and therefore maximum potential to absorb gas molecules of ammonia.

Fig. 2 demonstrates the experimental and model- calculated temperature of the coolant water on the shell side for the counter-current absorber in one of the tests. Discussion on the results in the thesis revealed that the absorption rate is probably being affected by hydrodynamic of the film and the variations in thermodynamic properties will affect the hydrodynamics of the film and vice versa and therefore one way to improve the robustness of the FFAB model is to consider the simultaneous effect of hydrodynamic of the film in a coupled manner with the heat and mass transfer process.

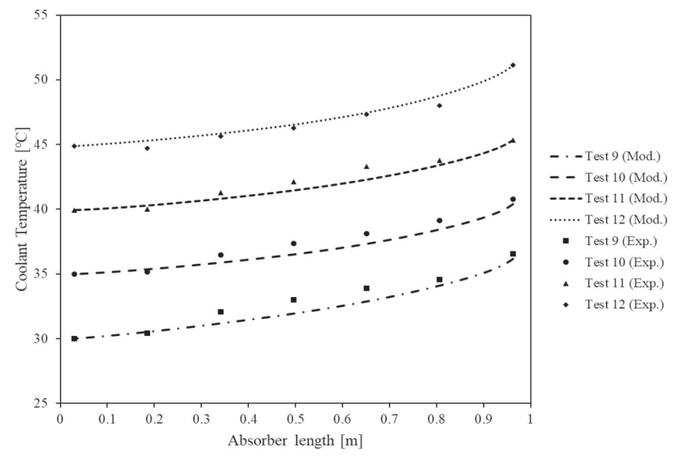

Fig. 2
Experimental and model-calculated temperatures for the tests for counter-current absorber with evaporator temperature of heat pump set at 5°C

THERMODYNAMIC MODELLING AND PROCESS DESIGN OF A CO_2 CAPTURE UNIT WITH AMINO ACID SALTS SOLUTIONS FOR COMBINED CYCLE DECARBONISATION

Antonio Conversano - Supervisor: Prof. Manuele Gatti

The work entitled "Thermodynamic Modelling and Process Design of a CO_2 Capture Unit with Amino Acid Salts Solutions for Combined Cycle Decarbonisation" combines experimental and modelling research activities aiming at the assessment of a CO_2 capture process operating with non-precipitating amino acid salts solutions coupled with a natural gas combined cycle. During the study, the post-combustion capture unit has been designed targeting 90%$_{mol/mol}$ CO_2 removal, and the energy penalty on the power island has been estimated in order to calculate the cost of electricity produced from the plant with capture, and the cost of CO_2 avoided.

The analysis overcomes the gaps recorded from the literature due to the lack of comprehensive vapor-liquid equilibrium data sets and equilibrium constants, and it is finalized to a techno-economic evaluation as from the following methodology:

- Initially, a screening of a selected group of amino acid salts solutions has been carried out, running experimental campaigns at bench scale. Preliminary simulations of the absorption process in the facility have supported test design, and the experimental test results have been analyzed with an in-house data analysis algorithm. Absorption performance evaluation of the different tested solutions has guided towards the selection of 43.7%$_{w/w}$ potassium lysinate as a solvent of interest for further investigation;
- An empirical Kent-Eisenberg thermodynamic correlation endowed with Debye-Hückel activity coefficient model has been proposed to estimate the missing equilibrium constants and evaluate CO_2 solubility for a solvent loading region characterized by lack of vapor-liquid equilibrium data. Starting from the aforementioned modified Kent-Eisenberg edition, a predictive and thermodynamically sound Deskhmukh-Mather model has been proposed;
- An in-house code of the absorption unit simulated with a rate-based model has been developed and validated against monoethanolamine pilot data from the literature. The model has been adapted to design the capture process operating with the identified potassium lysinate solution in a conventional configuration and suitable operating conditions selected based on cross sensitivity analysis on the absorber volume and solvent regeneration duty;
- In order to complete the techno-economic assessment, the heat of absorption has been calculated using van't Hoff equation. Consequently, the reboiler duty for solvent regeneration and plant energy penalty assessment has been estimated at different operating conditions (i.e., loading, liquid-to-gas ratio);
- The techno-economic assessment of a natural gas combined cycle coupled with a post combustion capture unit operating with the identified amino acid salt solution has been delivered to evaluate suitable performance, energy and economic indicators;

The results of the techno-economic assessment have been compared against a reference CO_2 capture commercial system operating with 30.0%$_{w/w}$ monoethanolamine solution, and an emerging advanced capture technology relying on 30.1% $_{w/w}$ (5m) piperazine solution with solvent regeneration under pressure.

ADVANCED APPLICATIONS OF CALCIUM-LOOPING FOR CO_2 CAPTURE IN CEMENT PLANTS AND FLEXIBLE POWER PLANTS

Edoardo De Lena – Supervisor: Prof. Matteo Carmelo Romano

Objectives and Scope

The aim of the PhD research project is to carry out techno-economic studies on innovative solutions for CO_2 capture in cement plants and power plants by Calcium Looping (CaL) processes. CaL is an emerging technology for CO_2 capture that uses CaO-based sorbent to remove CO_2 from process flue gases, according to the carbonation reaction $CaO+CO_2 \rightarrow C_aCO_3$.
Starting from the first configuration, proposed by Shimizu in 1999, the work carried out in this PhD thesis focuses on the following novel aspects with respect to the state-of-the-art:
A. The investigation of novel process configurations for the integration of CaL process in cement plants.
In fact, cement production is estimated to account for about 8% of anthropogenic CO_2 emissions, including process emissions in the order of 1.5 $GtCO_2$/y from the calcination reaction of C_aCO_3 into CaO. Therefore, long term scenarios for the cement industry indicate that CO_2 capture and storage (CCS) systems are needed to fully decarbonise the cement sector.
B. The study of the possibility of using thermochemical sorbent storage to improve both the cost-effectiveness and flexibility of fossil-fired power plants. In fact, renewable energy sources are providing new challenges for the electricity system. Furthermore, to contain greenhouse gas emissions, by 2050 most of fossil fuel fired plants should adopt CCS systems. Therefore, it is essential to investigate the performance and control strategies of next generation fossil-fired power plants coupled to CCS, to ensure a smooth transition towards a more sustainable power generation sector.

