

DOCTORAL PROGRAM IN ENERGY

Chair: **Prof. Carlo Bottani** The doctoral program in Energy is intended to prepare students for research and professional practice in energy science and engineering, focusing on strategic technologies for efficient energy conversion and utilization which aim to meet the urgent challenge of a sustainable energy supply.

The program, which emphasizes depth and originality of research, combines personal research activity in a chosen specialty with taught courses in the fundamental and engineering sciences that are basic to the energy field. The elective curriculum allows the student to establish the fundamental base from which to concentrate his or her study in an area of special interest. Theoretical, analytical, experimental, and computational aspects of the various fields are covered by the courses and research opportunities offered by the Energy Department. The technical areas spanned by the doctoral program are deeply rooted in the research activity of the Department and include the whole range of thermo-fluid-dynamic processes required to convert primary energy sources into useful forms of energy, as well as to the rational and environmentally friendly use of energy in stationary and mobile plants, either terrestrial or aerospace. This includes the study of clean combustion processes for a large variety of fuels, the selection of proper working fluids and the optimization of thermodynamic cycles to generate or cogenerate mechanical and electrical energy, heat, refrigeration, synthetic fuels, the study of reverse cycles for air conditioning and refrigeration, the design of components like steam, gas and hydraulic turbines, compressors, pumps, internal combustion engines, heat transfer equipment, etc. Equally important are all basic and applied aspects related to energy saving, the control of environmental guality and comfort (indoor and outdoor, including bio-climatic design and innovative envelope technologies), energy efficient products and components, intelligent integration of natural and artificial light, building automation systems, technological issues related to the exploitation of renewable energy sources, the environmental and economic impact of energy transformations. More recently, the Department addressed novel research themes such as integration of high temperature fuel cells with gas turbines, micro-cogeneration, the production and use of synthetic fuels, particularly hydrogen, carbon capture and sequestration techniques, energy recovery from municipal solid waste, geothermal heat pumps and power stations, advanced nuclear reactors.

Besides the subjects of study involved, the doctoral program implements the following educational path:

Basic training to research

Business and manufacturing worlds are justified in recognizing the doctoral program as providing a higher level of education. Indeed an important fraction of the curriculum is devoted to general subjects such as: mathematics, computational techniques, thermo-fluid-dynamics, combustion, measurements and controls. Courses dedicated to doctoral students are organized either by the Energy Department or in cooperation with other doctoral programs.

Training to experimental techniques

The school gives much weight to practical experience and experiment in the laboratory. Students are encouraged to take advantage of the wide availability of laboratories within the Energy Department and the associated Universities.

International experience

The world-wide interconnection of research and productive activities requests the extension of teaching at least to the European circle. The doctoral program encourages students to stay abroad, even for long periods, in order to follow courses, workshops, congresses or to undertake research in gualified laboratories. The doctorate is awarded upon the completion of a program of advanced study and the performance of significant original thesis research. The professional skill acquired in the doctoral course allows research doctors to carry out, organize, plan and manage research activity in the field of energy at an international level and provide the basis for successful careers both in industry and academia. Possible professional outlets for graduates include:

- 1. public and private institutions in the field of energy (national producers of energy services, manufacturers of energy related equipment, etc.).
- 2. energy intensive enterprises for which the Italian law 10/91 requires the position of the "energy manager". In small companies an employee with a master degree could cover properly this position. For larger firms the research doctor has the maturity, skill

and experience to take upon himself the responsibility for this job.

3. small or medium size high-technology companies for the coordination of Statefinanced research programs both at national or European levels. The preparation of the requested documents and the management of the research programs require a specific skill which is usually not available within these firms more and more often involved in research activities financed by public funding.

Starting with the new 25-th doctoral cycle (2010) this doctoral program and the Energy doctoral program are unified in the new Energy and Nuclear Science and Technology doctoral program.

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

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- Ayadi Osama Supervisor: Prof. Mario Motta Tutor: Prof. Livio Mazzarella
- Bianchi Enrico
 Supervisor: Prof. Enrico Tronconi
- Tutor: Prof. Gianpiero Groppi • Bonalumi Davide
- Supervisor: Prof. Ennio Macchi Tutor: Prof. Stefano Campanari
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Their research and most significant results are presented in the following pages.

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CHARACTERIZATION AND PERFORMANCE ASSESSMENT OF AIR PERMEABLE **BUILDING COMPONENTS**

Andrea Alongi

Air permeable walls can be used to achieve the functional integration between building envelope and ventilation plant: multi-layered walls, including permeable layers which are crossed by indoor ventilation air. act as heat exchangers and a filters of the ventilation system. This technology is usually called dynamic insulation. After the literature review, the first step in the research path has been the theoretical study of the physical problem, with the introduction of a mathematical approach aimed at the evaluation of the thermal interaction between the fluid and solid phase in porous media. The second step has been the thermophysical characterization of porous materials of some interest in building breathable walls. This step has been followed by the development of an algorithm for numerical simulations of dynamic insulation components under transient conditions, which can be useful both for research and design purposes. Finally, since such achievements may require an empirical validation to assess their reliability, an experimental apparatus has been designed and built.

As far as the theoretical approach is concerned, after a careful study of the dedicated bibliography, the volume average method has been chosen to deal with

the heat transfer problem related to porous media. The average procedure applied to a representative elementary volume (REV) of the porous medium has led to an averaged energy equation, which describes the phenomenon from a macroscopic over both materials: the first has point of view, taking into account microscopic interactions at the same time, through an effective thermal conductivity. This quantity is related to some main parameters: first of all, the thermal conductivities of both the fluid and the solid part of the domain; secondly, the porosity; finally, due to the mathematical approach used, two more quantities appear, which are related to the local values of velocity and temperature deviations from the respective average values: thermal tortuosity and dispersion These two parameters act as a correction of the simple volume averaged value of thermal conductivity, and need an additional set of equations for the problem closure. Considering now the fluid dynamic from a macroscopic point of view, we have chosen a corrected Darcy equation, where filter velocity and pressure gradient are linked together by air permeability and Ergun coefficient of the material The need for a detailed analysis of some materials, which could be used in building dynamic insulation components, has

arisen from this first part of the work, and has been developed in the second.

