



Modeling of solid oxide fuel cells

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Solid oxide fuel cell (SOFC) is a high temperature (800–1000 °C) power source, which can directly convert the chemical energy of a fuel into electrical energy via electrochemical reactions. As the energy conversion process is straightforward, the electric efficiency of SOFC (>50 %) is considerably higher than that of conventional heat engines (<40 %). Compared with low temperature fuel cells, such as proton exchange membrane fuel cells (PEMFC) or alkaline fuel cells (AFC), SOFCs are fuel flexible and can make use of various hydrocarbon fuels as internal reforming of hydrocarbon fuels can take place in the porous anode. In particular, the poisonous CO for PEMFC can even be used as a fuel by SOFCs for power generation [1]. The high operating temperature of SOFC also enables the use of non-noble metal catalyst, such as Ni. Thus, the cost of SOFCs is lower than that of PEMFCs, although it is still much higher than conventional thermal power plant. Moreover, the waste heat from SOFC stack is of high quality and can be recovered by integrating the SOFC stack with other thermodynamic cycles for combined heat (heating or cooling) and power (CHP) cogeneration, leading to high system efficiency. For instance, the SOFC system can be integrated with heat exchangers and absorption chillers to produce electrical power, hot water and cooling air simultaneously to meet the energy demand of hotels [2].

The key issues limiting the wide applications of high temperature SOFCs include the high system cost and

performance degradation. Lowering the operating temperature from 800–1000 °C down to 600 °C or even 400 °C can substantially reduce the system cost due to wider choice materials and reduced cost for the balance of plant (BOP) [3]. At reduced temperature, the sintering kinetics of the porous electrodes is greatly reduced, leading improved durability. In addition, the theoretical efficiency of SOFC increases with decreasing temperature. However, the actual performance of SOFC with traditional materials decreases significantly with decreasing temperature due to the decreased oxygen ion conductivity of the electrolyte (i.e. yttria stabilized zirconia: YSZ) and decreased catalytic activity of the electrodes (i.e. Lanthanum strontium manganite: LSM). Therefore, extensive efforts have been made to search for alternative electrolyte and electrode materials to enable efficient operation of SOFCs at reduced temperatures [4, 5].

From engineering point of view, the performance of SOFC at reduced temperature can be improved by optimizing the SOFC structural parameters and controlling the operating conditions [6, 7], which can be done efficiently by mathematical modeling of SOFCs. The Special Topic section of this issue presents five contributions by active researchers from Asia, Europe and North America on SOFC modeling at various scales.

To understand the microstructure properties of the porous anode, the focused ion beam-scanning electron microscopy (FIB-SEM) technique is used to reconstruct the 3D microstructure of SOFC anode before and after 500 h operation [8]. Analyses are then conducted to obtain important information for SOFC anode, such as the specific interfacial area, the triple phase boundary (TPB, sites for electrochemical reactions) density, phase volume of Ni and YSZ. It is suggested that the reconstruction size should be enlarged for analyzing the microstructure properties after

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long-term operation. The results are important for understanding the microstructure evolution of the SOFC electrodes. However, the FIB-SEM technique is expensive and time-consuming. A 2D stereological method is thus developed by Zhang et al. [9] to estimate the 3D geometric properties of SOFC electrodes. The 2D method can be used to analyze the electrode porosity, volume fractions of solid phases, inner surface/interface area, and TPB length with good agreement with the 3D results. However, efforts are still needed to improve the 2D method for analyzing the percolation and tortuosity properties of the SOFC electrodes as the different phases may not be well percolated in the 2D image.

Different from conventional sponge-like porous structures, finger-like channeled structures can be fabricated by advanced mesh-assisted phase inversion method. A continuum model is developed by Chen et al. [10] to investigate how the finger-like channeled structure affect the gas transport and thus the performance of SOFCs. The multiphysics model fully considers the fluid flow, electron and charge transport, and chemical/electrochemical reactions in SOFC. It is found that the performance of SOFC is improved by over 5 % by the finger-like channeled support structure with syngas as fuels. Further performance improvement is also possible by optimizing the finger-like channels, such as the channel diameter and inclined angle.

As a single SOFC cell can only deliver limited power and voltage, multiple SOFC cells need to be electrically connected by interconnectors to form an SOFC stack for practical applications. The coupled transport and reaction phenomena in an SOFC stack are studied by Xu et al. [11] using a multiphysics numerical model. The important thermal stresses in an SOFC are evaluated for different SOFC designs. It is found that the thermal stress can be decreased by using wider anode interconnector. The study provides important information for stack design and optimization.

The reversible operation of SOFC enables SOFC to be used as an energy storage device—converting excess renewable power into hydrogen fuel by steam electrolysis (charging mode) and converting the hydrogen fuel into electrical power when the renewable power is insufficient (discharging mode). Jin and Huang [12] developed a novel iron-air battery based on the SOFC technology. The iron-based redox cycle unit (RCU) is used for storing or releasing hydrogen via the steam-iron reaction. The

coupled processes in the SOFC and the RCU and the interaction between the two sections are investigated using a high-fidelity multiphysics model. It is found that the current density and depth of discharge have great effect on the performance for an intermediate temperature battery (about 550 °C). For high temperature battery, improving the exchange current density of the SOFC is found most important to improve the efficiency of the battery.

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