AutoRE

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References and Abstracts of Scientific Publications

AutoRE

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Executive summary

This report provides a full list of the scientific publications made within the AutoRE project in chronological order. This includes both peer reviewed scientific publications where open source links to the documents are provided, together with presentations given at workshops and conferences.

The AutoRE project partners have produced over 20 scientific publications during the course of the project. Further publications are planned after the completion of the AutoRE project, particularly as part of the final project workshop to be held at the EFC19 conference in Naples in December 2019

Table of content

1 Introduction and scope of the document

This deliverable 6.3 report is a part of Work Package 6 of the AutoRE project. It provides a full list of the scientific publications made within the AutoRE project in chronological order. This includes both peer reviewed scientific publications where open source links to the documents are provided, together with presentations given at workshops and conferences.

As requested by the FCH-JU Project Officer, a zip file containing copies of all the project publications is included as part of this report.

2 List of Project Scientific Publications

1. Bove R, AutoRE (Automotive deRivative Energy system), poster presented at Programme Review Days 2016 of FCH JU, 21-22 Nov 2016, Brussels, Belgium: open access- https://www.fch.europa.eu/sites/default/files/Nov21_Session1_Panel%203_Slot%204_AutoRE_Bove%20%28ID%202891302%29.pdf

2. Facci A L, Loreti G, Ubertini S, Barbir F, Chalkidis T, Eßline R-P, Peters T, Skoufa E, Bove R, Numerical assessment of an automotive derivative CHP fuel cell system. Proceedings of the 8th International Conference on Applied Energy ICAE2016. DOI: 10.1016/j.egypro.2017.03.495, published in Energy Procedia, Vol 105, pp1564-1569, May 2017: open access- https://www.sciencedirect.com/science/article/pii/S1876610217305362

   Abstract: In this paper we model the performance of a PEM-based CHP system. Such a system represents the first layout under investigation within the AutoRe project, which aims at developing an automotive derivative CHP stationary system based on PEM fuel cells with an electrical power in the range 50 kW - 100 kW. The CHP system is fed with natural gas (NG). The model is developed in Aspen-plus with proprietary Fortran codes for the FC and the PSA. Two configurations are studied: with one and with two fuel cell stacks. The performance is presented in terms of electric and thermal power outputs and efficiencies.

3. Peters T A, Stange M, Bredesen R, Pd-based membranes as key-enabling technology for H_2 production, recovery and purification, Presentation at the World Hydrogen Energy Conference 2016 (WHEC2016, June, 13-16, 2016), Zaragoza, Spain

4. Peters T A et al, Palladium (Pd) membranes as key enabling technology for pre-combustion CO_2 capture and hydrogen production, Presentation at the 13th International Conference on Greenhouse Gas Control Technologies (GHGT-13, Nov 14-18, 2016), Lausanne, Switzerland

5. Peters T A, Gas Separation Technologies; Activities on Membrane and non-Membrane Technologies in SINTEF, Presentation at DR HIPERGAS workshop (Jan 27, 2016), Leuven, Belgium

6. Peters T A et al, Palladium (Pd) membranes as key enabling technology for pre-combustion CO_2 capture and hydrogen production, Presentation at AMPEA workshop Materials for membranes in energy applications: gas separation membranes, electrolysers and fuel cells (Feb 7-8, 2017), Oslo, Norway, https://www.sintef.no/contentassets/e136731e6d2144e9a7cb38ac947151a3/summary-of-the-workshop.pdf

7. Peters T A et al, Palladium membranes - from innovation to industrial application, Presentation at CLIMIT SUMMIT (Mar 7-8, 2017), Oslo, Norway, http://www.climit.no/en/record-interest-in-climate-related-conference-in-oslo

8. Stange M, Fontaine, M L, Peters T A, Bredesen R, Scale-up and demonstration of inorganic membranes for gas separation and membrane reactors, Presentation at the 3rd European Workshop on Membrane Reactors (Mar 9-10, 2017), Verona, Italy http://www.ispt.eu/media/Flyer-MR4PI2017.pdf

9. Peters T A et al, 'Palladium (Pd) membranes as key enabling technology for pre-combustion CO2 capture and hydrogen production - from lab-scale to demonstration', Presentation at 9th Trondheim Conference on CO2 Capture, Transport and Storage. (TCCS-9), June 13-14, 2017, Trondheim, Norway https://www.sintef.no/projectweb/tccs-9

10. M. Mirković, J. Šimunović and F. Barbir, Converting an automotive fuel cell system to a stationary power generation system, Poster at 9th International Exergy, Energy and Environment Symposium IEEES9, 14-17 May 2017, Split