We have considered fibrous insulation (e.g. rock wool) and no-fines concrete. Numerical simulations have been performed been simplified approximating fibers with parallel and ordered cylinder arrays, orthogonally displaced in relation to fluid flow and thermal flux. The calculus domain has been defined with six levels of porosity. Conversely, the REV of the concrete-based material has been described in detail: cubic samples have been produced, cut and used for a photographic survey. Images have than been analyzed with three basic purposes: first, the evaluation of porosity; second, the definition of the REV size. based on the porosity and the autocorrelation function; finally, the definition of edges from the vectorization of the interface between the solid and the fluid phase (obtained using an edge-detection algorithm). Thermophysical properties of the compound solid matrix have been obtained by means of TPS measurements. At the end of this process, twelve meshes have been prepared. For both materials, parametric boundary conditions have been applied for inlet air velocity and temperature. CFD simulations results on REVs have been used to evaluate

regression equations for thermal tortuosity and dispersion, as a function of porosity and Peclet number (while no dependence on temperature gradient has been noticed). Such numerical results have also been used to derive correlation between pressure drop across the REV and the average air velocity. Considering fibrous materials, a linear regression equation has been obtained, while a quadratic one has been found for nofines concrete. The latter has also been validated by means of experimental analysis, performed on parallelepiped-shaped samples, and shows a good agreement with empirical data. Besides the materials characterization, some efforts have been made in the definition of a simulation algorithm aimed at the evaluation of multilayered dynamic insulation building components in transient boundary conditions. In order to have a detailed description of the temperature distribution inside the wall, we have decided to introduce a one-dimensional finite difference numerical model. the air velocity across layers More in detail, space derivatives have been approximated with central differences, time derivative has been treated with a full-implicit approach. All boundary conditions have been derived defining the energy conservation equations over appropriated reference volumes.

The numerical model is able to handle calculus domains representative for the building technology under discussion, generally comprising external and internal cavities, and an arbitrary number of permeable and notpermeable layers. The external air gap is simulated assuming a heat transfer coefficient equal to the one used for the indoor environment. Permeable layers model is based on fundamental parameters (effective thermal conductivity, permeability and Ergun coefficient), which are calculated as a function of userdefined conditions, according to all previously mentioned regression equations (restricted to fibrous insulation and nofines concrete, at this stage). Conversely, not-permeable lavers are based on user-defined constant parameters. The internal air cavity is modeled as a single temperature node, and its thermal resistance is calculated considering convective and radiative heat transfer separately. In addition to the temperature distribution computation, is calculated as a function of pressure gradient across the wall. Thanks to both numerical and order-of- magnitude analyses, we have been able to demonstrate that, with time steps typical for walls simulation, a quasistatic approach to the velocity evaluation is sufficiently reliable.

At the end, the described algorithm has been used to define a TRNSYS Type, which allows the user to simulate the kind of wall under discussion. when it is integrated in a building, taking into account the coupling with all other structures. At the same time, we have developed an experimental apparatus aimed at the reproduction of both indoor and outdoor environments, in steady state or transient temperature conditions. Moreover, the ventilation system adopted is able to control air flow. both in terms of velocity and direction, allowing the user to investigate the effects of various working configurations. At this stage, a no-fines concrete wall has been built, with 55 embedded thermocouples for the temperature distribution measurement. In the future, the experimental arrangement will be used to validate all numerically derived correlations, both for fibrous insulation and no-fines concrete, and will allow us to test the consistency of the developed finite difference model. Moreover, once the validation process is over, it will be possible to search for stratigraphies and control strategies optimized for climate conditions typical for Mediterranean countries.

SOLAR COOLING SYSTEMS UTILIZING CONCENTRATING SOLAR COLLECTORS; DESIGN, EXPERIMENTAL EVALUATION & OPTIMIZATION

Osama Ayadi

The food industry relies heavily on the vapor compression refrigeration cycle for food preservation and processing. Unfortunately, due to the scarcity of electricity resources that can run conventional cooling equipments in developing countries high post-harvest losses happen. Consequently, the possibility to utilize solar energy for cooling is considered as an attractive solution.

Concept Development

This thesis reports on the design and performance evaluation and optimization of a novel solar cooling concept that allows a high temperature lift. By applying this concept, very low temperatures (about –10 °C) on the cold side can be achieved in hot climates while a dry air cooled condenser that does not require water is being used. Under these operating conditions, thermodynamic analysis revealed that high efficient solar collectors are needed, and thus the system configuration consists of an air-cooled single-effect water ammonia absorption chiller that is driven by a medium temperature heat source (e.g. parabolic trough or linear Fresnel reflector collectors).

Experimental Setups

The development of the system

concept and the detailed design were implemented through dynamic simulations using the TRNSYS's simulation platform. For this purpose mathematical models of the concentrating collector and the absorption chiller were implemented. Two pilot plants based on this concept were designed and installed; The first was installed for a beverage factory in Tunisiaand consisted of a Linear Fresnel reflector collector (88 m2) connected to a waterammonia absorption chiller (13 kW), the latter cools a cold water-glycol storage (3 m3). The second experimental setup was installed for a dairy factory in Morocco, the system consisted of a parabolic trough collector (59 m²) coupled to a water-ammonia absorption chiller (13 kW) that can deliver cooling directly to the load or to a phase change material PCM cold storage (2 m³) when no cooling load exists.

Experimental Activities

A monitoring system, based on the unified monitoring procedure developed within the experts group of Task 38 SHCP-IEA, was designed and all monitoring sensors have been calibrated and a data acquisition system was programmed using the software LabVIEW. The average electrical COP of the solar cooling system was



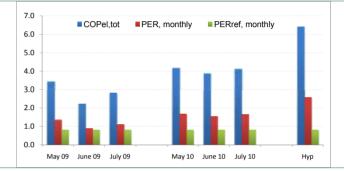
1. The first experimental setup in Tunisia: the solar collector, the absorption chiller and the cold storage.

in the range of 3 during the months of (May to July) 2009, the value has been improved to the range of 4 during the same months of the year 2010. And the ratio between the cold production and the primary energy consumed (PER) was improved from 112.5% during the months of (May-July) 2009 to reach a value of 162% during the same months of the year 2010 (Figure 3).

Models Validation

The results of the extensive experimental work on the pilot plants have been also used to calibrate and validate the TRNSYS models. For the Linear Fresnel Reflector (LFR) collector model, this was done by identifying the model parameters by coupling the TRNSYS simulation





2. The second experimental setup installed on the roof of the Moroccan dairy factory.

software model to the generic optimization software GenOpt. For the absorption chiller model, data acquired from the operation of the system during 2009 and 2010 were analyzed using a parametric-empirical approach to correlate cooling power and chiller's thermal COP to its operating conditions.

