Solid Oxide Fuel Cell Material Structure Grading Using COMSOL Multiphysics®

M. Andersson[1], B. Sundén[1]

[1]Department of Energy Sciences, Lund University, Lund, Sweden

Abstract

Introduction: Fuel cells (FCs) are promising as an energy producing device, which at this stage of development will require extensive analysis and benefit from numerical modeling at different time- and length scales. FC science and technology cut across multiple disciplines, including materials science, chemistry, electrochemistry, interfacial science, heat transfer, mechanical engineering and catalysis. The FC is not a new invention and its principle dates back to 1838. However, the FC technology is approaching the commercial phase, with an enormous future potential. To reach commercialization the cell and system production costs (comparative to other technologies) must be decreased as well as the cell performance and the lifetime increased.

Use of COMSOL Multiphysics®: A model in three-dimensions is developed to illustrate a planar intermediate temperature (IT) solid oxide fuel cell (SOFC). The transport equations are coupled to kinetics describing electrochemical and internal reforming reactions and are segregated in 5 different groups: 1. velocity field, pressure distribution and pressure corrections, 2. temperature distribution, 3. ion and electron distribution, 4. mass fraction distribution on the air side (O2/N2) and 5. mass fraction distribution on the fuel side (H2/H2O/CO/CO2/CH4). The segregated solver is applied for 9,279,000 degrees of freedom and the solution tolerance is set to 0.0005 for each segregated group. Grid-independence was achieved at 1,399,000 elements. The calculation time is around 24 hours on a single computer with 16 GB RAM and a CPU with 3.40 GHz. It should be noted that it is hard to give an exact value for the calculation time since the model is built in several steps, where each step start its calculation from the previous one.

Results and Conclusions: It is concluded that a graded pore structure decreases the gas-phase concentration differences between the fuel and/or air channel and the three-phase boundary (TPB), i.e., the concentration polarization decreases and also the Nernst potential increases from a higher concentration of fuel (at the anode TPB) and/or oxygen (at the cathode TPB), i.e., the current is increased. It is shown that the ionic Ohmic polarization can be decreased when the material is designed with a decreased ionic tortuosity in the TPB region. A material structure with an increased effective thermal conduction lowers both the local temperature at the TPBs and the maximum cell temperature, which can increase the cell lifetime. It is shown that a graded porosity can be used to maximize the TPB area-to-volume ratio. The high mechanical strength is maintained for the rest of the anode which is used as the cell support and for possible internal reforming reactions. In practice, the porosity, pore- or particle radius graded electrodes can be manufactured by advanced ceramic techniques or by electrophoretic co-deposition. Finally, it

should be mentioned that a highly optimized graded structure may contradict fuel flexibility.