Methodology

The thesis work was mainly performed using software (e.g. in-house code GS, Aspen, Thermoflex) to conduct process simulations for estimating the system performances (such as specific CO_2 emissions, LCOE, cost of CO_2 avoided, etc...). The experimental activities were also included to characterize the materials used as CO2-sorbent. These activities were developed in the laboratories of the INCAR research centre in Oviedo (Spain).
All analyses were carried out in close cooperation with European industries, research centres and universities. The methodology and boundary conditions were defined in the framework of the European projects CEMCAP, Flexical and Cleanker.

Main results and Conclusions

Regarding the applications in cement industry, from the analysis performed in this thesis it can be concluded that:
1. The increase in CO_2 equivalent reductions in the system inevitably means an increase in the energy consumption of the plant, either as fuel (CaL plants) or electricity (oxyfuel plants).
2. If the technical feasibility of working with very low air infiltration in the rotary kiln is proven and if the supply of additional electricity with low CO_2 emissions can be guaranteed, full oxyfuel process seems to be the preferred solution.
3. In case where air infiltration in the rotary kiln cannot be avoided (or significantly reduced), and if there is the possibility to use low-price fuel and/or fuel with which CO2 credits can be obtained (such as biomass or refuse derived fuel), the processes based on CaL technologies become competitive.
4. Among CaL systems, integrated processes are more efficient and economically more competitive, but pilot scale experiments are needed to validate the technical feasibility at industrially relevant scale.
5. The optimal technology also depends on the raw material/limestone properties of each specific plant. In particular, (i) materials that favor the formation of Ca-Si compounds are not recommended as CO_2-sorbent materials, and (ii) in processes where it is possible to have a separate supply of limestone and additives, integrated CaL configurations are favored.
Fig. 1 shows the cost of cement for the different processes analyzed in this work as function of carbon tax.
As regards applications in flexible power plants, the possibility of exploiting the thermochemical storage of the sorbent (Flexical case) allows to reduce the cost of electricity by around 4–5% with respect to the case without energy storage (Baseline case), independently of the value of the carbon tax and plant availability, as shown in Fig. 2.
Moreover, it allows to increase operability of the plant on the balancing market, with variation of +2% power output compared to the nominal load and -13% power output compared to the minimum load. Therefore, it can be concluded that, through appropriate technical measures, the thermochemical energy storage of the CaL system sorbent, can be exploited to achieve the dual objectives of increasing plant flexibility and cost reduction. The advantage of the storage system is greater the lower the capacity factor of the system. It will therefore be increasingly advantageous in the coming years as the penetration of renewables for electricity production is expected to increase.

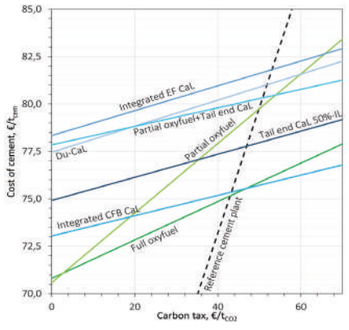

Fig. 1
Cost of cement as function of carbon tax for the different processes analyzed

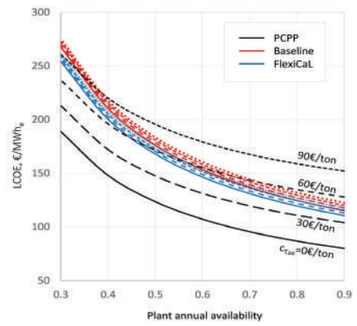

Fig. 2
Levelized Cost Of Electricity (LCOE) as function of the plant annual availability, in case of different values of carbon tax for the conventional Pulverized Coal Power Plant (PCPP, black), the Baseline (red) and the Flexical (blue) cases.

Points of Innovation

The innovative part of this PhD thesis was to analyze from an energetic, technical, economic and semi-quantitative point of view innovative solutions for CO_2 capture integrated in cement and fossil-fired power plants. The analysis allows the determination of the optimal configuration according to different operating conditions of the systems and market demands. An industrial patent application has also been filed for an innovative clinker production process, which is presented and analyzed in this thesis.

3D CFD MODELLING OF PREMIXED COMBUSTION IN NATURAL GAS SI ENGINES

Giovanni Gaetano Gianetti - Supervisor: Prof. Tommaso Lucchini

The main objective of this work is to develop a CFD methodology to model combustion process in premixed natural gas light-duty spark-ignition (SI) engines. A detailed description of all the processes that take place inside the combustion chamber is fundamental to obtain a stable and efficient combustion process and to guarantee control of pollutants formation. To this end, computational fluid dynamics simulations represents an efficient and powerful tool to study and understand the different phenomena involved as mixture ignition, laminar to turbulent transition, fully turbulent combustion and pollutant formation. CFD simulations were run using the open-source software OpenFOAM\ textsuperscript{\textregistered} coupled with the Lib-ICE code, which is a set of libraries developed by the Internal Combustion Engine Group of Politecnico di Milano, and using the RANS turbulence approach.
In the proposed comprehensive methodology a simplified deposition model was chosen to describe the ignition process. The turbulent flame propagation is reproduced by means of regress variable and flame wrinkling factor, following the Flame Area Model proposed by Weller. Laminar to turbulent flame transition instead is modeled using Herweg and Maly formulation coupled with a zero-dimensional flame kernel radius evolution. Burnt gases chemical composition are estimated considering two different approaches, one based on tabulated kinetics and the other on chemical equilibrium.
First, the combustion methodology was applied and validated on a premixed stoichiometric turbulent methane flame using experimental data on a piloted Bunsen burner and using two different formulations for the flame wrinkling factor. Then, the validation of the combustion model was performed using experimental data provided by Empa, the Swiss Federal Laboratories for Material Science and Technology, of a light duty SI engine fueled with natural gas. Two-dimensional simulations were run in order to perform a first assessment of the combustion model at different engine loads and speeds. Finally, the proposed methodology was used to study the influence of piston bowl geometry on turbulence distribution and consequently on combustion process, using the full 3D geometry.

ADVANCED MODELLING AND STABILITY ANALYSIS FOR NUCLEAR REACTORS

Carolina Introini – Supervisors: Prof. Antonio Cammi, Prof. Stefano Lorenzi

Because of the complexity of Generation-IV concepts, the trend of nuclear reactor analysis relies on high-fidelity 3D multi-physics modelling. Despite the advancements in terms of computational hardware and numerical methods, one of the main challenges of high-fidelity modelling remains the high computational cost, especially for all applications that requires quick and efficient multiple simulations of the same phenomena. A trade-off between computational cost and solution accuracy arises, which in the nuclear field it is extremely skewed towards the latter. Model order reduction techniques represent a viable strategy to reduce the computational times whilst preserving the solution accuracy, especially in the design and parameter optimisation phases. Once the reduced order model (ROM) is built starting from some available data, it becomes the optimal solution for multi-query scenarios. ROMs can also be used during the operation phase in control-related applications, to quickly predict the future evolution of the system following anomalies in the operating conditions and to compute those fields of interest for which experimental data are hard to obtain. Still, standard ROM techniques may not be able to provide the needed accuracy for the safety requirements, and they have some limitations that must be considered when studying their applicability.