Optimization

The validated models were used for further simulation campaigns aiming at defining the optimum operating points of the whole system and tracing a path towards the plant performance improvement. Several parameters of the control strategy have been studied through the coupling of TRNSYS simulation software with GenOpt optimization software. The results highlighted 3. Electrical COP and primary energy ration for the solar and the reference systems for different months.

the higher impact of some control parameters. Monitoring results showed that 44% improvement of the primary energy savings of the system has been achieved by applying the optimization procedure. Further optimization options, concerned with components design, showed that 45% improvement of the primary energy savings of the system could be achieved as can be seen in the data of the hypothetical month in Figure 3. 185

HEAT TRANSFER IN STRUCTURED CATALYSTS FOR STEAM REFORMING

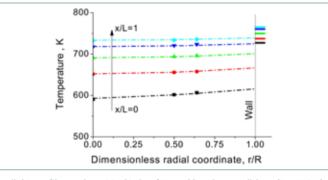
Enrico Bianchi

Introduction

The use of conductive catalyst supports, like metallic foams, is expected to enhance the performances of catalytic reactors, especially when heat transfer is a key factor like in highly endothermic (e.g. steam methane reforming) and exothermic (e.g. selective oxidations, methanation and Fischer–Tropsch synthesis) processes. In this context, opencelled foams are attractive also because of their high geometric surface areas, high void-fraction and high gas/solid heat- and mass-transfer rates. Despite of the increasing interest in such materials, there are neither enough data nor satisfactory correlations to evaluate their performances for the application in industrial structured reactors. In this doctoral work the heat transport properties of metal foams with different geometries and fabrication materials were characterized at process conditions representative of industrial operation, adopting a combined experimental and modeling approach.

Materials and methods

Both the effects of the thermal conductivity of the solid matrix, FeCrAl (k=16 W/m/K) vs. aluminium (k = 218 W/m/K), and of the fluid, N_{2} (k=0.026 W/m/K NTP) vs. He (k,=0.15 W/m/K NTP), were investigated over



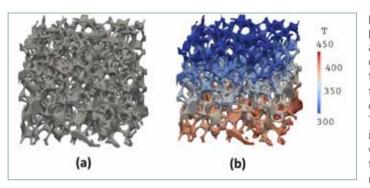
1. Radial T-profiles under a 20 NI/min of N₂ and heating conditions (T_{cp}=773 K).

foam samples with different cell densities (nominal 10-40 pores per inch, PPI) and porosities (89%-95%). Due to the geometrical complexity and the random orientation of the solid phase of the porous medium, the real geometry of foams is not easy to characterize unless using sophisticated methods of volume image analysis like micro computed tomography (μ CT): X-rays used to reconstruct an object from its projections with resolution in the micrometer range. Selected samples were so by micro-computed tomography (µ-CT) techniques. Experimental heat transfer runs were then performed in a lab-scale test rig with 10 cm long foams forced inside a 28 mm I.D. test pipe in an oven. The gas was fed to each foam sample at different flow rates (15-20-25-30-35 NI/ min) under heating or cooling

conditions. Steady-state T-profiles were then used to estimate the effective radial and axial thermal conductivities and the wall heat transfer coefficient of the foam bed. Furthermore the scanned images (µCT) enabled the reconstruction of a 3D volume to be used as virtual model for finite volume method (FVM) analysis of heat conduction.

Results and discussion

From the X-rays microtomography scans the specific geometrical surface of the geometrically characterized in full support, important for interphase transport properties and for catalytic applications, was determined and validated in comparison with literature models. On the other side, heat transfer experimental data showed a dominating role of solid fraction and its bulk material conductivity on the foam effective conductivity.



2. Al sample, 10 PPI nominal, 90% void fraction. (a) Sub-volume from X-ray u-CT: (b) T-distribution with FVM.

Figure 1 (c) presents the radial T-profiles measured in an Al foam sample where the high thermal conductivity of the support caused almost flat radial temperature profiles, with the whole T-gradient confined at the foam-tube wall interface. The effective conductivities determined for reconstructed sub volumes of the scanned samples (Figure 2a-b) confirmed then the conclusions from the experimental study.

The main effect of replacing N₂ with He in comparison experiments at the same condition was a reduction of the T-gradient at the wall, mainly attributed to the incremented thermal conductivity of the gas phase. From these considerations As a first result of this activity, the effective radial conductivity has been modeled as the sum of three contributions: conductive, convective, radiative. Moreover

as outcome of the experimental investigations, appraisals of the wall coefficient were collected. Also for this parameter a predicting correlation was developed, consisting of a convective term and a static term.

Finally to explore the potential advantages of foam supported catalysts, a model simulating a methane steam reforming rector was developed, implementing the thermal coefficicents get from the previous analysis. The model was first validated with literature data for traditional pellet technology, then results for structured reactors have been collected.

Significance

the effects of different heat transfer mechanisms on the thermal coefficients were measured factorizing such

parameters into their equivalent purely conductive, dispersive and radiative contributions: a correlation for estimation of these parameters in function of the foam properties and flow conditions was proposed. The other outcome of this investigation is the possibility, with an optimized foam support. to get structured reactor for methane steam reforming comparable or even better. in term of conversion, outlet temperature and pressure drop, respect to the actual technology. In conclusion this systematic study confirms the potentially superior heat transfer properties of metallic open-celled foam supports when used in place of traditional packed beds of catalyst pellets.

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THERMO-ECONOMIC INVESTIGATION OF AQUEOUS AMMONIA COMPARED TO AMINE CARBON CAPTURE FOR COAL-FIRED POWER PLANTS

Davide Bonalumi

The main focus of this thesis is the study of the post combustion carbon dioxide capture process using aqueous solutions of ammonia. The bench-mark technology is based on amine solutions. The main drawbacks for the amine-process are the high heat consumption for the regeneration, around 4 MJ per kg of carbon dioxide captured and the high degradation rate of the reactant. The process that applies aqueous ammonia solution is a promising alternative. It is proposed commercially with two The models have been validated different absorption conditions obtained principally cooling or chilling the flue gas. Alstom, the company that is developing the process with lower temperature, patented it with the name Chilled Ammonia Process (CAP). According to the company this system has a very low energy demand. In addition the ammonia has no degradation problems and is less expensive than amine.

