NUMERICAL HEAT TRANSFER AND OTHER TRANSPORT PHENOMENA AND MODELING APPROACHES WITH RESPECT TO CHEMICAL REACTIONS IN FUEL CELLS

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Keywords: Fuel cell, heat transfer, mass transfer, transport phenomena, electrode, electrolyte, membrane, anode, cathode, reaction, modeling, simulation, micro, macro, computation fluid dynamics, reforming, water phase change, multi-phase flow.

Contents

Summary

There are various transport phenomena occurred in fuel cells, e.g., multi-component gas flow in cells and manifolds, heat and mass transfer of gas species in various functional components and sites. These physical processes are strongly affected by chemical/electrochemical reactions in nano-/micro-structured electrodes and electrolytes. For example, the electrochemical reactions generate or consume chemical species together with electric current production, which take place at the active sites (so-called three-phase boundaries, or TPBs) in all kinds of fuel cells. Furthermore, potential water phase change and two-phase flow in proton exchange membrane fuel cells (PEMFCs) and internal reforming reactions of hydrocarbon fuels in solid oxide fuel cells (SOFCs) are strongly coupled with the electrochemical reactions and other transport processes to make the analysis and modeling even more difficult.

It is a common practice that, for modeling and analysis at the unit-cell and component level, typically CFD-based approaches might be suitable. Microscopic modeling approaches are required to analyze the various processes in, e.g., catalyst layers and active surfaces, while on the fuel cell stack and system levels, methods like lumped parameter analysis and overall heat/mass balances are more suitable. This paper outlines the various kinds of the approaches for modeling and numerical analysis, in terms of their characteristics, applicability and limitations.

1. Introduction

It is clear that extensive research activities have been carried out on fuel cells worldwide during last decades, with particular interest and focus on solid oxide fuel cell (SOFC) and proton exchange membrane fuel cell (PEMFC) systems. High performance, low cost and high reliability have been considered as the primary aspects and concerns for fuel cells to compete with well-developed fossil fuel power generation devices, such as internal combustion engines. However, the most research interests have focused on new material development, processing and manufacturing techniques for specific systems. As expected, currently available fuel cell materials appear to be adequate for near-term markets with higher cost entry points, and industries now focus on fuel cell design and optimization for better performance, improved durability, cost reduction and better cold-start characteristics, and system studies including hybrid or integrated fuel cell systems.

In these cases more attention should be placed on detailed analysis of transport processes in fuel cell functional materials, components and unit cells, even at micro- and nano-scale levels. This is because the majority of the physical and chemical processes take place in such small regions that are inaccessible to experimental measurement. Furthermore, water-phase change/multi-phase flow in PEMFCs and internal reforming reactions of hydrocarbon fuels in SOFCs are strongly coupled with the electrochemical reactions and other transport processes in the catalyst layers to make the physical phenomena extremely complicated. On the other hand, extensive research work is also needed for fuel cell stacks for the purpose to efficiently deliver required power output at the load operating voltage, and to achieve proper water/thermal management for an integrated power plant including various units.

Scientific models and simulations have been extremely important tools for many industrial applications. On the one hand, the micro-scale approaches, e.g., Density Functional Theory (DFT) and Molecular Dynamics (MD), and the meso-scale ones, e.g., Monte Carlo (MC) and Lattice-Boltzmann methods (LBM), take into account the effects of the multi-functional materials microscopic structures on the charge-transfer (electrochemical) reactions at active sites, the surface chemistry and the gas-phase chemistry based on elementary reaction kinetics (individual chemical reaction steps between intermediates) in the porous electrodes. On the other hand, there are well-developed computational fluid dynamics (CFD) codes, which are widely applied to optimize design or investigate the structures of a flow at a macroscopic scale. Similarly commercial codes are available for simulating integrated power system including several units. It is possible to use such simulation tools to make improvements to product design where physical design and testing are too expensive or not even possible.

This paper concerns the current status of fundamental models and analysis approaches for fuel cells and systems. It should be mentioned that this work is limited to PEMFCs and SOFCs. However, there are various models for other fuel cells, e.g., molten carbonate fuel cell (MCFC) in Gundermann *et al.* (2008) and Brouwer *et al*. (2005), and for fuel cell material and applications in Peighambardoust *et al*. (2010).

2. Multi-phase Transport Processes and Reactions in Fuel Cells

The fuel cell is not a new invention, since the electrochemical reaction was discovered already in 1838-39. The interest in fuel cells has been growing exponentially. Fuel cell systems are still an immature technology in early phases of development, as can be noted due to a lack of a dominant design, few commercial systems and a low market demand. The creation of strategic niche markets and search for early market niches are of a vital importance for the further development. It is expected that mass production will start when a dominant design is found, and then production cost will significantly decrease due to the economy of scale.

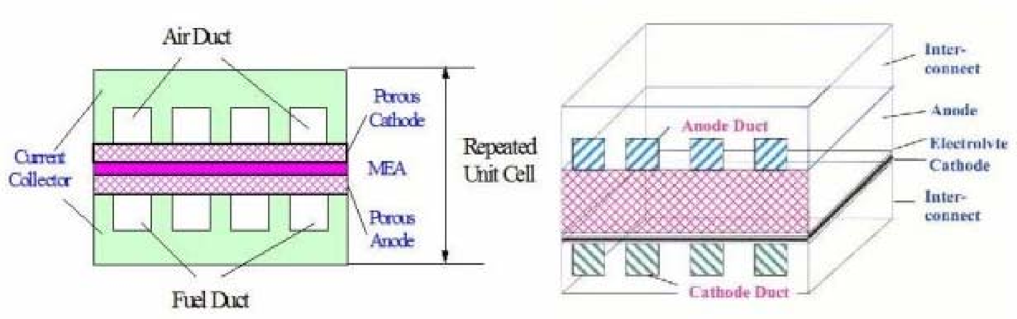
The fuel cells can be examined from different points of view: as an electrochemical generator in a viewpoint of electrochemical reactions at continuum level, as a heat and mass exchanger in a perspective of fluid dynamics and transport phenomena, or as a chemical reactor in viewpoints of chemical reactions depending on fuel composition and heat effects associated with the electrochemical conversion (Andersson *et al*., 2010).