Abstract- Fuel cell automobiles are already on the market. Significant scientific and engineering efforts have been made to satisfy automotive requirements in terms of performance, size and weight, durability and cost of the automotive fuel cell system. It has been calculated that such fuel cell systems could be produced at a cost below $50 per kW if produced in sufficiently large quantities applying mass production processes. The goal of this study, performed within the AutoRE project, was to determine what modifications on an automotive fuel cell should be made to make it suitable for stationary power generation and cogeneration applications (combined heat and power CHP). Automotive fuel cells are in the range of 50 to100kW. Such power range could be applicable for commercial and industrial buildings. The most obvious difference between automotive and stationary fuel cell applications is the fuel. While the automotive fuel cells run on high purity hydrogen stored onboard in high pressure tanks, the stationary units should use natural gas–more readily available fuel. Therefore, a stationary fuel cell system should include a fuel reformer and a hydrogen clean-up unit. Because a lower content of hydrogen in reformate would result in loss of power, a stationary fuel cell should be somewhat de-rated. In addition, the reformer may contain additional auxiliary components that need power supply which further reduces the fuel cell system power output. Small amounts of carbon monoxide in reformate may significantly affect fuel cell performance and durability. Usually, stationary fuel cells use CO tolerant catalyst (such as Pt-Ru). Automotive fuel cell systems are designed to operate at higher pressures (2.5 to 3 bar) which in a stationary unit must be matched by the reformer or a hydrogen compressor must be included in the system. In addition, an automotive fuel cell system may employ hydrogen recirculation which may require hydrogen supply at even higher pressure. However, reformate cannot be recirculated, so the unused hydrogen

would have to be burned. The available sources of heat are the reformer, after burner, fuel cell coolant and fuel cell exhaust. Waste heat from an automotive fuel cell is usually available at 80°C or higher. The AutoRE project will address all of these issues and result in a prototype which will be tested to define and verify the capability of automotive derivative CHP fuel cell systems to fulfill the requirements of commercial and industrial buildings, and to identify the technology elements of the system requiring further improvement.

11. Kelsall G J and Ubertini S, 'AUTORE (Automotive Derivative Energy System): 2 Years In', Proceedings of EFC2017, European Fuel Cell Technology & Applications Conference - Paper EFC17823, pp 457-458, Dec 12-15, 2017, Naples, Italy: open access- http://www.enea.it/it/seguici/pubblicazioni/edizioni-enea/2017/proceedings-efc-2017

    Abstract: AutoRE is a multi- partner project funded under the FCH-JU FCH-02.5-2014 call, aimed at demonstrating an automotive derivative fuel cell integrated with a natural gas reformer to make the required high purity hydrogen. The system prototype, to be demonstrated at GE's Rugby site in the UK, has a targeted electrical efficiency of 38-40%, with parallel component developments, such as hydrogen separation membranes, undertaken to increase the efficiency of a subsequent commercial system to >45%. The market for the product will be 50-100kWe applications in industrial and commercial buildings in combined heat and power (CHP) mode. At this scale, the fuel cell based CHP system has potential cost of electricity and emissions advantage over competing technologies. The project is now in its third year, with the build of the prototype system significantly underway. This paper gives the status of the project as reported at the mid-term meeting.

12. Facci A L, Loreti G, Peters T and Ubertini S, 'Numerical modeling of an automotive derivative PEM fuel cell CHP system with selective membranes, Proceedings of EFC2017, European Fuel Cell Technology & Applications Conference -EFC17027, pp 55-56, Dec 12-15, 2017, Naples, Italy : open access- http://www.enea.it/it/seguici/pubblicazioni/edizioni-enea/2017/proceedings-efc-2017

    Abstract: We present possible alternative configurations of a CHP plant based on an automotive derivative PEM fuel cell. Starting from a baseline CHP plant using the pressure swing adsorption (PSA) technology to separate hydrogen, we evaluate an alternative configuration by substituting the PSA with selective membranes.

13. Facci A L and Ubertini S, 'Analysis of the performances of a fuel cell CHP system under different energy demand and climate scenarios'. Proceedings of EFC2017, European Fuel Cell Technology & Applications Conference - EFC17028, pp 57-58, Dec 12-15, 2017, Naples, Italy : open access- http://www.enea.it/it/seguici/pubblicazioni/edizioni-enea/2017/proceedings-efc-2017

    Abstract: In this paper we assess the effective performance of a cogeneration plant based on low temperature PEM fuel cells in different energy scenarios. We vary the energy demand (office apartment district, clinic, hotel, and supermarket) and the climatic condition (Hot, Cooling Based, Moderate, Heating based, and Cold). We also consider two control strategies: one that minimizes the energy cost, and one that minimizes the primary energy consumption. The plant performance is analyzed comparing the energy cost and the primary energy consumption to the business as usual scenario. The payback time is also evaluated to assess the economic feasibility to the plant.