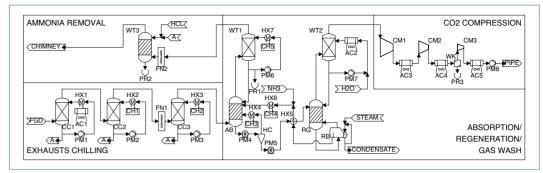
In this work the impact that this option of capture has on a hosting power plant is evaluated. The post combustion capture process takes place through chemical reactions in liquid phase. The solutions obtained are electrolytic. An energy evaluation of the processes, electrical and thermal energy demand, is described thru the thermodynamic

properties of such electrolyte means specific thermodynamic models. The capture processes are studied with the commercial software Aspen Plus. Two different thermodynamic models are coupled with the program: the Electrolyte Non Random Two Liquid (e-NRTL) and the Extended UNIQUAC. The first one is built-in Aspen Plus, the second one is used in collaboration with the Technical University of Denmark (DTU) that has developed and coupled the model with the software. against experimental data. The Extended UNIOUAC model with fitted parameters for the NH₂-CO₂-H₂O system reproduces the experimental results more accurately than the available e-NRTL model.

The report of the European Benchmarking Task Force (EBTF) has been adopted as guideline to define and study a reference case. It is represented by a Ultra Supercritical coal-fired steam power plant retrofitted with an amine-type capture plant. The amine employed is the MonoEthanolAmine (MEA). The power plant is simulated with the software developed by the Energy Department of Politecnico di Milano (GS) while the capture plant is investigated with the commercial software for process engineering simulation Aspen Plus. The

MEA-type process has been simulated with the built-in parameters for e-NRTL model of Aspen Plus. For the capture plant integrated with a power plant is proposed an economic evaluation. The principal indexes for describing the performance of the retrofitted power plant adopted are the SPECCA and the cost of electricity (COE). For the reference case the value of SPECCA has been calculated to be 4.2 MJ/kg and COE to be around 89 €/MWh_a. The scheme of plant for the CAP is represented in Figure 1.

For CAP has been carried out a parametric investigation with e-NRTL model proposed by the software Aspen Plus. The design parameters identified are: (i) ammonia initial concentration in the aqueous solution, (ii) ammonia-to-carbon dioxide ratio in the absorber, (iii) regeneration pressure, (iv) regeneration temperature, (v) absorber chiller evaporation temperature. The ammonia-to-carbon ratio in the absorber is the ratio of the number of ammonia moles entering the reactor through the lean solution line and the number of carbon dioxide moles entering through the exhaust line. The evaporation temperature values apply to the three chillers processing: (i) the exhaust gas, (ii) the lean solution and (iii) the solution



1. Schematic layout for CAP (CCx: Contact Coolers; HXx: Heat Exchanger; PMx: Pump; FNx: Fan; ACx: Air Cooler; AB: Absorber; CHx: Chillers; RB: Reboiler; RG: Regenerator; WTx: Wet Tower; CMx: Compressor).

PARAMETER	UNIT	REF	BEST CASE
Net electrical power	MWe	758	603
Net electrical efficiency, ne	%	45.2	36.0
Capture efficiency, η_{co_2}	%	NA	88.4
Specific CO ₂ emission, E	kg _{co2} /kWh _e	0.679	0.099
SPECCA	MJ/kg _{co2}	NA	3.5

Table 1. Results of the energy analysis of the reference and the best case plants.

PARAMETER	UNIT	BEST CASE
Reboiler heat duty, qCO2	MJ/kg _{co2}	2.66
Electrical loss due to:		
-steam extraction	kWh _e /kg _{co2}	0.1777
-exhaust chilling	kWh _e /kg _{co2}	0.0181
-abs/reg/wash	kWh _e /kg _{co2}	0.1258
-ammonia removal	kWh _e /kg _{co2}	0.0044
-compression	kWh _e /kg _{co2}	0.0183

Table 2. - Results of the energy analysis of the best case plants.

recycle, prior to entering into the absorber. The total number of simulated combinations is 129, among these a best case is identified. A simplified scheme of plant for CAP is simulated both with the e-NRTL model and with the ad-hoc calibrated Extended UNIOUAC. Their results have been compared. Since the better replication of

experimental data by Extended UNIOUAC the results obtained with this model have been exploited to correct the best case determined means the parametric investigation. The integration of this configuration with the same power plant considered for MEA-type capture plant has been investigated. In Table 1 are reported the results.

The integration gives SPECCA index equal to 3.5 MJ/kgCO₂ and the electrical efficiency is 36.0%. In Table 2 are reported the energy demand for the CAP. From the economic evaluation the Cost of Electricity results 83.9 €/MWh .

The main issue for the CAP is the ammonia slip through the treated gases. As alternative to the extensive water wash the acid water wash has been considered. To reduce the impact of the ammonia slip control on the COE, by limiting the expenditure for consumables, has been evaluated the option to obtain marketable byproducts. It has been considered a wash carried out with HCl and with H₂SO₄. For sulphuric acid has been also evaluated the possibility to exploit the SO₂ contained in the coal-fired flue gas. Due to the low content of sulfur in the used coal the best value for COE is around 82 €/ MWh, applying the hydrochloric acid.

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EXPERIMENTAL INVESTIGATION OF THE HEAT TRANSFER ON RIBBED SURFACES

Damiano Fustinoni

Heat transfer in forced convection inside rectangular channels is a very interesting matter for industry since it is encountered in critic heat transfer applications like gas-turbine blade cooling, as well as in devices largely used such as plate-fin compact heat exchangers. In designing these devices, high values of the heat transfer area per unit volume are looked for; however, if this parameter is increased over a given value, thermal performances start worsening. In fact, the higher the surfaceto-volume ratio the narrower the passages, so air velocity has to be lowered to limit the pressure drop; but narrow passages and low air velocities lead to a flow laminarization that is of course characterized by a guite poor convective coefficient which eventually defeats completely the benefits of area increase. To overcome this limit, designer enhances heat transfer by configuring surfaces with a large variety of fins and ribs, which are an efficient and costeffective solution. Thus, a large number of experimental studies examine the fluid dynamics and the heat transfer over these enhanced surfaces. Many papers are concerned with convection in turbulent regime through rectangular channel with ribroughened surfaces, that is a very interesting solution specially for gas-turbine blade cooling. In

