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# A parametric analysis of thermodynamic losses in an anode of a solid oxide fuel cell

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**Abstract.** In this paper, generation of thermodynamic losses in the micro-channels of a Solid Oxide Fuel Cell electrode is discussed. Diffusive-convective equation is implemented to compute local concentrations of reagents. The model accounts for both the Fick's, and the Knudsen's diffusion. For a number of cases the total losses are decomposed to isolate the contributions of the diffusion, the current conduction, and the chemical reaction irreversibilities.

## 1. Introduction

Fuel cells are devices, which allow direct conversion of chemical energy of fuels into electrical energy. The electrodes of a Solid Oxide Fuel Cell (SOFC) are composed of a porous, multiphase ceramic-metal composite. Each phase in the composite has a specific transport function. In an SOFC anode, the oxygen ions are conducted by an oxide phase, electrons obtained in the half-reaction are collected by a metallic phase, and the gaseous reagents are transported in an open network of pores. In most cases, the intricacies of SOFC microstructure are accounted for using macroscopic parameters, such as phase volume fraction or tortuosity. These parameters can be estimated on the basis of porosimetry or nanotomography. The nanotomographic analysis of an SOFC electrode was first performed by Wilson et al. [1] in 2006. However, the digital reconstructions of electrode samples may also be used directly to construct a computational domain for numerically solving three-dimensional transport equations. While uncommon, this approach has been implemented by several teams during the previous decade [2, 3, 4].

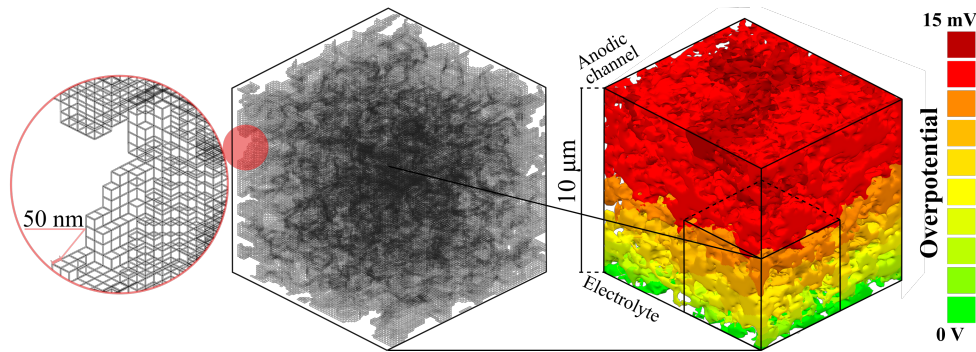
In the present research, a digital reconstruction of an SOFC electrode microstructure is used to create a three-dimensional, non-continuous computational domain, in which the microscale transport equations are solved. The resulting spatial distributions of electric potentials and reagent partial pressures are used to analyze the local irreversibilities, and their direct causes.

## 2. Methodology

A Nickel-YSZ (Yttrium Stabilized Zirconia) porous anode, fueled with a 97 : 3 mixture of H<sub>2</sub> and H<sub>2</sub>O, is considered. The proposed model included empirical relationships for material and species properties. Cylindrical Pore Interpolation Model [6] with local linearization was used to account for the gas flow in the transitional regime between the limits of the continuum, and the



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**Figure 1.** The electric overpotential of the anodic ion-conducting phase computed in a 3D microscale mesh. Total overpotential: 0.05 V, Total pressure: 100 000 Pa, hydrogen partial pressure at the anodic channel boundary: 97 000 Pa, Temperature: 1073 K.

free-molecular diffusion. The mathematical model is based on a system of Poisson differential equations for each species included in the model: the oxygen ions, the electrons, and the gaseous reagents, coupled with the Butler-Volmer model for fuel cell reaction rate. The model is based around the following set of equations:

