Minisymposium at the
7th International Conference on Porous Media
18-21 May 2015, Padova, Italy

Multiscale modeling of transport processes in Fuel Cell and hydrogen economy related applications

Relevant theme: Computational challenges in porous media simulation

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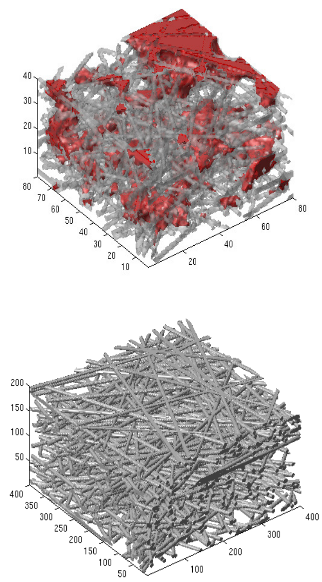
Fuel cells (FCs) are electrochemical devices efficiently converting the Gibbs Free energy of hydrogen oxidation into electricity and comprise a key enabling technology for the future energy strategies. FCs are constructed by a series of technologically advanced porous layers that allow for the efficient transport of the reacting species and products towards and from the catalytic surfaces of the Membrane Electrode Assembly (MEA), where the reactions take place and the electric current is collected.

Typical porous FC components include among many others; the **Gas Diffusion Layers** (GDLs), which are made of carbon fibers in order to provide a high porosity pathway for the species, the **Microporous Layers** (MPLs), which are made of carbon nanoparticles, treated with a hydrophobic agent, that significantly improve water management in the system, and the **Porous Electrodes,** that provide the three-phase boundary between the electron conductive material, the ion conducting membrane and the gas permeable medium, where the reactions take place.

Such FC components combine a series of transport properties: high permeability, excellent electric conductivity for the selection of the produced electric current towards the external circuit, excellent thermal conductivity to allow for the heat management during the exothermic oxidation reaction and joule heating of internal components.

The numerical modeling of transport processes, including flow and heat transfer, in such components is thus of crucial importance for the characterization and assessment of commercially available materials (e.g. carbon paper, carbon cloth), and the understanding of their contribution to the overall performance of the integrated FC systems. At the same time, the diversity of length scales involved (e.g. micrometers at GDLs vs nanometers in MPLs) in such materials makes modeling a taunting task that can benefit significantly from multiscale numerical approaches combining methods ranging from the atomistic all the way up to continuum scale modeling of transport processes. This is a highly challenging computational concept receiving at the moment continuously increasing attention also due to the strong technological impact of a viable hydrogen economy.



Stochastically reconstructed GDLs of CIGRACET carbon paper (EREL Lab, NCSR Demokritos)

The proposed minisymposium aspires to bring together scientists from the rapidly growing field of transport processes studies for hydrogen-related applications using pore scale, pore network and continuum scale modeling. Although emphasis will be on FC components, contributions associated with relevant applications such as hydrogen purification, storage in solids etc, are also expected.

[1] Yiotis et al. *Journal of Power Sources* **269** (2014), 440-450.
[2] Pauchet et al, *International Journal of Hydrogen Energy* **37** (2012), 1628-1641.
[3] Ceballos L. and Prat M., *Journal of Power Sources* **195** (2010), 825-828.