spite of these numerous studies, however, there is still a rather poor experimental database on rib-roughened surfaces due to the large variety of configurations and dimensions. For this reason, an experimental investigation on heat transfer characteristics of forced convection inside ribbed channels was performed. This thesis presents experimental results on the average heat transfer characteristics of a forced two Pt100 thermoresistances. air-flow through a rectangular channel with the lower and upper walls is measured by eight T-type surfaces with different kind of ribs. Comparisons with data for a top wall and five on the bottom flat rectangular channel are also presented. The experimental duct cross-section is 120 mm wide and taps located upstream and 12 mm height, and the channel is operated with the lower and upper walls at fixed temperature whereas the sides are adiabatic. All the ribs have a square cross section and they differ in three parameters: side dimensions (2 or results on the behaviour of the 4 mm), geometrical configuration (transverse ribs, tilted ribs with the angle between rib axis and flow direction equal to 60°, V-shape ribs and V-shape broken), pitch-to-side ratio p/e (10, 20 or 40). Upstream the ribbed channel, there is an entrysection, which consists of a 800 mm long rectangular duct with the same transverse dimensions as the test section but with flat and adiabatic walls, in order to attain a developed velocity profile at the test channel inlet.

Air flow rates have been varied in order to investigate Revnolds numbers, based on the duct hydraulic diameter, between 600 and 8000. The average Nusselt number is determined. at various Reynolds numbers, from the temperature differences between the air and the wall at both the inlet and the outlet sections of the heated zone. The air temperature is measured by The temperature of the heated thermocouples, three on the wall. The test channel is also equipped with two static pressure downstream the heated area to measure the pressure drop for the evaluation of the Darcy-Weisbach friction factor. In addition to these average data, this work also presents some local heat transfer coefficient by means of IR-thermography. In particular, it is considered the flat channel and a rib configuration

with transverse rib (p/e = 10, 4mm side length). Indeed, local heat transfer characteristics over are very useful from both a conceptual and practical standpoint, since they provide an insight into enhancement mechanisms, so that they are an efficient tool in guiding geometry optimization. Among the available techniques for heat transfer measurements, infrared thermography is very attractive because it allows a not-intrusive. full-field surveying of the surface temperature with a high spatial resolution. However, the heat flux distribution over the surface is required to determine the heat transfer coefficient from the surface temperature distribution. Consequently, the test section was properly modified by operating the lower wall at fixed heat flux while mounting at the upper one a 120 mm x 80 mm window made of germanium, i.e. a material highly transparent to radiation within the 3-5 µm wavelength range (τ =0.95) that allows optical access to the infrared-camera. Consequently, the upper wall, has not been heated. On the other hand, it is well known that the heat transfer coefficient in turbulent forced convection inside a duct is practically independent of a large extent of thermal boundary conditions. In order to assess the

experimental procedures, the heat transfer coefficient and the pressure drop have been measured for forced air-flows through a test section with flat walls. Very good agreements with the available correlations have been found. In particular, concerning the Nusselt number, the Shah and London correlation and the Gnielinsky correlation have been considered for the

laminar and the turbulent flow respectively; similarly, for the friction factor, the Shah and London correlations have been used Then thirty-four different ribbed

configurations are studied. The flow regime seems to be turbulent from the lowest value of Revnolds number, at least for the configurations with the shortest pitch. The Nusselt number shows a power law dependence on Reynolds number with the same exponent as in the flat channel (about 0.8), but it is two or three times larger. The friction factor for all the tested configurations increases up to an asymptotic value, thus becoming independent of the Reynolds number. This is quite similar to the typical trend observed for flows inside ducts with walls characterized by an equivalent sand roughness. Heat transfer and friction data have been also jointly analysed by means of three several performance comparison criteria, currently used in the optimization of the heat exchanger performance, e.g., at constant mass flow rate, at fixed pumping power, and at fixed heat transfer rate. For each geometry a correlation among the Nusselt number,

the Reynolds number, the

dimensionless pitch (p/e), the

blocking factor (e/D_L), and the

angle between a rib and the

main flow direction is derived. Considering the whole database, the correlations here presented show an error within 6%, which reduces to 2% while correlating only the data for turbulent flow. Thermographic images of the ribbed surface clearly indicate the effect of the ribs on the flow structure. In fact, at a distance equal to 5 p/e downstream a rib, where the reattachment of the fluid vein takes place according to literature, a minimum value of temperature is found. Finally, two theoretical insights are also presented: the fluid dynamics on rough walls and the analysis of turbulent dissipation. In the future these approaches, supported by the DNS and experimental analysis of the flow field by means of PIV, may help to classify the very large number of geometries in groups characterized by the same thermal fluid dynamic effects.

EXPERIMENTAL STUDY OF POLYBENZIMIDAZOLE BASED HIGH TEMPERATURE POLYMER ELECTROLYTE FUEL CELLS

Samuele Galbiati

In the last decades Polymer Electrolyte Membrane Fuel Cells (PEMFCs) attracted increasing attention as energy conversion systems mainly due to their high efficiency, high power density, low emissions and modularity. Such features make PEMFCs suitable for both stationary and mobile applications in the perspective of distributed power generation and of internal combustion engines replacement. and costs, representing an The currently improved PEMFC technology is based on perfluorosulfonic acid (PFSA) polymer electrolyte membranes, among which the most popular is Nafion[®]. PFSA polymers exhibit high proton conductivity only when fully hydrated due to their typical water-based proton transport mechanism. This requires reactants humidification and limits fuel cell operational temperature below water boiling point (normally 60-80°C) to prevent water evaporation. Consequently some severe constraints are introduced in **PEMFC** applications:

- · a reactants humidification system is necessary,
- reaction kinetics are slower than at higher temperatures,
- · cogeneration is not attractive due to low temperature heat recovery,
- tolerance to fuel impurities is poor due to easy CO adsorption on electrodes catalyst.