The objective of this PhD work is to develop and investigate advanced ROM strategies for the study of traditional and innovative nuclear reactor designs, overcoming the limitations associated with ROMs by integrating the proposed techniques with data assimilation (DA) approaches. Traditional ROM algorithms present only seldom integration between the available experimental data and the simulation, and once the ROM is created, it operates as a black box. Additionally, the most widespread ROM techniques need to know the underlying equations of the system under analysis, which are usually approximated as linear for simplicity thus introducing further uncertainties, and some of the physical phenomena occurring in the real-world system may not be known a-priori. With increasing complexity in the systems under study, the paradigm is shifting towards equation-free and DA methods. Data assimilation techniques lie between model-based and pure data-driven methods, as they use both experimental data and the information coming from the numerical model. Uncertainty, noise fluctuations and approximations heavily influence both source of information: by combining the two, the experimental data can help inform the model about the state of the system with local information, and the model can help discriminate between instrument and stochastic uncertainty of the observation, while being able to predict the evolution of the system beyond the available measurements. This dynamic integration can then improve the predictive accuracy of the model and identify the locations where sensors may be more useful.

In general, computational reduction approaches aim at retaining the governing dynamics of the system whilst significantly reduce the computational cost of performing multiple simulations. The fundamental assumption behind ROM techniques is that a few dominant bases can accurately describe the behaviour of the system. The selection of the set of optimal basis modes is critical to create a lower-dimensional but accurate approximation of the system. As such, ROM techniques relies on a computationally expensive offline stage to extract the dominant modes and build the ROM, based either on experimental data (data-driven ROM) or high-fidelity PDE snapshots (FOM) for a limited number of parameters (model-based ROM). In both cases, this costly step is performed only once, and the obtained cheaper ROM can be used in the online phase for running multiple simulations, also for additional values of the parameters for which the FOM solution is unavailable.

This work develops and improves three different ROM approaches for the analysis of nuclear reactors, each with distinct advantages and limitations, to tackle different issues and challenges. These techniques go beyond the current state-of-the-art modelling solutions for nuclear reactors by providing an adequate trade-off between computational cost and accuracy, as well considering their potential future application for control and real-time analysis. For all three techniques, the OpenFOAM computational fluid-dynamic model of the TRIGA Mark II research reactor represents the benchmark test case for verification and validation. Despite its technology, this reactor is a very good benchmark case even for Generation-IV concepts, because it has many similar characteristics.

At first, Dynamic Mode Decomposition (DMD) was optimised for the analysis of nuclear reactor core. DMD is an equation-free method which can extract the time-varying characteristic of the system and the governing dynamic structures from the available data, without the need of any underlying knowledge about the governing equations. DMD also allows the evaluation of a low-dimensional surrogate of the dynamic matrix, on which dynamics and stability analysis can be performed using advanced techniques such as Non-Modal Stability Analysis (as done in this work). Indeed, the results show how, through the extraction of the dominant dynamical structures, this technique is able to extend the model prediction beyond the last available snapshot, especially when dense observations are available. In terms of computational time, the DMD is the fastest method in terms of online reconstruct.

Proper Orthogonal Decomposition (POD) is based on solving the FOM for only a selected number of instances of the parameters; these FOM solutions are then used to construct the ROM. Based on this computationally demanding offline step, performed only once, many computationally inexpensive online simulations for different instances of the parameters can be performed. In this work, the main drawbacks of this approach (the need of having high-fidelity PDE solutions and the loss of local information related to the less energetic modes) are overcome by enriching the ROM model using additional information coming from experimental data: this is done by integrating the Kalman filter (KF) with the POD reduction techniques (POD-KF) in the offline stage during the construction of the ROM itself. This model was applied to an instrumented channel of the TRIGA reactor, showing remarkable improvements in the reconstruction of the fields of interest compared to the standard POD.

Among all reduction order techniques, the Generalised Empirical Interpolation Method (GEIM) allow to tackle at the same time both the problem of optimal sensor positioning and the reconstruction of the state of the system in real-time. The GEIM is an equation-free method based on a greedy procedure to extract both the bases functions and a set of interpolating points from the available data; this information is then used to solve the problem of sensor positioning and of real-time reconstruction, both direct and indirect (for fields for which experimental data are not available). This method was tested on the TRIGA reactor core starting from experimental data on temperature, successfully identifying the best locations for sensors and offering quite good convergence compared to the standard ROM method for CFD. Globally, the POD-KF has better accuracy but longer computational times and, most importantly, it can reconstruct only fields for which FOM data are available. On the contrary, with the GEIM remarkable results are obtained for the reconstruction of fields for which measurements are not available.

In general, this thesis work shows the advantages and the feasibility of employing ROM-DA methodologies for the analysis of complex engineering systems such as nuclear reactors. Due to their flexibility, the proposed techniques can be applied to different reactor concepts.

EXPERIMENTAL AND MODELLING ANALYSIS OF OPERATIONAL HETEROGENEITY IN A VANADIUM REDOX FLOW BATTERY FOCUSING ON THE DESIGN OF INNOVATIVE FLOW FIELDS FOR LARGE-SCALE DEVICES

