

CFD Contribution on Fuel Cell Development

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The need to move away from fossil energy sources has never been so strong. One of the technologies under the spotlight in recent years is certainly that of Fuel Cells (FC). Direct Methanol Fuel Cells (DMFC), Solid Oxide Fuel Cells (SOFC) or Molten Carbonate Fuel Cells (MCFC) represent different developing paths of this technology, but they all share a couple of benefits with respect to other energy conversion devices: they have no moving parts and a quite simple working principle. But how can we push forward the development of FCs?

Computational Fluid Dynamics (CFD) has been proven to be a powerful research aid in different fields of engineering. Similarly to other simulation tools (0D and 1D), 3D CFD opens up possibilities for parametric studies in a cost and time effective approach. Whether it's evaluating the effects of air-fuel mixture formation in an engine [1], comparing the performance of several types of air foils [2] or calculating the drag coefficient of a car with variable spoiler angles [3], this is what everyday CFD has to deal with.

Different types of FCs require different considerations, so let's focus on FCs for mobility: in this large family of by-products [4], Low Temperature Proton Exchange Membrane Fuel Cells (LT PEMFC) have been identified as the most suitable for vehicle implementation given their low operating temperature (80-100°C) and thus fast transient phase. This does not mean that this technology doesn't show issues: current and voltage requirements force engineers to use a stack configuration of FCs, making it harder to keep the overall temperature field of the device under control, thus resulting in poor cell performance. Thermal management is a common problem for all FC types. A peculiar problem of LT PEMFC is flooding: the redox reaction taking place in the Membrane Electrode Assembly (MEA) generates water. A humid MEA is able to enhance transport phenomena [5], but too much water could flood the pathways of reactant gases [6].

And, once again, the "deeper" we go in the stack configuration, the harder it is to regulate water removal rates. CFD can help us understand key design factors and improve overall FC performance. It is possible but quite difficult to prepare an experimental setup and observe water accumulation inside a working PEMFC: you could use plexiglass Bipolar Plates (BP) instead of metal ones, but the wettability of the surface will be affected.

Researchers developed several models to investigate different aspects of the interaction between water and MEA. These interactions may be divided in three main areas:

- Does the design of the channel influence water removal rates? Simulations show that the height and width of the channel, the presence of a "U" turn, and the wettability of BPs are key factors that determine critical dimension of the droplets and their behaviour (do they detach? do they roll? do they lift?) [7-9];
- Does the design of the interlaced surface of the Gas Diffusion Layer (GDL, the outer layer of MEAs) influence water removal rates? In [10] it seems clear that the texture of the GDL can improve water transport, and the dimension of the pores can also reduce delays in detachment of droplets [11];

- Does the design of porosity/permeability of MEA layers influence water removal rates? The approach shown in [12] led to an increase in PEMFC performance after a thickness and porosity optimization study.

FC development presents itself as an extremely multidisciplinary process, even more if one starts to consider its implementation on a vehicle. It is a device still far from its optimal state, and the coupling between experiments and CFD simulation certainly represents the most promising way to fully develop this technology.

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