Considering on-site hydrogen production by natural gas reforming, high purity levels (CO concentrations below 20 ppm) can be obtained only with a multi stage fuel processing system provided with watergas shift and partial oxidation reactors. This feature, together with the necessary presence of gas humidifiers, remarkably increases plant complexity obstacle in the spread of fuel cell systems. Several attempts have been made to rise fuel cell temperature in order to overcome these limitations. This goal can be achieved through the use of basic polymers combined with proton conducting acids. Such systems are also named acidbase complexes and exhibit good proton conductivity in the temperature range between 100°C and 200°C. The resulting fuel cells are named: High Temperature Polymer Electrolyte Fuel Cells (HT-PEMFC). Higher working temperature enhances reaction kinetics, extends catalysts tolerance to fuel impurities and eases fuel cell heat recovery. These features, together with the unnecessary reactants humidification, open new possibilities for the use of polymer membrane fuel cells in real applications, especially where gas reforming units are employed to supply

fuel. In particular the use of polybenzimidazole (PBI) polymer membranes imbibed with phosphoric acid emerges as the best option due to its high thermal stability and proton conductivity. Important steps in understanding the basic principles of HT-PEMFC are necessary due to the early stage of this technology. This work represents an experimental investigation on HT-PEMFC fundamental properties with the aim to provide insight in some of the unclear points that still concern this technology. Particular efforts are dedicated to the study of internal mass transport phenomena, to the clarification of the interaction of water with the phosphoric acid doped PBI system and to the analysis of degradation. The investigated fuel cells are fed with pure hydrogen and air and are tested using a specially designed and built experimental apparatus which can be easily modified to carry out different measurements thanks to its modular concept. Different instruments can actually be connected and the test station can be adapted to perform several types of measures. The uncertainty of the measurements is controlled and minimized with the use of calibrated instruments and with the evaluation of their combined uncertainty. The behavior of the tested fuel

cells is investigated by means of polarization curves and continuous mass balance and Ohmic resistivity measurements. During the whole experimental activity the single internal fuel cell components are periodically monitored thanks to specifically implemented electrochemical techniques such as Electrochemical Impedance Spectroscopy (EIS), Cyclic Voltammetry (CV) and Linear Sweep Voltammetry (LSV). The main outcomes of this work are here listed:

• The performance of the fuel cell is sensitive to temperature and air stoichiometry, but is not influenced by the hydrogen stoichiometry in the investigated range of conditions. The Ohmic resistance of the membrane slightly decreases when the polymer is well hydrated. • The presence of an anomalous air crossover rate was detected in one of the tested fuel cells thanks to the mass balance analysis of the exhausts. Such phenomenon is generally known as crossover leakage and represents a typical failure mode. Its effect on the fuel cell performance was estimated and a methodology for in-situ detection of gas crossover was developed. In the specific case, the fuel cell voltage was not affected by this internal gas leakage, but a sensible increase

in hydrogen consumption

recoverv was measured.

and quantified, water

moves due to different

that compromises the energy

• An important water transport

concentration, pointing out

a diffusive mechanism. With

dry reactants water migrates

across the MEA was detected

- from the cathode, where it is produced, to the anode across the polymer electrolyte. Conversely, when hydrogen is intensively humidified, as would be in a syngas-fed fuel cell, water transport can be reversed and water moves from anode to cathode. In every tested condition the water concentration at anode outlet is higher than the one at cathode outlet and shows increasing trends that underline a non linearity in water transport.
- The influence of humidification on the fuel cell performance was studied in detail analyzing its effect on the single fuel cell components by means of EIS and CV. The acid was found to play a fundamental role, actually when humidified reactants are fed, the phosphoric acid in the MEA shifts its equilibrium to the more conductive orthophosphoric form. As a consequence the number of proton conducting molecules in the membrane and in the electrodes increases. For this reason the conductivity of the membrane and of the electrodes becomes higher. At the same time the three phase zone in the electrodes grows contacting more catalyst particles and enlarging the catalyst active area. Therefore both the Ohmic resistance of the MEA and the kinetic resistance of the electrodes positively decrease. Nevertheless, the partial pressure of the reactants becomes lower and offsets these positive effects, causing a global drop in the fuel cell voltage.

• The degradation of the fuel cell under reference operating conditions was measured and confirmed on two different fuel cell samples. A faster degradation rate was measured when the temperature was increased from 160°C to 180°C. The degradation of the single components was investigated by means of EIS and CV and the main reason of fuel cell performance drop was individuated in the decrease of the catalyst active area. Hysteresis was detected when changing the operative condition and its reason was attributed to slow internal equilibration mechanisms related to hydration, but further study is needed to clarify this point. The mass transport properties of the GDLs. the Ohmic resistance of the membrane and its crossover rate did not show noticeable variations during this activity and seem to be minor issues.

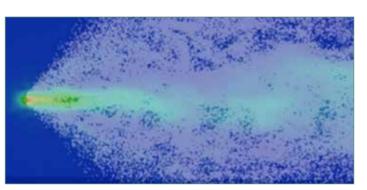
• Different fuel cell configurations have been experimentally studied by changing the cathode gas diffusion layer material in order to investigate its impact on the fuel cell. The investigated Gas Diffusion Lavers resulted in the same fuel cell behavior due to the important thickness of the catalyst coating. This parameter resulted extremely important, therefore the optimization of electrodes thickness and porosity is essential for a proper fuel cell operation.

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VALIDATION AND ASSESSMENT OF A CFD METHODOLOGY FOR FIRE SAFETY ENGINEERING APPLICATIONS

Luca lannantuoni

In the Fire Safety Engineering (FSE), when standard requirements do not provide a good establishment, the Performance Based Design (PDB) approach is the most effective solution to design protection systems for civil buildings and infrastructures. This circumstance often occurs for historical buildings, for huge or complex buildings and for tunnels. The present work focuses in particular about road and subway tunnels, because of the rapid increase of underground transportation systems demand and of their emergency management due to the high risk of fires. There are two major areas of interest for FSE analysis of that systems: the thermal response of structures and the efficacy of smoke management strategies. In fact, smoke can travel within a tunnel rapidly and it is the most hazardous factor to human beings and structures; therefore the main focus is on smoke management. Three different kinds of methodologies have been classified as basic tools to study the smoke propagation in case of fire: pseudo-thermal scale models, full scale tests and numerical models. Experimental activities are difficult because they are expensive: it is expensive designing smoke management systems with fullscale fire tests because these



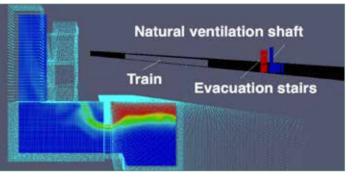
1. Spray simulation of a water mist nozzle operating at 100 bar with a flow rate of approximately 20 l/min and an average characteristic diameter of 50 microns.

systems would require covering all possible scenarios including all necessary computational design tools.

