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Modeling and simulation supporting the application of fuel cell & hydrogen technologies

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ABSTRACT

This work aims to demonstrate the importance and usefulness of multiscale computational approaches and tools, as well as of reliable input data and verification procedures for fuel cells & hydrogen (FCH) technology applications. For that purpose, three typical case studies on the use of simulation models/tools at various scales for specific applications are examined. More specifically, these cases concern:

(i) the optimization of materials design for Fuel Cells via a novel process-based methodology; particularly the stochastic reconstruction and accurate characterization of carbon fiber-based matrices, which are commonly used as Gas Diffusion Layers (GDL) in Proton Exchange Membrane Fuel Cells. The computational approach employs a rigorous model simulating the spatial distribution of the graphitized resin that is typically used to enhance the structural properties and thermal/electrical conductivities of the composite GDL materials;

(ii) the investigation of hydrogen safety related issues and scenarios, where characteristic examples of Computational Fluid Dynamics (CFD) studies and associated benchmarking activities in particular applications are presented;

(iii) the optimization of hybrid Renewable Energy (RE) – hydrogen systems at real scale in remote/isolated communities like off-grid islands where cost effectiveness with regard to the produced energy is a critical factor.

Besides the scientific and technical aspects, we would like through these examples to stress how complementarities and synergies between numerical and experimental research can greatly assist in closing knowledge gaps & developing innovative designs, and may contribute toward defragmentation of relevant efforts, more effective collaboration between researchers and provision of validated simulation tools.

1. Rationale

It is well known and widely acknowledged that modeling and simulation can offer substantially to the development, application at all levels and public acceptance of new technologies across disciplines. This work focuses on the support that modeling and simulation efforts have provided and continue to provide for the development at all scales (from micro- to macro-) and market deployment of Fuel Cell & Hydrogen (FCH) technologies. The latter are considered as a promising candidate for the future energy mix as they offer the potential for increased penetration of Renewable Energy Sources (RES) and essential reductions in the emission of greenhouse gases and other pollutants [1].

The FCH scientific community has repeatedly identified a number of R&D needs with regard to computational infrastructure and tools that would enable higher efficiency, creativity and productivity of research encompassing the whole spectrum of FCH processes and systems [http://www.h2fc.eu/portal.html]. Such needs include:

- Defragmentation and improvement of computational infrastructure and tools for FCH research.
- Covering existing needs for simulation support in a wide range of FCH topics, like H_2 storage, H_2 safety, Fuel Cell (FC) performance, Integrated RES-H_2 systems, etc.
- Assuring quality and reliability of simulation services, through systematic model validation/inter-comparisons/new developments.

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- Creating a validated software suite for the assessment of FCH systems key performance parameters for use by interested researchers and stakeholders.

In the present paper, we demonstrate briefly the capabilities offered by modeling and simulation with the aim of covering existing needs in a wide range of FCH topics, including (but not limited to) storage, safety, FC performance, integrated systems, etc. Three particular examples are presented spanning a wide range of applications and scales.

2. Microscale reconstruction and characterization of materials for FCH technologies

2.1. Stochastic reconstruction of FC components

Fuel Cells (FCs) are compact, yet complex, electrochemical energy conversion devices that efficiently produce electrical power from the chemical energy released during the oxidation-reduction reaction of hydrogen with an oxidizing agent, such as oxygen. FCs are very versatile devices, that can operate under a very wide temperature ranges (e.g. less than 100 °C for PEMFCs (Proton Exchange Membrane FCs) to more than 500 °C for SOFCs (Solid Oxide FCs)) and use as fuel several gases rich in hydrogen, including natural gas, ethane and propane [2,3]. These features combined with their high energy conversion efficiencies (measured as the ratio of the produced electrical power to the provided chemical power) in the order of 50% and the high gravimetric energy content of H_2, in the order of 120 MJ/kg compared to 44 MJ/kg of petrol, make FCs a very attractive option for powering a wide range of applications, both mobile and stationary, from vehicles to submarines and large-scale Uninterrupted Power Supply units for the urban electricity grid.

Typical FCs consist of stacks of several layers of composite materials that perform different highly specialized functions. The reacting gases (typically H_2 and O_2) are introduced into the Membrane Electrode Assembly (MEA) through appropriately designed flow channels (bipolar plates) and diffuse through porous Gas Diffusion Media (e.g. the Gas Diffusion Layer in Proton Exchange Membrane FCs (PEMFCs)) towards the catalytic electrodes, where the electrochemical reactions take place [4,5]. The energy conversion efficiency of the MEA can be limited by a series of factors associated with the design and chemical/transport properties of the composite layers that make up the stack. These include irreversibilities due to Joule heating effect (ohmic overpotential), the finite rates of diffusing species from the flow channels to the catalytic surfaces (concentration overpotential) and the energy associated with the activation of electrochemical reactions at the catalytic surfaces (activation overpotential) [6].