14. Facci A L and Loreti G, 'Numerical analysis of a CHCP system combining an absorption chiller

and a low temperature PEM fuel cell', Proceedings of EFC2017, European Fuel Cell Technology & Applications Conference - EFC17029, pp 59-60, Dec 12-15, 2017, Naples, Italy : open access- http://www.enea.it/it/seguici/pubblicazioni/edizioni-enea/2017/proceedings-efc-2017

Abstract: The utilization of absorption chillers to fulfill the refrigeration demand boosts the effectiveness of CHP systems. In this paper, we analyze the performance of a CHCP plant that integrates a low temperature PEM fuel cell and an absorption chiller. The plant, is simulated through a thermochemical model implemented in AspenPlus. Then, we evaluate the effective performance of the CHCP plant, in a real energy management scenario.

15. Facci A L and Ubertini S, 'Meta-heuristic optimization for a high-detail smart management of complex energy systems'. *Energy conversion and management*, 160, 341-353, Jan 2018- open access: http://dspace.unitus.it/handle/2067/3076

Abstract- Distributed generation and, in particular, cogeneration and trigeneration are generally considered viable solutions to reduce energy consumption and mitigate the environmental impact of developed economies. Nonetheless, such systems need to be carefully designed and managed to effectively meet all the economic and environmental expectations. The design of a distributed generation plant and the choice of its proper management policy are complex tasks that require effective support methodologies and tools. In this paper, we develop a methodology to determine the optimal control strategy for a trigeneration plant. The model enforces mass end energy balances and accounts for the nonlinear and the basic dynamic behavior of each energy converter, for the time varying energy prices and environmental conditions, for maintenance and cold start costs, and for the possibility to store energy. We built on a methodology previously developed and we dramatically broaden its field of application to complex smart grids with a very high temporal detail, by cutting down its computational costs. To this aim, we implement an heuristic procedure that reduces the computational complexity of the non linear optimization problem. The total cash flow, the primary energy consumption, the plant efficiency, and the CO2 emissions, beside the instantaneous set-point of the plant, are among the most relevant results of the model. The model is first validated through 11 test-cases specifically designed to stress the possible weaknesses of the heuristic procedure. The validation evidences that the proposed procedure does not introduce further approximations to the mathematical model. The global optimum is retrieved for all the considered cases. Afterwards, we apply the proposed methodology to a realistic energy management scenario: the assessment of a fuel cell based trigeneration plant for a civil building for a whole year. The discussion highlights the effectiveness of the proposed method for different applications including the optimization of the control strategy for existing plants, the design of new distributed generation systems, the assessment of innovative energy conversion technologies, and the evaluation of national energy policies.

16. Facci A L and Ubertini S, 'Analysis of a fuel cell combined heat and power plant under realistic smart management scenarios', Applied energy, 216, 60-72, Jan 2018- open access: http://dspace.unitus.it/handle/2067/3075

Abstract- Proton exchange membrane fuel cells are a promising and mature technology for combined heat and power plants. High efficiency (in particular for small size devices), practically zero pollutant emissions, noiseless operation and fast response to transient demand make these energy systems excellent prime movers for residential and commercial application. Nevertheless, due to large capital costs, their utilization and commercialization are still limited to demonstrative projects. In this scenario we are working on a research project, called AutoRe, which utilizes an automotive derivative fuel cell for a cogeneration plant to create a synergy between two non competitive industries (automotive

and stationary plants) and to realize a significant economy of scale that will drastically cut the costs of fuel cell based cogenerative plants. In this paper we perform a thorough techno-economic analysis of the AutoRe (AUTomotive deRivative Energy system) power plant. A number of realistic energy management scenarios are constructed by varying the energy demand, the climatic condition, the energy cost, and the efficiency of the surrounding energy system. The control strategy is determined on an hourly basis, by minimizing the cost or the primary energy consumption through a graph based methodology. The resulting global parameters are compared to a reference scenario where electricity is acquired from the grid and heat is locally produced through a natural gas boiler. We consider 5 different building types (Office, Apartment district, Clinic, Hotel, Supermarket), 5 different climatic conditions (Hot, Cooling Based, Moderate, Heating based, Cold), and 2 different surrounding energy systems (USA and Europe). The results show that overall the proposed plant is economically sustainable and effective in reducing the energy costs and the primary energy consumption. Nevertheless, the building type and the energy prices impact on the return on investment, while the climatic condition affects the relative cost and energy variations. In the US scenario the management based on cost and primary energy minimization exhibits similar patterns. On the contrary, in Europe cost minimization might increase the primary energy consumption with respect to the reference scenario.