There is an increasing demand for performance-based design in this field, due to the various benefits from this approach. Fire performance strategy is thereby assessed to maintain a safe environment for occupants to escape and to preserve structures. To determine whether the system is effective the criteria is defined and scrutinized. Anytime the hypothesis significantly changes during its lifecycle, the system's performance needs be checked to verify that the safety criteria are met.

Up to now, there are not well established guidelines for applying the PBD approach to address the huge variety of

system design optimizations, but it is well known that among other computational techniques, CFD methodologies are more promising to forecast the evolution of a given fire scenario to verify, maintain or improve the required safety levels of the proposed fire-fighting strategy; they play a significant role when analyzing fire consequences. specifically where complex flows need to be resolved. Emergency strategies assessment is of primary importance and since the strategies involve one or more active systems to provide smoke and fire control, a deep understanding of their own and mutual influences on the consequences of the fire is of paramount interest. This is hardly done by experiments, since ventilation systems and water spray systems effectiveness depends upon a



2. Smoke propagation in a subway tunnel along the evacuation path at 120 s since the fire has started under natural ventilation conditions.

great number of parameters. These scenarios can be split into two areas, those related to natural ventilation design in subway systems, and those related to water mist effect on smoke in road tunnel fire fight- ing strategies. These two scenarios are selected because they state a comprehensive description of all the relevant phenomena involved in fire simulations.

Water mist systems are very interesting because they are a promising and innovative technology for tunnel applications (they are effective in pool fires suppression, air disruption and oxygen depletion, etc..) but up to now few experiments were carried out and there are no standards for their application in tunnel fire fighting design. Within this research a common commercial

water mist spray model's performance is investigated (Figure 1) after a previous evaluation of the nozzle and spray characteristics. Through the validation of a proper numerical set-up it is possible to minimize the high uncertainty that affect the description of the scenario. To do such analysis, the characterization, validation and assessment of the model is of paramount importance and the literature available on the subject is unsatisfactory. An analysis was carried on upon de-stratification effects on smoke due to water cooling, which may implicate danger for people evacuating.

The other important aspect which is not well covered by standards and for which CFD simulation come in help, and that is investigated in the present work, is the design of ventilation shafts for smoke management (with a focus on natural ventilation, since it is a good opportunity because it doesn't require mechanical equipment to be installed and started to evacuate hot combustion products). Hence, CFD simulations are carried on with the primary intent to help the lack of experiments in the design and optimization of these systems (Figure 2).

A rigorous approach have been applied in order to ensure, where possible: grid independence, reproducibility, sensitivity of the model (with particular reference to water spray simulation) and results were backed by experimental validation whenever it was possible. In fact, buoyancy driven flows induced by fire require a validated numerical set up to forecast natural ventilation scenarios to assure the minimum possible uncertainty. For this reason small-scale and large scale compartment fire tests are used to support simulation results, based upon a well established and documented small scale fire test (Steckler et al.) and large scale fire test (Memorial Tunnel).

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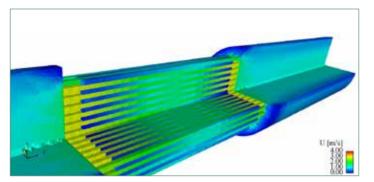
MULTIDIMENSIONAL SIMULATION OF INTAKE AND EXHAUST SYSTEMS FOR INTERNAL **COMBUSTION ENGINES**

Andrea Montorfano

Multi-dimensional **Computational Fluid Dynamics** (CFD) techniques applied to Internal Combustion Engines (ICE) problems are the topic of the present work.

In the first part, an original approach for the simulation of wall-flow Diesel Particulate Filters (DPF) by the Finite Volume Method is presented. Filtrating walls are modeled as porous membranes with an associated pressure drop term, while monolith channels are simplified as one-dimensional arrays of FV cells. By this method, total number of cells in the FV mesh is reduced by a significant amount and, at the same time, minimum cell size is increased. Porous resistance is modeled with the Darcy formula and it is applied to porous faces as a surface force term in the momentum equation. Friction between gas and porous walls is modeled using classic 1D correlation. Due to the greatly reduced computational cost, it is possible to simulate within the same fluid domain both the fullscale particulate trap and the inlet-outlet pipes. Results are obtained both at the global scales and at the filter channel scale (see Figure 1).

The model includes also particulate matter transport and deposition with a scalar



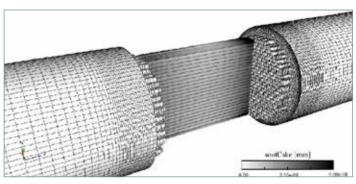
1. Contour plot of velocity field inside a DPF monolith together with the inlet and outlet ducts. Sampled velocity inside the channels follows the theoretical predicted curves.

transport (Eulerian) approach in order to study the filter loading cycle. Soot is advected within the flow as nonreacting chemical specie and it is removed from the exhaust gas flow by a surface sink term applied to porous surfaces. Trapped soot increases walls filtrating efficiency and decreases permeability, thus increasing hydrodynamic resistance. Non-uniformities in soot deposition inside the trap monolith can be studied with this approach (see Figure 2).

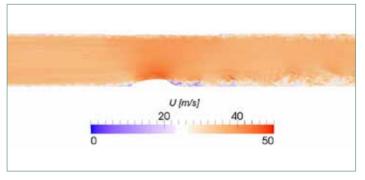
Simulations have been validated by comparison against experimental data. The solver exhibits great accuracy both in terms of global quantities and at length (separation and channel-scale level and also very good predictive properties. In the second part of the research, Large Eddy Simulation

of the ERCOFTAC test case n. 83 (wall-mounted hump, see Figure 3) is presented. Fully turbulent. incompressible flow (Re =1,000,000; Ma = 0.1) is forced over a hump profile that causes separation. A recirculation bubble is formed downstream of the hump profile, up to the reattachment point that is located about one hump length downstream of the separation.

