Puma Mind

Physical bottom Up Multiscale Modelling for Automotive PEMFC Innovative performance and Durability optimization

Duration:

from 17/12/2012 to 17/12/2015

Application Area:

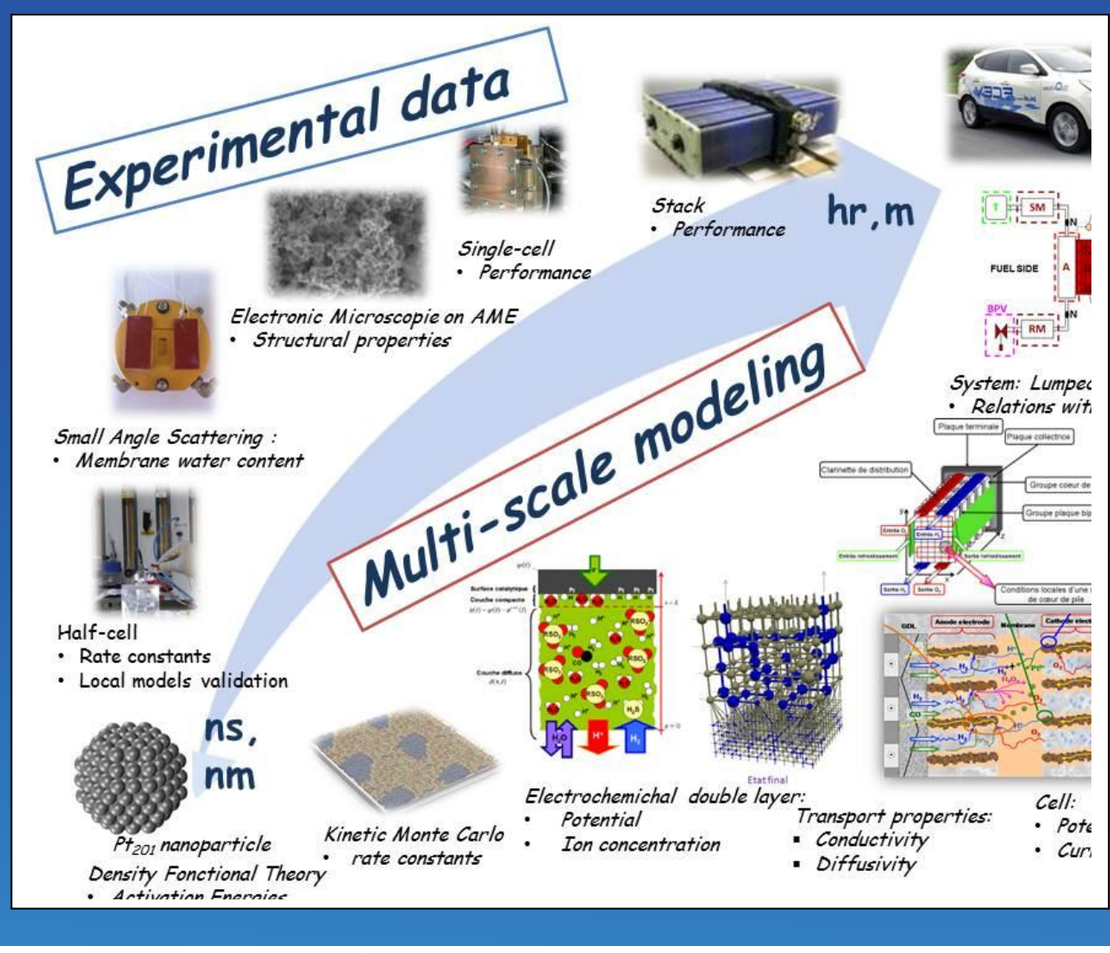
Automotive Power Generation

Budget:

Total budget: 4 100 000 €
FCH contribution: 2 300 000 €

Partnership / consortium list:

Coordinator: CEA;
1 – CEA / LITEN, France, 2 – , Germany, 3 –UNISA, Italy, 4 – , Spain, 5 – HSO, Germany, 6 – ENSL, France, 7 – JRC, Belgium, 8 – SFU, Canada, 9 – VODERA, England, 10 – IDIADA, Spain, 11 – LRCS, France



Summary / main objectives of the project:

The main goal of PUMA MIND is to establish a predictive multiscale modelling tool of PEMFC durability as function of its components composition and operating conditions that should be representative of automotive applications. More precisely, this modelling tool will adhere to an integrative approach combining:

- **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 at multiple scales (from the material to the cell level) and allowing 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 optimization of the operating conditions.**

Perspectives:

Next year will be dedicated to

- **the on-going development of the performance and degradation models at various scales and coupling these scales (DFT calculations including solvent contribution, KMC simulation and local degradation model, electrodes, GDL and membrane transport properties, diagnostic tools)**
- **Experimental validation (RRDE, Half-Cell, Single cell, SAS)**
- **Fuel Cell roadmap, workshop organization**

Contribution to the Programme Objectives:

OBJECTIVES OF	RELATED PROJECT ACHIEVEMENTS
"Development of multi-scale modeling and numerical simulation tools for increasing the performance and durability of PEM fuel cells. These computer-based tools are to be validated through experimental work"	• **DFT** calculation of **adsorption energies** on a Pt_{201} nanoparticule (Nano scale). • **Kinetic Monte Carlo** for kinetic constants calculation based on DFT results (mesoscale). On-going development. • **Models coupling the nano/meso/micro scales** (under Matlab/Simulink). • Lumped-**control oriented models** based on micro scales inputs. • **In-situ** investigations: **SAXS** (ESRF, Grenoble) for PEM water content. • **Ex-situ** Post-mortem **GDL Computed Tomography** for **reconstruction. Effective properties calculation.**
"Lifetime predictions,… research to establish methodologies as well as tools for modelling, operational controls and diagnostics"	• On-going development of an **online diagnostic model** to optimize the operating conditions. • On-going **modelling** of **degradation mechanisms** at various scales : Carbon corrosion, Platinum coarsening, PTFE aging. Development of a local degradation model. • In-situ investigation of the **water content in PEM with aging** (**SAXS**).

Dissemination:

- Workshop "Multiscale modelling of PEMFC", June 12-13, 2014 in Grenoble, France
- Tutorial and Organized Symposium on multi-scale modelling within the 64th Annual Meeting of the ISE, September 8-13, 2013, Queretaro, Mexico
- A tutorial on multi-scale modelling at the CECAM workshop (Julich Research center, Germany)
-10 Publications (done or planned) in scientific journals
-10 Communications (done or planned) in international conferences
-1 book (Polymer Electrolyte Fuel Cells: Science, Applications and Challenges, A.A. Franco, Ed., CRC Press, Taylor and Francis group, FL, USA (2013).

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Puma mind
Modelling PEM Fuel cells