

The talk on "Modeling and Structural Optimization of Solid Oxide Fuel Cells" summarizes the research conducted in the context of the relevant PhD at the Technical University of Denmark (DTU). This research lies on the cross section between multi-scale modeling of flow in open channels and porous media, electrochemical diffusion and reaction, in combination with Shape and Structural Optimization techniques. More specifically, we have deployed two lines of action for dealing with this problem.

On the one hand, we perform optimization of a Solid Oxide Fuel Cell in the macro scale in two dimensions. Focusing on the anode interconnect, we wish to come up with an optimum interconnect design for a half-cell arrangement. This should be in principal achievable, since the interconnect needs to satisfy two major requirements. On the one hand, it needs to secure the intake of fuel into the half-cell, fact that would require an as low hydraulic resistance as possible, i.e. ideally an open channel and on the other hand to exhibit an as high as possible electronic conductance, which in the ideal case would mean an area blocked completely by a material with high conductivity such as coated stainless steel. The balance between these two competing, oppositely driving forces indicates as a starting point that there should be a design that satisfies in the best way both. Similar problems have been successfully treated by structural optimization approaches and this is one of the first attempts to apply this combination of set of tools to fuel cells. Describing in a nutshell the methodology followed, we use Comsol's ability to create Matlab scripts which incorporate the desired physics of the problem (Partial Differential Equations, treating the setup as continuum) and we combine these scripts with the ones containing the optimization routines like the Method of Moving Asymptotes (MMA). Success in obtaining such a design, greatly affects the overall half-cell's energy output which is used as objective function, rendering the Solid Oxide Fuel Cell more competitive in the sustainable energy market. The optimization takes place on increasing levels of model complexity and coupling. As another product of this work, it was further proven possible to derive analytical expressions for the net power provided by the cell under certain simplifying assumptions, which however in many cases can be used as rule of thumb or fast, order of magnitude, calculations.

The other approach is based on attacking the problem in the micro-scale. Departing from the homogenization method for getting an up-scaled equation for the diffusion of ion vacancies in a fuel cell's cathode, we derive formulas that express the Area Specific Resistance (ASR) of the electrode as a function of geometric parameters, such as the tortuosity, the porosity and the area available for reaction for certain preselected micro-structures. Furthermore, we apply optimization techniques to lead the ASR to minimization for each one of the micro-structures under study.