Mirko Messaggi – Supervisor: Prof. Matteo Zago

Vanadium redox flow batteries are electrochemical devices for the storage of energy, in which electric energy is converted into chemical energy of different vanadium species which are dissolved in a solution of water and sulphuric acid or hydrochloric acid, and stored into electrolyte tanks. This process is allowed by the oxidation and reduction of the vanadium ions between its four stable oxidation states, from II to V, occurring in each side of the device: the V^{IV-V} couple at positive electrode, while the couple V^{II-III} at negative electrode. One of the main advantages of vanadium redox flow battery technology is the decoupling between stored energy and power, since the capacity of the battery is determined by the volume of electrolyte stored inside the tanks, while the power is regulated by the electrochemical performance of the cell stack. Furthermore, the systems are easily scalable to MWh-order-of-magnitude energy storage applications. Other positive aspects are the fast response of the system to load changes and fast start-up and the possibility to easily revert the charge imbalance of electrolytes caused by crossover of vanadium ions through the membrane. Moreover, VRF batteries can assure an extended operative life undergoing to numerous deep charge-discharge. The technology also presents drawbacks that currently prevent a spread commercialization, such as a limited power density because of local mass transport issues which hinder the overall performance, a limited knowledge of the degradation mechanisms which hampers efforts to improve the useful life, and a not-negligible effect of cross contamination on efficiency and exchanged capacity over long time period. Literature studies show a highly heterogeneous distribution of current density over the electrode area, limiting the overall performance of the battery and contributing in hindering the commercial spread of the technology. This heterogeneity can be ascribed to the complex electrolyte transport through the porous electrode, which is determined by the deep interplay among the electrode morphological properties, the distributor geometry and the electrolyte properties. This aspect is faced in literature with different approaches such as innovative geometries of the distributor, novel high-specific-active-area carbon electrodes with enhanced kinetics and improved mass transport properties, or optimizing the operative conditions. All the investigations are carried out without a spatial resolution of performance and electrochemical impedance, with no possibilities to catch the effect of the local reactants starvation that may occur during operation because of the depletion of reactants along the flow field. For this reason, the employment of a segmented cell hardware is fundamental to understand the physical phenomena involved in the determination of local performance and its heterogeneity. In literature the development of a segmented cell hardware for VRFB investigation finds limited applications.

The scope of the present work is the investigation of the VRFB performance and its heterogeneity in order to deepen the understanding of the physical phenomena that are responsible for performance distribution. Among the various aspects, the focus of the research is mainly on the role of the distributor, and of its interplay with the porous electrode, on the performance and its local profile inside the battery. Not only the performance, but also its evolution through time is subject of the research, to tackle the evolution of the cell performance related to the choice of the distributor. After having enhanced the comprehension of the phenomena, the focus moves to a better overall performance of the device, aiming to the reduction of the operational and degradation heterogeneities, lower auxiliaries consumption and a stability through time. Finally, the main results obtained on a laboratory scale device are investigated on a larger scale battery, with electrode area comparable to commercial applications.

In order to answer to the needs of the scope of the work of the project, the research methodology includes an experimental investigation of a single cell with local resolution, thanks to a dedicated hardware designed for the purpose. This hardware allows the complete electrochemical characterization of the device, not only from the overall point of view, but also from the local point of view, performing polarisation curves, charge/discharge cycles and electrochemical impedance spectroscopy. The investigation is carried out not only on the all-vanadium configuration of the device, but also on auxiliary configurations which allow to separately study positive and negative electrodes, the so-called *symmetric cells*. In order to help the interpretation of the locally-resolved experimental data collected, a modelling investigation is carried out starting from simpler and fast 1D and pseudo-2D analytical physics based models, which are versatile tools to analyse experimental polarizations and EIS identifying the main sources of losses, up to a more complex 3D numerical model coupling fluid dynamics and electrochemistry, essential for the design of novel flow field layouts. The main findings of the research activities on a laboratory scale device are then applied to a large-scale device to prove their validity.

The research activities allowed to develop an effective method to characterize the performance of VRFB and to design an innovative flow field, based on the coupling between experimental and modelling tools. It was highlighted how the convective fluxes inside the porous electrode are crucial in determining the performance and its heterogeneity, and how a design approach of innovative distributor geometries should aim to raise their intensity and uniformity to be effective. Thanks to the tools developed, a locally modified innovative distributor was designed, revealing promising results in terms of performance, low pressure drop, limited heterogeneity and stability of performance in time. The effectiveness of the proposed solution was then verified on a large scale device more representative of a real life application, following a scale-up process which considered the trade-off between the reactants depletion over the electrode area and the enhancement of the convective fluxes inside the porous electrode, always trying to maintain a limited pressure drop.

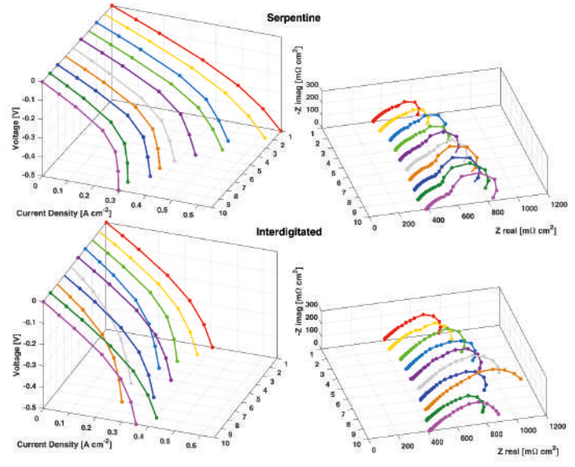

Fig. 1
Locally resolved polarization curves (left) and electrochemical impedance spectra (right) for a positive electrolyte symmetric cell with different distributors.

NUMERICAL AND EXPERIMENTAL INVESTIGATION OF LASER-DRIVEN RADIATION SOURCES FOR MATERIALS CHARACTERIZATION

Francesco Mirani - Supervisor: Prof. Matteo Passoni

Atomic and nuclear analytical methods are among the most powerful tools for materials characterization. Despite their exceptional capabilities, many techniques are subject to significant limitations, preventing their large-scale diffusion. Indeed, as in the case of particle accelerators, the exploited radiation sources are large and expensive. Moreover, they can provide only one kind of particle. Therefore, complementary techniques often require very different types of equipment. Lastly, when electrostatic accelerators are exploited, the energy is not easily tuneable with detrimental consequences in terms of flexibility. Therefore, analytical techniques like Particle Induced X-ray Emission (PIXE), Energy Dispersive X-ray (EDX) spectroscopy and Photon Activation Analysis (PAA) can greatly benefit from the adoption of a more compact, cost-effective and multi-particle radiation source. In this respect, laser-driven particle acceleration could be an attractive alternative to conventional sources. Unlike conventionally accelerated particles, laser-driven electrons and ions are emitted quasi-simultaneously. Their energy can span from a few up to tens of MeV, and they are characterized by a broad momentum distribution. The particle energy can be easily tuned by changing the laser intensity or acting on the target properties. For instance, compared to conventional metallic foils, the adoption of near-critical double-layer targets (DLTs) allow enhancing both the energy and number of the accelerated particles.