2.1. Fuel Cell Basics

The major processes relevant to the fuel cell characteristics are similar in SOFCs and PEMFCs. These processes consist of the gas-phase species transport, electrochemical reactions, electronic and ionic transport, and heat transfer and temperature distribution. A unit-cell structure of fuel cells, as shown in Figure 1, includes various components, such as fuel and oxidant ducts (or channels), electrolyte (polymer electrolyte membrane for PEMFCs), anode and cathode diffusion layers, catalyst layers in between them, as well as current inter-conductors/-connectors.

Unit cells are further organized together into stacks to supply the required electricity. In a fuel cell stack, the gas transport processes consist of the fuel and oxidant gas flows which are separated through the gas manifolds where no electrochemical reactions occur. The fuel and oxidant gases flow along cell ducts (or channels), where there is absorption of the reactants and injection of reactive products from/to the active sites. In the porous layers (electrodes), transport of the reactant gases occur towards triple-phase boundary (TPB, where electrode, electrolyte and gas meet) between the electrolyte and the electrodes, and the exhaust gases are rejected to the cell ducts (or channels) through the open pores. The exhaust gases from each cell are discharged through the gas output manifolds.

The electrolyte is non porous material, for instance, Y_2O_3 stabilized ZrO_2 (YSZ) in SOFCs. At an operating temperature (between 600-1000 °C for SOFCs and around 80 °C for PEMFCs), the electrolyte becomes non-conductive for electrons, but conductive to oxygen ions (in SOFCs) and hydrogen protons (in PEMFCs). The SOFC cathodes are mostly made from electronically conducting oxides or mixed electronically conducting and ion-conduction ceramics. The anode consists normally of nickel/yttria stabilized zirconia (Ni/YSZ) cermet. SOFCs can be designed with planar, tubular or monolithic structures. The planar design is normally more compact, compared to the tubular design, i.e., a higher specific volume power can be obtained. Tubular and planar SOFCs can be either electrolyte-, anode-, cathode- or metal-supported. An electrolyte-supported cell has thin anode and cathode (~50 μm), and the thickness of the electrolyte is more than 100 μm. This design works preferably at temperatures around 1000 °C for SOFCs. In an electrode-supported SOFC either the anode (anode-supported) or the cathode (cathode-supported) is thick enough to serve as the supporting substrate for cell fabrication, normally between 0.3 and 1.5 mm. The electrolyte is in this configuration very thin, and the operating temperature can be reduced to an intermediate range.



(a) (b)

Figure 1. Schematic sketch of a unit cell for: a) PEMFC, and b) SOFC.

For PEMFCs a polymer membrane is used in between anode and cathode. The membrane is made by substituting fluorine for hydrogen in long chain polymers and the process is called perfluorination. After this, a side chain is added, ending with sulfonic acid. The perflourination of the polymer gives it the chemical resistance and mechanical strength while the addition of sulfonic acid gives it the property to carry the positive ions (hydrogen ions in this case). Therefore, the electrolyte in PEM fuel cells is sometimes also called proton exchange membranes. Despite the differences in terms of materials, it is obvious that all the fuel cell electrolytes should essentially have the following properties, such as: they should be chemically resistant, and sufficiently strong so that they can be casted in very small thicknesses.

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Biographical Sketch

Dr. Yuan works as a senior researcher and the project leader for heat transfer and transport phenomena in energy systems and a supervisor for PhD students at the Department of Energy Sciences, Lund University, Sweden.

Jinliang received his LicEngn Degree in February 2001 and presented his PhD degree thesis in February 2003. He was promoted as Docent (an honorary degree in Sweden) in April 2006. Dr Yuan is a visiting professor for several universities and a research institute in both Sweden and China.

Supported by the external funding agencies, his current research work concerns comprehensive understanding of catalytically chemical reaction mechanisms and multi-functional material structure effects on various transport processes in components of fuel cell systems, in terms of micro-/nano-structures and configurations, water/thermal/mass balance and integration, and overall fuel cell/stack performance as well. The research is approached by theoretical and numerical analysis validated by experimental data. The computer codes have been further developed and applied for the research projects; commercial software has been applied to estimate the heat amount being exchanged in fuel cell systems, in terms of heat transfer rate requirement by considering the effects from compressors, humidifier and PEMFC stack operating conditions; The research is of fundamental as well as of applied character, and has links to overall fuel cell modeling/design system analysis, as well as other investigations considering reacting transport processes in real-world industrial applications.

Jinliang has been very active in formulating project proposals, and several projects have been granted by agencies. Dr Yuan has established a good network with industry and universities, and is now strongly involved in international collaboration both concerning projects and as reviewer of papers for journals and conferences. He severs also for an international journal as in the editorial board, and has delivered several invited lectures and keynote presentations internationally. As a teacher/adviser, he has been involved in several courses for undergraduates and PhD students both in China and Sweden. More than 100 papers of various kinds have been extensively published in international journals or conference proceedings.