PUMA MIND

Physical Bottom-up Multiscale Modelling for Automotive PEMFC Innovative Performance and Durability Optimisation

CALL TOPIC	Innovative materials and components for PEM electrolysers
START-DATE	17 December 2012
END-DATE	17 December 2015
TOTAL BUDGET	€4,100,000
FCH JU CONTRIBUTION	€2,300,000
OTHER CONTRIBUTION(S)	

PARTNERSHIP/CONSORTIUM LIST

Coordinator: CEA (France)

Partners: German Aerospace Center (DLR), Universita degli Studi di Salerno, AECSIC (Spain), Hochschule Offenburg, Ecole Normale Superieure de Lyon, JRC, Simon Fraser University, Vodera Ltd, Idiada Automotive Technology SA.

PROJECT WEBSITE/URL

www.pumamind.eu

PROJECT CONTACT INFORMATION

Pascal Schott and Manuelle Quinaud

pascal.schott@cea.fr, manuelle.quinaud@cea.fr

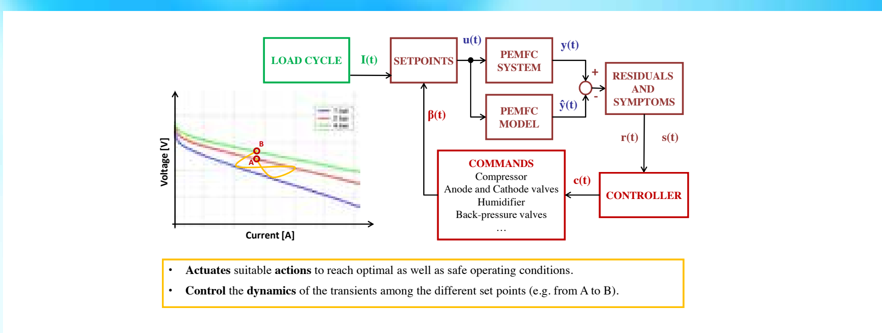
MAIN OBJECTIVES OF THE PROJECT

Puma Mind aims at establishing a predictive multi-scale modelling tool for PEMFC performance and durability as function of its components and operating conditions (automotive applications) as follows:

- a detailed model of the electrochemical phenomena;
- a detailed model of the transport processes;
- a 1D cell-level multi-scale model describing the competitive mechanisms and calculating their relative influence on the macroscopic performance and durability under current cycled conditions;
- a 2D cell-level multi-physics CFD model to predict instantaneous efficiency;
- an innovative diagnostic and control-oriented physical model for online PEMFC diagnosis and real-time optimisation of operating conditions.

PROGRESS/RESULTS TO DATE

- Adsorption energies (WP2): linear relationship to estimate adsorption energies as a function of a simple geometric descriptor, the generalised coordination number. Easy to calculate and to integrate in the micro-scale models (WP3, WP4).
- Multi-scale coupling between the electrochemical double layer model including a kinetic Monte Carlo description of the adsorbed species and the meso-scale/micro-scale transport model (MS-LIBERT code, WP3).
- Integration of the electrochemical and transport data in a 1D multi-scale model (EDMOND, WP4).
- Macro-scale model linked to system models ready for the integration of degradation models to address performance and durability at system level (WP5).
- Development of on-board monitoring tools to quantify the major losses of the fuel cell, and to enable building comprehensive strategies to reach optimal and safe conditions (WP6).



FUTURE STEPS

Next year will be dedicated to:

- Further atomistic calculations and their integration at the meso-scale;
- Comparison between the kinetic Monte Carlo and the mean field approach for the integration of the electrochemical data;
- Sensitivity study at the 1D multiscale model level to demonstrate the relative impact of the mechanisms involved, and enable further reduction of the electrochemical and transport modules for their integration in the macro-models;
- Integration of degradation (Pt dissolution and chemical degradation of the membrane) in the models;
- Improvements in the development of on-board diagnostic tools and control strategies to ensure both performance and durability.

CONCLUSIONS, MAJOR FINDINGS AND OUTLOOK

- Modules are under development at each scale and their integration is on-going thanks to strong interaction between the partners.
- Performance models are set up and degradation will be implemented next year.
- System-level models are ready for incorporation of the reduced models from the lower scale.
- Comprehensive strategies for performance and durability optimisation are under development.
- The first workshop on multi-scale modeling for PEMFC was held at CEA Grenoble, France, on 12-13 June 2014.

CONTRIBUTION TO THE PROGRAMME OBJECTIVES

SOURCE OF OBJECTIVE/TARGET (MAIP, AIP)	ASPECT ADDRESSED	PROJECT OBJECTIVES/ QUANTITATIVE TARGETS	CURRENT STATUS/ ACHIEVEMENTS TO DATE
MAIP	Development of modelling tools for PEMFC performance and durability	DFT calculation of adsorption energies on a Pt_{201} nanoparticule (nanoscale)	Linear relationships for the estimation of the adsorption energies. Suitable for taking into account the degradation of the catalyst
		Kinetic Monte Carlo for the description of the adsorbed species in the electrochemical double layer (meso-scale). Calculation of the surface potential according to a calculated electric permittivity and a given distribution of the size of the nanoparticles. On-going development.	Coupling of kinetic Monte Carlo and transport model. Ready for comparison between kinetic Monte Carlo and the mean field approaches for the modelling of the electrochemical double layer
		Integration of the modules at the meso-scale Study of the interplay (sensitivity study) Methodology for the reduction of the micro-model	Integration of the electrochemical module and the transport module in the micro-scale model
		Bridge between the micro-model and the system-level models	Performance model at the system level is ready for the incorporation of the reduced models from the lower scales, and ready for the incorporation of the degradation mechanisms
		Design of on-board experiments to quantify the major losses in the FC depending on the operating conditions. Design of comprehensive control command strategies to promote performance and durability	Methodology for the model reduction at the system level is well established On-board quantification of the major losses is developed Control command strategies are under development for improving performance and durability
		Ex-situ post-mortem GDL computed tomography for structure reconstruction and effective properties calculation	CT scans performed on the fresh and aged GDL. Results are under analysis
		In-situ investigations: SAXS (ESRF, Grenoble) for PEM water content	Neutron experiments were carried out to validate the water management models

FUEL CELLS AND HYDROGEN JOINT UNDERTAKING