Because of their potential compactness and cheapness, several applications of laser-driven particle sources are the object of intense research. However, among the considered fields, the elemental characterization of materials is one of the least investigated. Indeed, only one work on this topic was present in literature before the start of this PhD thesis. Lastly, materials characterization techniques require excellent particle beam reliability. Considering laser-driven radiation sources, they are still subject to a certain degree of shot-to-shot instability. Nevertheless, the required reliability could be achieved by optimizing both the experimental setup and the particle detection system. Besides, the shot-to-shot reproducibility can be enhanced by improving the laser pulse stability and optimizing the target manufacture. This PhD thesis, funded by the European Research Council (ERC) project ENSURE (Exploring the New Science and engineering unveiled by Ultraintense ultrashort Radiation interaction with mattEr), aims at investigating the possibility of exploiting laser-driven radiation sources for the elemental characterization of materials. The analytical techniques under investigation are PIXE, EDX and PAA. Among all possible laser-driven particle acceleration regimes, Target Normal Sheath Acceleration (TNSA) is considered because, while being recognized as one of the most stable and best-understood mechanisms, it provides both electrons and ions at the required energies. Besides,

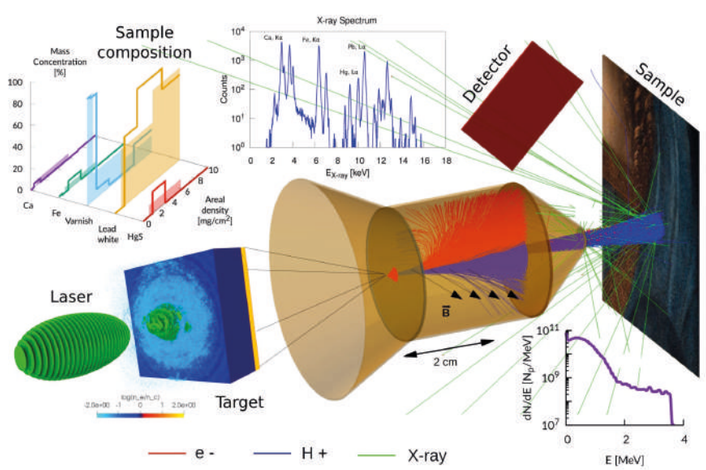

Fig. 1
Conceptual scheme of laser-driven materials characterization.

to ensure the particle energy and number demanded by the applications exploiting reduced laser requirements, the adoption of DLTs is considered. Considering the mentioned goal, several important tasks are accomplished. While the source stability can be raised acting on both the laser and target side, the present work focuses on the latter. Considering DLTs, the adopted sub-micrometric commercial substrates are affected by non-negligible local thickness uncertainty. Thus, a primary task of this work is to develop a strategy for the DLT substrates (or bare targets) manufacture, considering the sub-micrometre thickness range and achieving exceptional thickness uniformity. To this aim, the possibility to exploit the Magnetron Sputtering deposition technique is investigated. After the near-critical carbon foam deposition, the resulting DLTs should be the essential component of a laser-driven particle acceleration apparatus for materials characterization. As previously mentioned, laser-driven radiation sources are intrinsically different compared to conventional ones. Therefore, I perform a theoretical instigation of the laser-driven PIXE, EDX and PAA feasibility. This activity requires the exploitation of suitable numerical tools (e.g. Particle-In-Cell and Monte Carlo) and the development of theoretical models. Additionally, the work aims to carry out the preliminary design of a compact laser-driven apparatus for materials science applications and to unveil the full potentials, in terms of analytical capabilities, of laser-driven PIXE, EDX and PAA. Last, the possibility of performing different materials characterization techniques with a laser-driven radiation source must be experimentally demonstrated. Therefore, the results of a laser-driven PIXE and EDX proof-of-principle experiment at an international laser facility are presented and discussed. In conclusion, the outcomes of this PhD work confirm that materials characterization can be performed in existing laser facilities hosting 10 – 100 TW class lasers.

TURBOMACHINERY OPERATING IN THE NON-IDEAL COMPRESSIBLE FLUID-DYNAMIC REGIME: A STEP TOWARDS NEXT-GENERATION POWER SYSTEMS

Alessandro Romei - Supervisor: Prof. Giacomo Bruno Azzurro Persico

Energy efficiency is a broad topic that can fit different fields, from transportation to buildings and power systems. In this research work, the attention is posed to energy-conversion systems that convert thermal energy to electrical energy. Historically, the conversion from thermal to electrical energy heavily relied on steam-based Rankine cycles or air-breathe Joule-Brayton cycles. Although these technologies are well-established for fossil fuels, they can perform sub-optimally when the aim is to exploit other kinds of hot sources, e.g., waste heat, biomass, and solar to name a few. A major step in efficiency improvement can be represented by developing tailored technologies for the specific energy-conversion problem without adapting existing solutions that may be intrinsically limited from a thermodynamic perspective. Within this framework, organic Rankine cycles (ORCs) and supercritical carbon dioxide (sCO_2) power systems are promising solutions that can outperform conventional technologies based on steam and air for a variety of applications and temperature levels.

Notwithstanding their theoretical potentialities, both ORCs and sCO_2 cycles are penalized by a lack of design experience that may hinder their penetration on the market. In particular, the overall plant efficiency is intimately related to the achievable efficiency of the turbomachinery components, whose design practices cannot rely on several decades of experimental activities and in-field operation. A straight reworking of established design criteria may lead to shortcomings, owing to the unconventional gas dynamics underlying ORCs and sCO_2 turbomachinery, which considerably differs from the one based on the ideal-gas thermodynamics. Intending to develop tailored design rules that can enable high-efficient ORC and sCO_2 turbomachinery, the contribution of this research activity is twofold: first, to advance the present knowledge on turbomachinery operating in the so-called non-ideal compressible fluid-dynamics (NICFD) regime, and second, to provide a number of numerical tools that can be instrumental for the design and the analysis of such complex devices. To this end, the research work can be split into three main pillars:

I. The development of an automated shape-optimization technique based on high-fidelity computational fluid-dynamic (CFD) simulations. Regardless of the specific application, the tool is conceived to provide high-efficient turbomachinery profiles while inherently coping with a generalized thermodynamics. To tackle the prohibitive computational cost that would require a straight CFD-based optimization, a surrogate strategy is introduced. As a result, the computational cost is reduced by building a response surface of the target quantity of interest with a limited number of CFD runs. The surface response, based on the Kriging interpolation, is then minimized (or maximized) with genetic algorithms. The local reliability of the surface response is updated at each iteration by including the optimal individual in the initial design pool. The optimization tool is then applied to a variety of test cases, involving stator and rotor cascades, transonic and supersonic flow regimes, ideal-like and significantly non-ideal flows, and accounting for single and multiple operating conditions. The increase in the efficiency for all reported cases indicates that shape-optimization techniques can be effectively used for the design of turbomachinery for which well-established design rules are presently not available.

