Numerical Modelling of a Microtubular Solid Oxide Fuel Cell Using COMSOL MultiphysicsÈ

Paulina Pianko-Oprych[1], Ekaterina Kasilova[1], Zdzisğaw Jaworski[1]

1. West Pomeranian University of Technology, Szczecin, Institute of Chemical Engineering and Environmental Protection Processes, Al. Piast· w 42, 71-065 Szczecin, Poland.

Introduction: The main purpose of this work was development of CFD model of a single microtubular Solid Oxide Fuel Cell (mSOFC). The CFD model has to be able to predict the mSOFC performance. On the other hand it was assumed that the model has to be simple enough to be applicable in the system simulations.

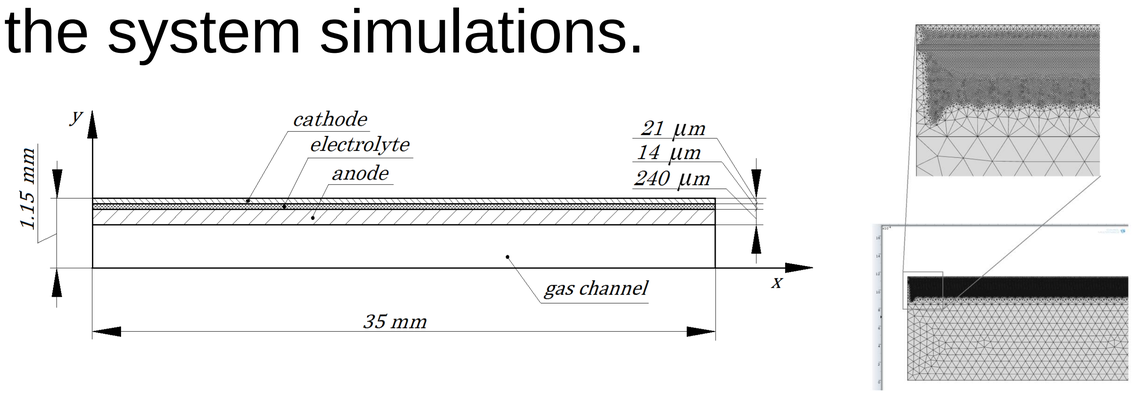

Figure 1. Geometry of the ½ cross-section of the mSOFC (not to scale) [Howe & Kendall, 2011] and mesh in the computational domain

Computational Methods: A two-dimensional simplified fuel cell model was built to take into account an electrochemical reaction. Sets of the governing equations for momentum, energy and the species transport were simultaneously solved giving local profiles of temperatures, electrical current density and concentrations in the computational domain. Numerical code of Computational Fluid Dynamics name COMSOL Multiphysics 4.3 with Batteries and Fuel Cell module was used in the simulations.

Table 1. Set of equations solved in the CFD model

Navier-Stokes equation – fuel channel	$\rho\frac{\partial\bar{u}}{\partial t}+\rho(\bar{u}\cdot\nabla)\bar{u}=\nabla\cdot\left[-pI+\mu\left(\nabla\bar{u}+(\nabla\bar{u})^T\right)\right]+F$
Darcy approach – porous cathode	$\bar{u}=-\frac{\kappa}{\mu}\nabla p$
Brinkman equation – porous anode – gas channel	$\frac{\rho}{\varepsilon}\left(\frac{\partial\bar{u}}{\partial t}+(\bar{u}\cdot\nabla)\frac{\bar{u}}{\varepsilon}\right)=\bar{F}-\nabla p-\left(\frac{\mu}{\kappa}+Q_m\right)\bar{u}+\nabla\left[\frac{1}{\varepsilon}\left\{\mu\left(\nabla\bar{u}+(\nabla\bar{u})^T\right)-\frac{2}{3}\mu(\nabla\cdot\bar{u})I\right\}\right]$
Mass conservation equation for porous flows	$\frac{\partial(\rho\varepsilon)}{\partial t}+\nabla\cdot(\rho\bar{u})=Q_m$
Mass transport of species "i" in the channel and electrodes	$\bar{j}_i=-M_i D_i\nabla c_i$
Species conservation equation and rate of production/consumption of i-component in the anode/cathode	$\frac{\partial}{\partial t}(\rho\omega_i)+\nabla\cdot(\rho\omega_i\bar{u})=-\nabla\cdot\bar{j}_i+R_i$ $R_i=M_i\frac{\nu_{i,m}i}{n_m F}$
Charge conservation equation	$\nabla\cdot i_k=Q_k$
Ohm law	$i_k=-\sigma_k\nabla\phi_k$
Butler-Volmer equation for a single-electron reaction	$i=i_0\left(\frac{c_i}{c_i^{ref}}\right)^{\gamma_i}\left\{\exp\left(\frac{\alpha_a F\eta}{RT}\right)-\exp\left(-\frac{\alpha_c F\eta}{RT}\right)\right\}$