The dramatic increase in computational power in recent years, combined with the development of robust parallel programming and code execution methodologies/technologies, have allowed for performing numerical simulations of transport processes in complex heterogeneous porous materials at unprecedented spatial scales and resolutions. It is nowadays possible to characterize FC components by solving the transport and conservation partial differential equations at sub-micrometer resolutions for computational domains of the same size as such of the actual components. The calculated microscale field for each transport variable can then be volume-averaged over the entire computational domain to obtain macroscopically meaningful effective transport properties for the subsequent solution of the macroscopic conservation equations in the entire FC assembly.

In the following sections, we present such a multi-scale approach for reconstructing and characterizing crucial FC components that can serve for the design and optimization of the internal FC structure. Our analysis relies on the accurate pore-scale digital reconstruction, either process-based or stochastic, of each FC component and the rigorous modeling of reactive transport processes to quantify the effects of microstructural characteristics on transport parameters. The volume-averaged transport properties are then applied to a computationally efficient REV-scale model (Representative Elementary Volume scale), where FC components are treated as effective continua, for the direct calculation of FC efficiencies. While we focus primarily on Gas Diffusion Layers (GDL) of PEMFCs as a case study, the proposed analysis can be readily applied to all other FC components and their combinations.

For the microscale characterization of GDLs, we have performed a series of 3D X-Ray micro-CT scans on a commercially available Toray TGP-H-090 carbon paper at a resolution of 1 μm/pixel. The obtained micro-CT images were subsequently binarized using the open-source Fiji-ImageJ software in order to filter image noise, remove image margins and produce digital void-solid domains of the scanned medium (Fig. 1(a)). The void volume fraction in all samples was found to be 0.77–0.79 and the sample average thickness 285 μm, both in agreement with the values reported by the GDL manufacturer.

The scanned images reveal the anisotropic microstructural characteristics of the GDL, which is composed of carbon fibers with an apparent diameter in the range of 7–9 μm, glued together with a wetting phase resin that covers primarily fiber intersections and smaller pores. The digital reconstruction of the fibrous skeleton, prior to resin impregnation, can be thus realized following the standard method of Schladitz et al. [8] where overlapping cylindrical segments are deposited in a 3D domain, with the projection of their principal axis randomly distributed in the xy-plane (azimuthal angle, φ), while the polar angle, θ (z-direction), obeys a

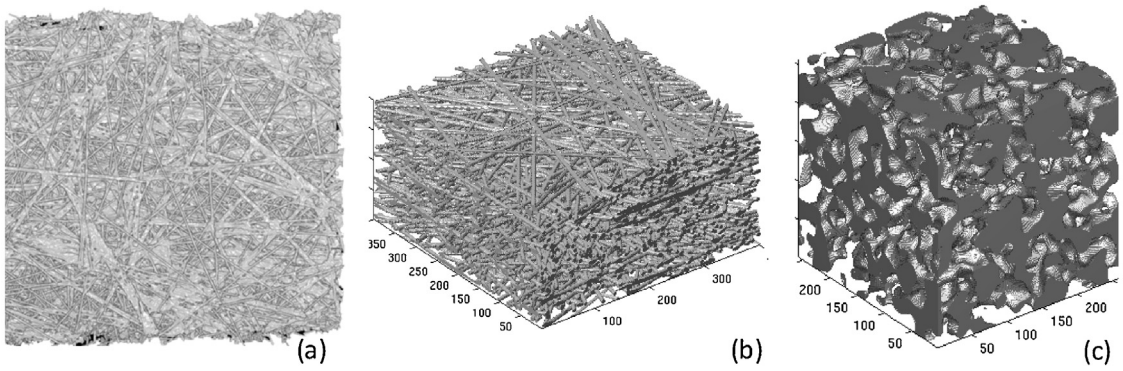

Fig. 1. (a) A digital representation of the surface view of a Toray TGP-H-090 GDL obtained using X-Ray microtomography at a spatial resolution of 1 μm/pixel. (b) A stochastically reconstructed GDL (only fibrous skeleton) using the methodology described in Ref. [7]. (c) A stochastic reconstruction of the Microporous Layer (MPL) of a SOFC using a Gaussian Kernel for the medium autocorrelation function. The units are in micrometers.