II. Many molecularly complex fluids that are routinely used in ORC power systems exhibit a thermodynamic region in which $\Gamma<1$, where $\Gamma=1+c/v\,(\partial c/\partial P)_s$. In this region, some peculiar effects, which are not admissible with an ideal thermodynamic description, can take place, e.g. the non-monotonic variation of the Mach number along expansions and the discontinuous increase of the Mach number across oblique shocks. Until this research work, such non-ideal effects were only studied in simple geometries without any technical relevance. Whether non-ideal effects in the expansion process could also occur in a turbomachinery and possibly affect its performance and operation was still unclear. An original contribution of this research is the first-ever computational assessment of non-ideal phenomena in supersonic turbine flows, observing both the non-monotonic variation of the Mach number against the pressure along an expansion process and non-ideal oblique shocks/rarefaction fans featuring an increase/decrease of the Mach number. In these thermodynamic conditions, the turbine performance is quantified and is found to be highly sensitive to the upstream total state. As such, an uncertainty-quantification strategy combined with CFD simulations is devised to propagate the uncertainty in the boundary conditions (representative of the operational uncertainty in field operation) into an uncertainty in the turbine performance, allowing for a rigorous quantification of the performance deviation in these peculiar operating conditions. The results of this analysis elucidate the role of Γ on the part-load behavior of the turbine, providing valuable information to the designer and minimizing the risk of potential pitfalls induced by non-ideal effects.

III. Complementary non-ideal phenomena are also encountered in characteristic flows of carbon dioxide for sCO_2 power systems. At first, the large volumetric departure from the ideal-gas model in the near-critical region poses some challenges to the aerodynamic design of the main centrifugal compressor. To this end, a comprehensive analysis of the maximum achievable efficiency in presence of such non-ideal effects is performed, and the subsequent impact on the power cycle is quantified. It is shown that competitive efficiencies can be obtained when accounting for the actual volumetric flow evolutions in the early stages of the design process. The analysis was limited to single-phase CO_2 flows, but local flow accelerations can also promote phase transition (both cavitation and condensation, depending on the intake thermodynamic state). The challenges connected with the simulation of two-phase non-ideal compressible flows are tackled in the last part of this PhD research. As a result, two CFD strategies that assume thermodynamic equilibrium are developed, conjugating the need for a reduced computational cost with an adequate solution accuracy. The first model, named "mixture model", includes an extra transport equation for the mass of the dispersed phase (with respect to the classical set of governing equations for compressible flows) with a source term that introduces the phase transition via a penalty formulation. The second model, named "barotropic model", reproduces the pressure-density relation of the mixture along the upstream isentrope to recover the standard set of governing equations for the mixture. The latter model provides predictions that are comparable with the former at a lower computational cost. As such, it may represent a valuable technical tool that can be routinely applied to the analysis and design of sCO_2 centrifugal compressors. As proof, the barotropic model is used to simulate a realistic centrifugal compressor for sCO_2 applications; specifically, the change in the compressor performance at variable intake thermodynamic conditions is evaluated, leading to the formulation of an extended similitude theory that explicitly accounts for both non-ideal and two-phase effects.

LOCAL HEAT TRANSFER MEASUREMENT INSIDE A RECTANGULAR RIB ENHANCED CHANNEL, FOR LOW-REYNOLDS FLOW REGIMES

Luigi Vitali - Supervisor: Prof. Alfonso Niro

Convective heat transfer enhancement is a key technological problem in many applications, and a non-exhaustive list includes turbines, where the increase of the temperature of the evolving fluid, which directly leads to an increase of the system efficiency, requires proportionally more efficient cooling systems, electronics, since the size and power of server farms is skyrocketing as more people rely on digital infrastructures, vehicles, either combustion- and electricity-based, solar technologies, either to cool down photovoltaic modules or for solar air heaters or, finally, nuclear plants, where a high heat output should be carefully managed.
While active techniques, which range from vibrating surfaces to the use electro magnetic fields, may achieve higher heat transfer performances with less pressure losses, passive techniques based on artificial roughness made by various patterns of ribs, groves or dimples, are typically preferred in industrial practice for their intrinsic reliability.
In a world where 3D printing is allowing engineers to design heat transfer components with an unprecedented geometric freedom, it is now more important than ever to thoroughly investigate basic phenomena like convective heat transfer enhancement in relatively simple and controlled systems, to reach a deep understanding of its mechanisms and to find a meeting point between experimental and numerical data. In particular, the first are hard to obtain and, so far, have been shown to provide good general results in aggregate, but are very dependent on the experimental parameters of the single trial. The latter, which may be easy or hard to obtain depending on the software and on the level of programming and modeling involved, may not be any more accurate than the experimental counterpart, especially when thermal models are involved.
While a rich bibliography is available on global heat transfer parameters for a plethora of configurations, as any obstacle in a flow can act as a heat transfer enhancer, in a fully turbulent regime, low-Reynolds regimes, i.e. laminar and transitional, are generally overlooked, but are relevant for applications like plate-heat-exchangers, from which the main experimental parameters of this work are derived. Moreover, the advancements of IR-cameras allow to retrieve high-resolution thermal maps, and consequently enhance the resolution of heat flux maps.
In conjunction with high-precision CFD techniques, it is now possible to deepen the detailed knowledge of convective heat transfer.
In this context, the objective of this project is to establish a technique to reliably and accurately measure the local convective heat transfer in a rectangular channel with 1:10 aspect ratio heated from below, to provide insights both for the explanation of the global heat transfer and pressure loss measurement campaigns carried out in an imposed temperature channel, and an experimental verification for new DNS/based numerical models which are in development at the Politecnico. In particular, the technique should be applied to the whole width of the channel as the behavior towards the edges is neglected in most scientific literature on the topic.
Also, at low-reynolds regime, the convective heat flux has the same order of magnitude with respect to conductive and radiative terms, which have to be carefully retrieved by creating custom models and by measuring conductive and radiative properties of the components at hand. The validation of the models used to retrieve the convective heat flux from the temperature measurements has been thoroughly investigated and described.
IR thermography is chosen for several reasons. Its technical strong points are the wider detectable temperature range, a higher sensitivity to local temperature gradients, and robustness with regards to environmental conditions. However, dedicated image processing techniques have been developed during the course of this work to calculate temperature gradients from images affected by noise, unwanted spatial features induced by the heater, and ribs in various arrangements.
The first experimental results are focused on the smooth channel and four rib configurations, namely transverse ribs, parallel, V up and V down, the last three with an angle of incidence of 60°, all with P/e = 20, e = 4 mm and e/H = 0.33
These results are new in the scientific literature, especially considering the Reynolds regime, i.e. 650 – 7500.
Among the results, the highlights are the retrieval of heat transfer enhancement due to the vortices induced by the corners in the smooth configuration, the higher performance of the V down configuration with respect to the others in the whole Reynolds range, and the trends of average heat transfer increment in the transitioning Reynolds regime.