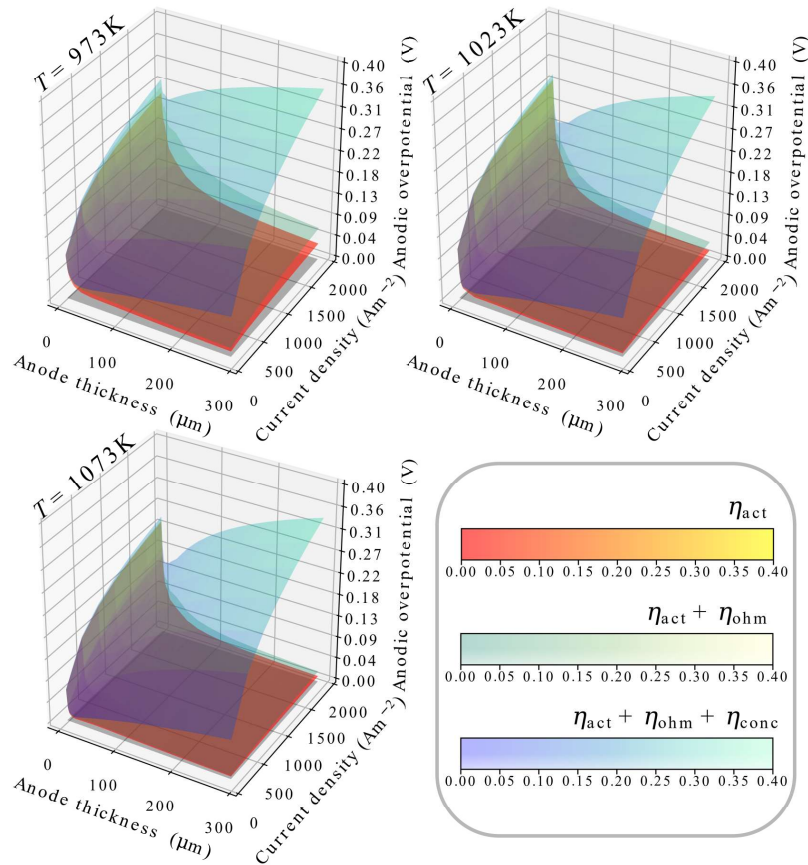
$$\left\{ \begin{array}{l} i = i_0 l_{tpb} \cdot \left[ \frac{p_{H_2}}{p_{H_2}^{bulk}} \exp\left(\frac{\alpha_{an,fwd} F}{RT} \eta\right) - \frac{p_{H_2O}}{p_{H_2O}^{bulk}} \exp\left(-\frac{\alpha_{an,bcw} F}{RT} \eta\right) \right] \\ \eta = \phi_{el} - \phi_{ion} - \frac{RT}{2F} \ln\left(\frac{p_{H_2}^{bulk} p_{H_2O}}{p_{H_2} p_{H_2O}^{bulk}}\right) \\ i = \nabla \cdot (\sigma_{el} \nabla \phi_{el}) \\ -i = \nabla \cdot (\sigma_{ion} \nabla \phi_{ion}) \\ \frac{i}{2F} = \nabla \cdot \left( \frac{D_{H_2}}{RT} \nabla p_{H_2} \right) \\ -\frac{i}{2F} = \nabla \cdot \left( \frac{D_{H_2O}}{RT} \nabla p_{H_2O} \right) \end{array} \right. \quad (1)$$

where  $i$  ( $A m^{-3}$ ) is the volumetric charge transfer rate,  $i_0$  ( $A m^{-1}$ ) is the equilibrium exchange current density for the reaction at the Triple Phase Boundary.  $\eta$  (V) is the activation overpotential, and  $j$  ( $A m^{-2}$ ) is the current density.  $\phi_{el}$  (V), and  $\phi_{ion}$  (V) are the electric potentials of the electron-conducting phase, and the ion-conducting phase, while  $\sigma_{el}$  ( $\Omega^{-1} m^{-1}$ )  $\sigma_{ion}$  ( $\Omega^{-1} m^{-1}$ ) are their respective conductivities.  $p$  (Pa) is the total pressure,  $p_i$  (Pa) is the partial pressure of the gas mixture component  $i$ .  $F$  ( $A mol^{-1}$ ) is the Faraday's constant,  $R$  ( $J mol^{-1} K^{-1}$ ) is the universal gas constant,  $D_i$  ( $m^2 s^{-1}$ ) is the specific diffusivity of  $i$ ,  $\alpha_{fwd}$ , and  $\alpha_{bcw}$  are charge transfer coefficients for the forward and the backward anodic reaction respectively. Superscript 'bulk' indicates the value at the channel boundary.