Results: CFD analysis of the single mSOFC led to the following conclusions:

Åelectrochemical model of the single mSOFC was developed and validated againts experimental data [Howe and Kendall, 2011]

Å sensitivity analysis of the electrochemical model was carried out to understand the influence of the stack heat transfer conditions on the mSOFC performance.

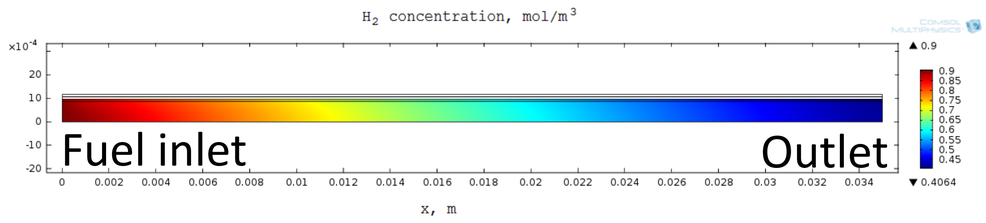

Figure 2. Hydrogen molar concentration field in the fuel channel

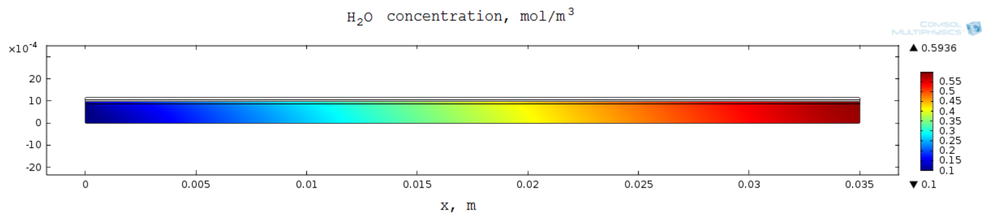

Figure 3. Water steam molar concentration field in the fuel channel

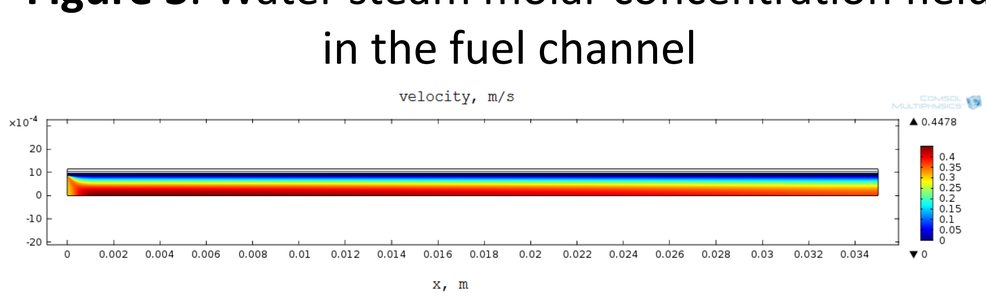

Figure 4. Velocity field in the fuel channel

Conclusions: A simple CFD model of the single mSOFC for pure hydrogen as fuel in the COMSOL software was developed for the purpose of future system simulations.

References:

1. Howe K. et al., 2011. Micro-tubular solid oxide fuel cells and stacks. J. of Power Sources, 196, 1677 ï 1686.

2. Howe K., Kendall K., 2011. Transient Performance of Micro-Tubular SOFCs and Stacks. ECS Trans., 35, 1, 419-423.

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