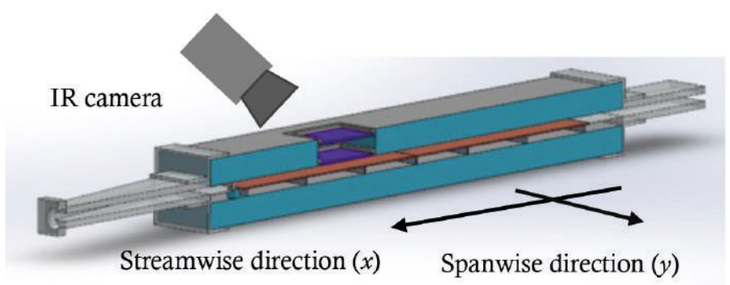

Fig. 1
Lengthwise section of the designed test channel for local heat transfer measurements.

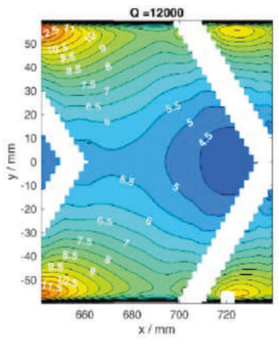

Fig.2
Nu/Nu_0 maps, 60° V-down ribs, Re 3100. Flow from left to right

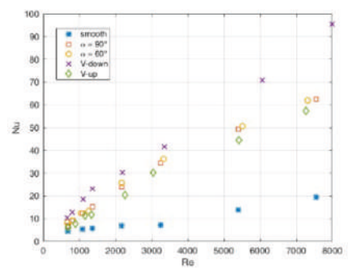

Fig.3
Average rib-to-rib Nusselt number, linear scale

MULTI-DIMENSIONAL NUMERICAL MODELING OF COMBUSTION IN COMPRESSION-IGNITION ENGINES USING TABULATED KINETICS AND TURBULENCE-CHEMISTRY INTERACTION

Qiyan Zhou - Supervisor: Prof. Tommaso Lucchini

The fundamental goal of the compression ignition engine development is to continuously reduce the fuel consumption and meet the progressively tighter emission legislations, which requires an optimal combination of the combustion chamber design, compression ratio, fuel reactivity, and injection strategy. To identify the most promising configurations and speed up the engine development process, the predictive CFD tools are needed to gain more insight into multi-physics phenomenon of combustion and carry out investigations that would prove to be experimentally laborious and expensive.

In this context, this thesis is dedicated to the development and application of a high-fidelity, robust, and fast CFD code for Diesel combustion modeling. In particular, the tabulated flamelet progress variable (TFPV) approach, which can incorporate detailed chemistry and turbulence-chemistry interaction with an affordable cost, has been comprehensively discussed: from its fundamental theory (the flamelet models), implementation in the Lib-ICE code, comprehensive validation in turbulent spray flames and practical Diesel engine, to its application in studying the combustion characteristics of Diesel sprays and exploring the gasoline compression ignition (GCI) concept.

The validation of the TFPV model was conducted in two parts, from the ECN Spray A configuration to the heavy-duty Diesel applications. In the first part, the TFPV approach was first assessed in modeling n-dodecane Spray A with multiple injections and compared with the representative interactive flamelet (RIF) model, being the state of the art in Diesel combustion modeling. The TFPV approach could give a better description of the flame stabilization process and ignition event of the second injection due to the use of progress variable and the consideration of local values of stoichiometric scalar dissipation rate. The soot model was calibrated, and different constants were used for RIF and TFPV models to have a good match with experimental data. In particular, the pre-exponential factor of the surface growth step was three times higher in the TFPV case due to the less presence of soot precursor (C_2H_2). Besides, the k-ω SST model was successfully applied in both non-reacting and reacting sprays with single and double injections. It showed similar accuracy as the k-ε model, demonstrating the possibility to utilize its benefits in describing the flame-wall interaction in practical Diesel engines. Second, the TFPV approach was extended to take into account the multi-component fuels. It was investigated and validated by simulating Diesel sprays with primary reference fuels -- binary mixtures of n-heptane and iso-octane. Two kinetic models from POLIMI and LLNL were evaluated and compared following the operation steps of the TFPV model considering different fuels, ambient temperatures, and oxygen concentrations. The subtle difference between the two kinetic models were well captured and preserved in each step of the TFPV model. The comparison between measured and computed ignition delay and lift-off length suggested that both kinetic models can be applied in practical engine simulations.

In the second part, the TFPV approach was first validated by simulating turbulent Diesel sprays from Spray A, Spray C, and Spray D, representing the change from light-duty to heavy-duty Diesel injectors in terms of nozzle diameters. The spatial coordinates were normalized with the effective diameters, where the same equivalence ratio was observed for different injectors at a certain location. In such coordinates, a smaller injector showed a faster penetration and a higher stoichiometric scalar dissipation rate in the near nozzle region, with a consequent reduction of ignition delay and an increase of lift-off length in the reacting spray simulations. The parametric variations of ambient temperature were later considered for the three injectors to comprehensively assess and validate the TFPV model. The trends of ignition delay and lift-off length with nozzle diameter were correctly captured by the TFPV model, while the computed ignition delays were less sensitive to the ambient temperature compared to the measured ones. Such discrepancy was overcome by extending the TFPV model, being also referred as "TFPV-HR" where the TFPV table is generated using tabulated kinetics based on homogeneous reactor assumption, to the "TFPV-DI" approach that directly integrates the ODE equations in unsteady diffusion flamelet calculations. Second, the TFPV approach was assessed and validated in practical heavy-duty Diesel engine simulations considering a wide range of operating maps. Two sets of grids were compared and tested for different relevant operating points to identify the most suitable mesh. Afterward, simulations were carried out in a heavy-duty engine for 20 operating conditions, allowing an extensive validation of the TFPV model, as well as the tabulated NOx model. Very encouraging results were achieved in terms of pressure, apparent heat release rate and NOx emissions over all these 20 points, proving the accuracy and validity of using the TFPV approach in engine design and development.