17. Peters T A, Bredesen R, Venvik H J, 'Pd-based membranes in hydrogen production: long time tests and contaminant effects', Chapter 6, in Drioli, E., Barbieri, G., (Eds.), Membrane Engineering for the treatment of gases, RSC Publishing, ISBN 978-1-78262-875-0, 2018. Link: http://dx.doi.org/10.1039/9781788010443-00177 , Open access: https://www.researchgate.net/publication/321781364_Pd-based_Membranes_in_Hydrogen_Production_Long-term_Stability_and_Contaminant_Effects

Abstract- H2 membrane separation technology has been identified as a key enabling technology for hydrogen as future energy carrier, in particular in conjunction with the capture and storage of CO2. Improved Pd-alloys and composite membrane structures are needed for this to become viable. In this chapter, the factors affecting the stability of Pd-based membranes, focusing particularly on the effect of structural changes and gaseous contaminants under long-term operation, are described. Approaches to enhance the stability and tolerance are introduced and discussed. Subsequently, an overview of the main application areas of Pd-based membranes is given, along with the stability demands of these applications. Finally, relevant long-term studies focusing on membrane stability are reviewed. It is concluded that considerable progress has been made with respect to the stability, with some applications close to commercialisation. Certain contaminants remain an issue, however, that are likely to require additional developments in gas cleaning technologies.

18. Loreti G, Facci A L and Ubertini S, AUTomotive deRivative Energy system (AutoRE): power plant modeling and optimization. International Workshop Noon-to-Noon with Energy and Environmental Challenges, Perugia Feb 15-16, 2018

19. Loreti G, Facci A L and Ubertini S, Selective membranes for hydrogen production in a realistic energy management scenario. Ph.D. Summer School AIMSEA Pisa, Sept 10-13, 2018

20. Kelsall G J, 'AutoRE (Automotive deRivative Energy system)', Programme Review Days 2018 of FCH JU, 14-15 Nov 2018, Brussels, Belgium: open access-
https://www.fch.europa.eu/sites/default/files/documents/ga2011/3_Session%202_AutoRE%20%28ID%204811648%29.pdf

21. Loreti G, Facci A L, Peters T and Ubertini S, Numerical modeling of an automotive derivative polymer electrolyte membrane fuel cell cogeneration system with selective membranes. International Journal of Hydrogen Energy, Vol 44, Issue 9, pp4508-4523, Feb 2019, doi.org/10.1016/j.ijhydene.2018.07.166, Open access: http://dspace.unitus.it/handle/2067/3121

Abstract- Cogeneration power plants based on fuel cells are a promising technology to produce electric and thermal energy with reduced costs and environmental impact. The most mature fuel cell technology for this kind of applications are polymer electrolyte membrane fuel cells, which require high-purity hydrogen. The most common and least expensive way to produce hydrogen within today's energy infrastructure is steam reforming of natural gas. Such a process produces a syngas rich in hydrogen that has to be purified to be properly used in low temperature fuel cells. However, the hydrogen production and purification processes strongly affect the performance, the cost, and the complexity of the energy system. Purification is usually performed through pressure swing adsorption, which is a semi-batch process that increases the plant complexity and incorporates a substantial efficiency penalty. A promising alternative option for hydrogen purification is the use of selective metal membranes that can be integrated in the reactors of the fuel processing plant. Such a membrane separation may improve the thermo-chemical performance of the energy system, while reducing the power plant complexity, and potentially its cost. Herein, we perform a technical analysis, through thermo-chemical models, to evaluate the integration of Pd-based H2-selective membranes in different sections of the fuel processing plant: (i) steam reforming reactor, (ii) water gas shift reactor, (iii) at the outlet of the fuel processor as a separator device. The results show that a drastic fuel processing plant simplification is achievable by integrating the Pd-membranes in the water gas shift and reforming reactors. Moreover, the natural gas reforming membrane reactor yields significant efficiency improvements.