The computational domain was constructed using three-dimensional micro-imaging data obtained with Focused-Ion-Beam Scanning Electron Microscopy (FIB-SEM). The problem is discretized using Finite-Volume Method, and solved using a Successive Over-Relaxation scheme to obtain local potential values (see Fig. 3). The numerical simulations were performed using an in-house code developed in C++.

### 3. Findings

The model allowed to compute potential distributions within the microstructure (see Fig. 3) of an SOFC's anode. Microstructure details and model validation are provided in another paper [5].

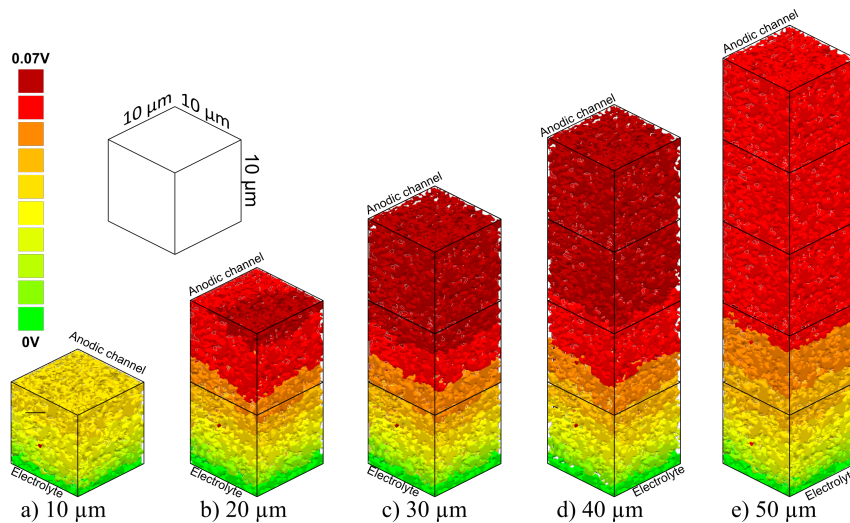


**Figure 2.** Anodic voltage losses at different electrode thicknesses and temperatures. Total pressure: 100 000 Pa, Hydrogen partial pressure at the anodic channel boundary: 60 000 Pa.

The results were used for the purpose of a parametric analysis aimed at determining the voltage loss  $\eta$  (V) occurring due to activation (subscript 'act'), current conduction (subscript 'ohm') and concentration (subscripts 'conc') irreversibilities (see Fig. 2). When the thickness is increased, the activation losses decrease. At the same time, concentration losses grow due to the increase in diffusion pathways. Combined, these two effects result in local minima, which become more apparent as the temperatures increase. Three-dimensional visualizations of selected cases are presented in Figure 3. It can be seen that the thickness of the active layer is increasing at a slower rate than the total electrode thickness. For very thin electrodes, the active layer appears to not be fully developed, suggesting a reaction site deficiency.

#### 4. Conclusions

The results allow for optimization of future microstructure designs, and for proper selection of the device's operation parameters. When the thickness is very low, the activation overpotential is high due to poor availability of the reaction sites. However, beyond an optimal value (20 μm – 40 μm), additional thickness results in greater losses related to the gas diffusion. An



**Figure 3.** Potential of the anodic ion-conducting phase for electrodes of various thicknesses - a 3D visualization. Simulation parameters:  $p = 100000$  Pa  $p_{\text{H}_2, \text{b}} = 60000$  Pa,  $T = 1023$  K,  $j = 2000$  A m<sup>-2</sup>.

increase in temperature  $T$  (K) decreases total losses and causes the optima to become more prominent. While adding thickness to the diffusive layer is often necessary due to its function as the cell's mechanical support, low resistance to diffusion should be ensured for the best electrochemical performance.

### Acknowledgments

Numerical code developed during National Science Centre's grant (SONATA-10, Grant No. UMO-2015/19/D/ST8/00839) was used. The parametric study was conducted thanks to the support of the Ministry of Science and Higher Education (Grant AGH No. 16.16.210.476). This research was supported in part by PL-Grid Infrastructure. Matplotlib Python library was used for data visualization.

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