The purpose is to study the influence of some setup parameters, namely, inflow boundary condition, subgrid model, grid size. Reference experimental data of the following quantities are provided: recirculation bubble reattachment point), Reynolds stresses, and pressure coefficient along the hump profile. The influence of the inlet



2. Contour plot of trapped soot cake thickness after 30 min loading.



3. Snapshot of instantaneous velocity for the hump test case. Data simulated with LES, synthetic turbulence inlet, LKDM SGS model

boundary condition is investigated by comparing the following models: fixed velocity profile, mapping plane and synthetic turbulence generation. Inflow boundary conditions the test case under study, since flow statistics (namely, mean velocity and Reynolds stresses) exhibit little or no variation when the inflow condition is

changed. Validation against experimental data has been only partially fulfilled, since the main flow structures could be reproduced only gualitatively. Subgrid model, conversely, has proved to have little influence on a major influence on the results. Two models have been tested: classic Smagorinsky (with Cs = 0.1) and Kim and Menon LKDM. They show an opposite behavior with respect to the

recirculation bubble size, which is overestimated by the former and underestimated by the latter SGS model.

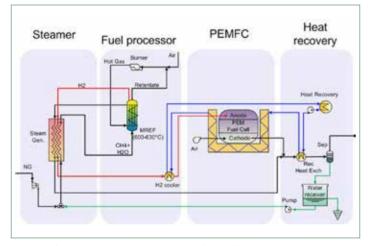
Cell size of the FV mesh plays a dominant role, since LES results are very sensitive to such a parameter. In particular, we found out that, for the present test case, too a coarse discretization can lead to completely unphysical results, which exhibit no separation at all.

MICRO-COGENERATION WITH PEM FUEL CELLS AND MEMBRANE REACTOR TECHNOLOGY

Leonardo Roses

Combined Heat & Power (CHP) technologies are distinctive mediums towards the conquest of an efficient management of energy resources. This PhD thesis studies the development of a residential scale PEM fuel cell based micro-CHP system for the provision of approximately 2 kW electric and 2-3 kW thermal power from natural gas (NG), with overall efficiencies in the range of 80-100 %, Within this setting, the scope of the work has set special focus on the technology for processing of natural gas.

The benchmark technology for small scale integrated NG processing and PEM based cogeneration is based on a series of catalytically activated reactions starting from reforming reaction at temperatures ranging 800 to 900 °C, followed by one or two levels of shift reactors at temperatures between 200 and 450 °C and finally CO reduction through preferential oxidation at temperatures around 200 °C in order to accomplish levels of CO below 10-20 ppm in the stream fed to the fuel cell. This technology, when integrated with a PEM fuel cell for power generation shows net electric efficiencies ranging between 30 to 35 % In this thesis an alternative technology is suggested: the membrane reactor system for hydrogen production, through



1. Layout for CHP system with membrane reformer for NG processing.

which the integrated CHP system could perform at higher electric efficiency of around 9 percentage points compared to the traditional option. Membrane reactor technology refers in general terms to the integration of a reacting process with membranes having the characteristics of being selectively permeable to a specific species, and by this means managing the addition or removal of that species from the reacting mixture. For the processing of natural (being methane its predominant component) the reaction of steam reforming of methane is considered, from which CO_{2} , CO and H₂ are produced. From this reacting mixture, by means of palladium based membranes which are perm-selective to hydrogen, this is removed and sent to the fuel cell anode. The extraction of hydrogen from the reforming reaction shifts the equilibrium conversion of methane towards higher values with respect to the hermetic reaction. In this way, higher values of conversion can be achieved at lower reacting temperature. Figure 1 shows the layout of the proposed system.

By means of the proposed fuel processing technique the main drivers behind the increase in electrical efficiency are the two. On one side the use of nondiluted hydrogen in the fuel cell allows the PEM system to operate at a higher voltage for a given current density, therefore

at higher electric efficiency. Moreover, the high purity of the hydrogen feed could reduce degradation effects on the fuel cell otherwise caused by CO poisoning of the anodic catalyst. The second main effect contributing to the higher electrical efficiency of the CHP system is the more efficient process for the production of hvdrogen.

Research is aimed towards numerical simulation as well as experimentation. The work comprises three approaches to the problem and then integrates them. The first one involves a systemic model for the integration of the fuel processor, the power generation system and thermal recovery. Then, detailed CFD and phenomenological models of membrane reactors of the fixed and fluidized bed type respectively were used for in-depth analysis of the innovative fuel processor. Finally experimental research was performed on a fluidized bed membrane reactor, and obtained results integrated into the prior two levels of modelling approach.

The systemic model was developed using the platform Aspen Plus[®]. Simpler versions of systemic integration of membrane reactor with PEM fuel cells had been found in literature, however in the original model described in this thesis not only the energy and mass balances are contemplated, fluidized bed membrane but taking an approach towards the design of the reactor, by considering the appropriate permeance expression of the membrane a calculation of the required area of palladium membrane is extracted.

Two different models deal with the simulation of specific configurations of the hydrogen separator: for once, a CFD model of a packed bed membrane reactor, and then a 1D- 2 phase phenomenological model of a fluidized bed membrane reactor. The CFD model integrates thermal-fluid dynamics with reaction kinetics and mass transport through the permeable membrane, allowing detailed analysis of the evolution of temperature, species and reaction kinetics along axial and radial directions. Some of the main observations brought after having evaluated the results of the model concern the definition of criteria for defining recommended operating conditions and configuration of the membrane reactor, with emphasis on steam to carbon, risks of carbon deposition, the use of sweep gas, and methods for thermal coupling. Comparing results of a packed bed membrane reactor with those for a fluidized bed membrane reactor under analogue operating conditions showed that the packed bed option could require up to 25 % larger membrane area in order to accomplish the same production of hydrogen, due to the presence of aggressive temperature profiles. An experimental campaign investigated the production of pure hydrogen by steam methane reforming in a reactor capable of producing 1.5 Nl/min of hydrogen output

using 4.5 micron thick Pd-Ag

membranes. Results from the

verification of the 1D-2 phase

experiments allowed for the

phenomenological model

giving detailed definition and observation of the non-ideal performance of the reactor under fluidization conditions and at temperature that provide slower kinetics in comparison with those of a traditional reformer at 800-900 °C. This performance was then translated into the systemic model of the CHP system (on Aspen Plus[®]). Thus, the resulting integrated model is able to reflect realistic performance of the fuel processor and its consequent effect on the CHP system. The CHP solution is optimized in terms of economic and environmental performance giving a proposed design of the fuel processor defining the operating conditions at 630 °C, 12 bar, and steam to carbon ratio of 2.0. Finally the proposed system is described with definition of the membrane reactor design and characterization of the main components for the integration of the CHP system.

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