The TFPV model was applied in exploring the GCI engine concept after the comprehensive validation. The temporal and spatial features of flame structure and soot formation for different PRFs were first investigated with so-called intensity-axial distance-time (IXT) plots. Then, ten PRFs, from RRF0 to PRF90 with 10% increment in isooctane mass fraction, were investigated and compared in a heavy-duty Diesel engine operating at the conventional high-temperature, short-ignition delay (HTSID) condition. The injection timing was altered from -5 to -13 CAD ATDC to optimize the combustion phase and engine performance for different fuels. The results showed that PRF70 exhibited the best performance at the tested condition, which reduced the soot mass to 5% of the baseline value without sacrificing fuel efficiency.

FEASIBILITY STUDY OF A COLOUR-BASED DISCRIMINATION TECHNIQUE FOR NEUTRON/GAMMA DETECTION WITH INORGANIC SCINTILLATORS

Gabriele Zorloni - Supervisor: Prof. Marco Caresana

Recent advances in inorganic scintillator science and technology brought to the development of an incredibly large number of materials to be employed for radiation detection. Solid state physics models improvements, in particular regarding the scintillation process, in synergy with the advancements in material science and technology, open the way to disciplines such as the so-called band gap engineering and energy level positioning. Large efforts are spent for the study, design and development of ad hoc inorganic scintillators for applications mainly related to high energy physics and medical imaging. Nonetheless, also the radiation protection community is taking advantage of such innovations, using these novel materials for dosimetry and environmental monitoring.
As a side effect of such efforts, a large number of new scintillator species with several different characteristics are available and require precise characterization studies. Those materials are characterized by different unique properties which can be used and combined to face radiation protection and monitoring challenges. Among their characteristics, several new materials are appealing to be employed as gamma-ray probes, thermal and fast neutron counting systems, charged particle detectors etc. A peculiarity of a series of new materials species, such as elpasolites, halides and garnets, is the particular behaviour of their scintillation process. Different dopants added to the host matrix appear to result in very specific spectral emissions, which, differently from the traditional scintillators, are very well resolved in specific spectral regions of the visible spectrum. This spectral information could in principle be employed for different applications.
One out of the traditional tasks of radiation protection and monitoring is the need of performing particle discrimination. Different particle types usually lead to huge variations in the related protection quantities and even small uncertainties in the discrimination process may lead to highly under-/over-estimate the risk associated to a certain radiation field. In particular, neutron/gamma discrimination is one of the major tasks for radiation protection, because of the large difference in the biological effects due to the two particles' types. Moreover, in almost all applications involving neutrons, a background gamma field is present. Several commercial and laboratory-made solutions are designed to manage such problems. The most traditional detector employed is based on 3He-filled tubes, but a series of drawbacks, in particular its shortage, are driving the research towards alternative solutions. Inorganic scintillator-based instruments are an appealing alternative, because of the robustness, low power consumption and the possibility to perform both gamma and neutron real time spectroscopy. Several techniques are employed with inorganic scintillators to face the neutron/gamma discrimination task, such as Pulse Shape Discrimination (PSD). However, these techniques demand an on-line signal processing. Thus, precise and simple alternatives can be attractive.
This thesis is aimed at studying a completely new technique to tackle the neutron/gamma discrimination challenge with inorganic scintillators. The driving idea is to take advantage of some out of the recently developed scintillators and combine their characteristics in a new manner. The possibility of retrieving the spectral emission information, together with a proper engineered geometry of the probe and of the electronic readout, could lead to the development of a new spectral-based particle discrimination technique, exploiting the specific emission of different scintillator species combined with their unique capabilities in detecting neutron and/or gamma-rays. Instead of distinguishing particles by means of analysing the photodetector signal, the proposed technique employs optical filtration directly on the emitted scintillation light. By the accurate design of the probe, and by employing two different readout circuits, it is possible to select a specific region of the emission spectrum, correlating the particle type with respect to the emission colour. The expected advantages of this technique are the relative simplicity of the readout electronics, the cost and power savings and an improved clearance of the discrimination threshold. In principle, once properly designed the detector, the colour-based discrimination can be considered as a quasi-digital physical-based technique, capable of uniquely determine the type of interacting particle, overcoming all the uncertainties related to the electric signal behaviour with respect to the discrimination purposes. In principle, the resulting uncertainties in recognizing the particle type are related only to the stochastic behaviour of the particles' interaction with matter itself.
Two types of solutions were explored, namely the phoswich arrangement and the monolithic crystal setup. The phoswich solution is based on coupling two different scintillator species, chosen considering their scintillation emission and the selective cross section to neutrons and gammas. By the proper geometrical design of the scintillator probe, one can build a system capable of discriminating the two particles' contribution basing on the point of interaction. The former information can be obtained through the optical filtration of the scintillation light. The monolithic solution employs the different mechanisms involved in the scintillation process of some peculiar scintillators. The selectivity of the quenching effects due to different particle types interactions on specific scintillation mechanisms can result in different spectral emissions. By selecting the spectral region through optical filtration, it is possible to retrieve the particle type information.
Several materials were studied, characterized and tested, in particular garnet scintillators (GGAG:Ce, LuAG:Ce, LuAG:Pr, YAG:Pr, both crystals and ceramics), halide scintillators (LiCAF:Eu) and elpasolite scintillators (CLYC:Ce). Specific instruments, sources and computational tools were employed for comprehensively analyse the technique. In particular, two prototype detectors were developed, custom-built and characterized, partially in collaboration with the industry, to accurately study the proposed technique.
The main challenges tackled by the thesis are the definition of the new technique, the development of specific experiments and radiation detectors to properly study the proposed method, the characterization of such demonstrators and the physical and optical characterization of the scintillator species used.
This intrinsically multi-disciplinary approach required the use of several instruments and techniques, both experimental and computational, as well as the need to collaborate with different partners. This brought to the rise of a project collaboration, named DECIDE, with the aim of producing dual-colour emitting monolithic ceramic phoswich scintillators to be employed as the radiation probe for future experiments.
The results obtained demonstrated the feasibility of the proposed technique to be employed as an alternative to existing particle discrimination techniques. Even though the instruments developed are not directly comparable with commercial instrumentation, they demonstrated to be valuable tools for the technique study and definition. The outcomes of the thesis, except from the neutron/gamma discrimination, could find application in other particle discrimination related problems, such as beta/gamma, alpha/beta or in completely different fields, such as medical imaging (PET-DOI) and the so-called coloured radiography.