22. Loreti G, Facci A L, Baffo I and Ubertini S ‘Combined heat, cooling, and power systems based on half effect absorption chillers and polymer electrolyte membrane fuel cells’, Applied Energy, 235, 747-760, 2019- https://www.sciencedirect.com/science/article/pii/S0306261918316805, Open access: http://hdl.handle.net/2067/3144

Abstract- Fuel cell based trigeneration plants, that utilize absorption chillers to convert waste heat into cooling energy, are a promising technology to satisfy heat, power, and cooling demand in warm climates. Polymer electrolyte membrane fuel cells, that operate at low temperature (<100°C), are the most technologically mature among the several types of fuel cells. Thermally activated cooling technologies are widely utilized in trigeneration plants to improve their efficiency. However, absorption chillers require relatively high grade thermal energy and their coupling with low temperature fuel cells is relatively untapped.

Herein, we perform a techno-economic analysis of a trigeneration plant based on low temperature polymer electrolyte membrane fuel cells and half-effect absorption chillers. A thermo-chemical model is developed to estimate the performance of a cogeneration plant based on low temperature fuel cells and of the half-effect absorption chiller. The behavior of such combined heat, cooling, and power plant is also analyzed within real energy management scenarios, considering different energy demands, climatic conditions, energy costs, and plant layouts. The control strategy of the power plant is optimized through a graph-based methodology previously developed and validated by the authors. Total energy cost and CO2 emissions are then compared to those of a reference scenario where electricity is acquired from the distribution grid, thermal energy is produced through a natural gas boiler, and a mechanical chiller is used for cooling.

The results show that the utilization of half-effect absorption chillers boosts the environmental and economic benefits for all the considered scenarios. We also demonstrate that the utilization of the absorption chiller reduces the imbalance between the results obtained for the different scenarios (i.e. climates), although economic and

environmental benefits associated to distributed generation are strongly influenced by the energy context.

23. Peters T A, Caravella A, ‘Pd-based Membranes: Overview and Perspectives’, Membranes 9, 25 (2019) 1-5- open access: https://www.mdpi.com/2077-0375/9/2/25.

Abstract- Palladium (Pd)-based membranes have received a lot of attention from both academia and industry thanks to their ability to selectively separate hydrogen from gas streams. Integration of such membranes with appropriate catalysts in membrane reactors allows for hydrogen production with CO2 capture that can be applied in smaller bioenergy or combined heat and power (CHP) plants, as well as in large-scale power plants. Pd-based membranes are, therefore, regarded as a Key Enabling Technology (KET) to facilitate the transition towards a knowledge-based, low carbon and resource-efficient economy. This Special Issue of the journal Membranes on “Pd-based Membranes: Overview and Perspectives” contains nine peer-reviewed articles. Topics include manufacturing techniques, understanding of material phenomena, module and reactor design, novel applications, and demonstration efforts and industrial exploitation.

24. Peters T A, Carvalho P A , Stange, M, Bredesen R, ‘Formation of hydrogen bubbles in Pd-Ag membranes during H2 permeation’, Int. J. Hydrogen. Energy (2019) accepted, https://doi.org/10.1016/j.ijhydene.2019.02.001- open access: https://www.researchgate.net/publication/331466578_Formation_of_hydrogen_bubbles_in_Pd-Ag_membranes_during_H2_permeation

Abstract- Palladium membranes used for hydrogen separation seemingly develop cavities filled with hydrogen, i.e. hydrogen bubbles, along the grain boundaries. These bubbles may represent initial stages of pinhole formation that lead to unselective leakage and compromise the long-term stability of the membranes. Alloying with Ag improves the permeability of Pd, but whether these H2 bubbles form in Pd-Ag membranes remained unknown. In this work, the microstructure of a Pd77Ag23 membrane was characterized by electron microscopy after H2 permeation testing for 50 days at 15 bar at temperatures up to 450°C. The results show that Ag does not prevent bubbles from emerging along high-angle grain boundaries, but reduces the number of potential nucleation sites for cavity formation by supressing the development of dislocation networks when H-saturated Pd is cycled through the miscibility gap. Both magnetron-sputtered and electroless plated membranes are afflicted by H2 bubbles, thus their formation seems determined by intrinsic properties of the material independent of the fabrication technique. The qualitative discussion enables to point directions for enhancement of membrane stability.

3 Conclusions

The AutoRE project partners have produced over 20 scientific publications during the course of the project. Further publications are planned after the completion of the AutoRE project, particularly as part of the final project workshop. This is scheduled as a special session for the at EFC19 conference to be held in Naples in December 2019 (http://www.europeanfuelcell.it/).

4 Acknowledgement

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