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Dr. Alejandro A. Franco studied theoretical physics in Argentina (Universidad Nacional del Sur and the Instituto Balseiro of the CNEA -Argentinean Nuclear Commission-). In January 2002, he joined the CEA in Grenoble to participate in a research project addressing micro-fuel cells. Until December 2002, he worked on the development and the characterisation of a new kind of solid fuel cell with anionic polymeric electrolyte and with magnetized catalysts. In January 2003 he started his PhD thesis which he defended in 2005: in his thesis he proposed a new theoretical approach based on infinite-dimensional Bond Graphs for the transient modeling of the physico-chemical phenomena in the PEFC. At the present, he is member of the permanent research staff of the CEA/LCPEM, and he is the CEA-Grenoble specialist on the modeling of electrochemical processes in PEFC environments: he is working package responsible of several French projects (*POLIMPAC*, *OPTICAT*, *DVD-AME...*) addressing the understanding of electrochemical mechanisms taking place on Pt and non Pt alloys catalysts, the impact of pollutants on PEFC performance, and the intrinsic catalytic and ionomer ageing. He was the supervisor of 4 Master students, he participated in about 30 French and international congresses and workshops, and he is the author of several scientific papers in first class journals and proceedings and of one international patent. In 2005, he was finalist for the Young Scientific Award of the International Society for Solid State Ionics.

“AGEING MECHANISMS IN POLYMER ELECTROLYTE FUEL CELLS: WHEN ELECTRODE DESIGN MEETS THEORY – *THE CEA-GRENOBLE APPROACH*“

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Electrode durability in state-of-the-art polymer electrolyte fuel cells (PEFCs) is one of the main shortcomings limiting the large-scale development and commercialization of this zero-emission power technology. It is largely observed that the micro-structural properties of Pt and Pt-alloy electrodes evolve during the membrane-electrodes assembly (MEA) operation, limiting the PEFC lifetime to 300–500 h under some power drive-cycle operating conditions representative of automotive applications [1]. These spatiotemporal micro-structural changes are strongly dependent on the electrode operating conditions and translate into cell potential degradation. Because of the strong coupling between different physicochemical phenomena, interpretation of these experimental observations is difficult, and analysis through mathematical modeling becomes crucial in order to establish microstructure-performance relationships, to elucidate MEA degradation and failure mechanisms, and to help improve both PEFC electrochemical performance and durability.

In order to help to solve the “PEFC cost/performance/durability equation”, several combined experimental and theoretical tools from fundamentals to systems (portable, automotive, stationary including coupled wind energy/hydrogen systems) are developed at the CEA-Grenoble from more than 15 years: in this talk, we will summarize some of these research efforts.

In particular, as an example of the CEA coupled applied/fundamental research strategy, we will discuss a multi-scale mechanistic theoretical approach describing the electrochemical processes in a Polymer Electrolyte Fuel Cell, including ageing mechanisms, and based on a novel non-equilibrium thermodynamics model of the catalyst/ionomer electrochemical interfaces recently developed by us [2-4]. This proposed model takes into account the cathodic oxidation/dissolution of platinum, the transport of dissolved platinum in the Nafion[®] phase, the carbon-supported platinum ripening and the carbon support corrosion. It carries out a coupling of these mechanisms with the internal dynamics of the electrochemical double layers taking into account the transport phenomena of protons and platinum ions in the diffuse layers, as well as the detailed HOR and the ORR and water dipoles adsorption in the compact layers. This continuous interfacial model is coupled with a continuous micro-scale model of the electrons, dissolved platinum and protons transports through the MEA thickness, and with a continuous micro-scale model of the reactants transport through the impregnated Nafion[®] layers [3-4]. The model represents explicitly the different physical phenomena as nonlinear sub-models in interaction, and some of its parameters can be estimated by using

atomistic approaches (*ab-initio*, reactive force field molecular dynamics...). It helps to analyse the sensitivity of the MEA response to the operating conditions (nominal current, reactant-gas pressure, temperature, Nafion[®] water content), to the compositions (platinum/Nafion[®] loadings) and to the temporal evolution of the electrochemical activity from ageing mechanisms [5-6]. The influence of time on impedance spectra pattern can also be simulated, using a Matlab[®]/Comsol[®] in-house developed code. The use of the infinite dimensional Bond Graph theory has allowed to hierarchize this multi-scale model in a modular way, so that it is reusable in another electrochemical contexts and it can be easily coupled to other physico-chemical phenomena (water transport, pollutants...[4,7]). Theoretical predictions are compared with experimental results obtained with dedicated in-situ and ex-situ tests performed with model electrodes and MEA (DLI-MOCVD, CNT-supported catalyts...) and specified benches (from mono-cells to systems). This work focuses on the diagnostic of the dynamic fuel cell operation, and depending on the PEFC final application, it could help to optimize the electrodes properties for improved performance and durability at low costs [5-6].

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