Numerical Modelling of Solid Oxide Fuel Cells: Role of Various Cell Parameters on Performance

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Osarobo Ighodaro*, Keith Scott

School of Chemical Engineering and Advanced Materials, Newcastle University, Newcastle upon Tyne, NE1 7RU, UK. * Corresponding author: o.o.ighodaro@ncl.ac.uk

Abstract

Solid oxide fuel cells (SOFCs) are expected to play a major role in future energy systems due to their wide range of applications, high energy efficiency, environmental friendliness and good fuel flexibility. While conventional high temperature SOFCs operate at about 1000ºC, there is growing interest in intermediate temperature SOFCs which operates between 600ºC and 800ºC allowing for wider range of materials, stability and reduced cost of production. A fully coupled computational fluid dynamics (CFD) model predicting the performance of a planar solid oxide fuel cell (SOFC) at intermediate temperature has been developed using the finite element based package (COMSOL Multipysics). The model solves governing equations for mass, momentum and charge transport as well as the kinetics of the electrochemical reaction, the effect of Knudsen diffusion is accounted for in the electrochemical reaction layer. Varying structural designs and operating conditions, is used in predicting the performance of the cell. The cell is modelled with yttria-stabilized zirconia (YSZ) electrolyte, Ni-YSZ anode support layer, Ni-YSZ anode reaction layer, strontium doped lanthanum manganite (LSM)-YSZ cathode reaction layer and LSM current electrolyte layer with hydrogen as fuel and air as oxidant. The predicted performance of the cell is validated with measured data found in literature. Sensitivity analysis on the effect of some cell parameters on cell performance was carried out. Results shows that decreasing the electrolyte and anode thickness improves cell performance, also reduction in cell temperature lowers cell performance due to increased activation and ohmic losses while increased operating pressure enhances cell performance due to reduced concentration losses.

1. Introduction

Solid oxide fuel cells are promising and are beginning to receive lots of attention because of their high energy efficiency, good fuel flexibility, wide variety of catalyst, low hazardous emissions and for the possibility of using them for combined heat and power (CHP).

In this study, a micro-scale model is developed, the model provides detailed information of a two dimensional mass and charge transport phenomena for an intermediate temperature SOFC. The study looks at the role of some parameters and the influence of operating conditions on performance.

In the past, several models have been developed to simulate the electrochemical processes and transport phenomena in anode supported SOFC, Hussain et al [ ], Jeon D.H[ ], Anderson et al [ ] and Bessler et al [ ], such model have been useful for designing and optimisation of SOFCS.

2. Approach and Assumptions

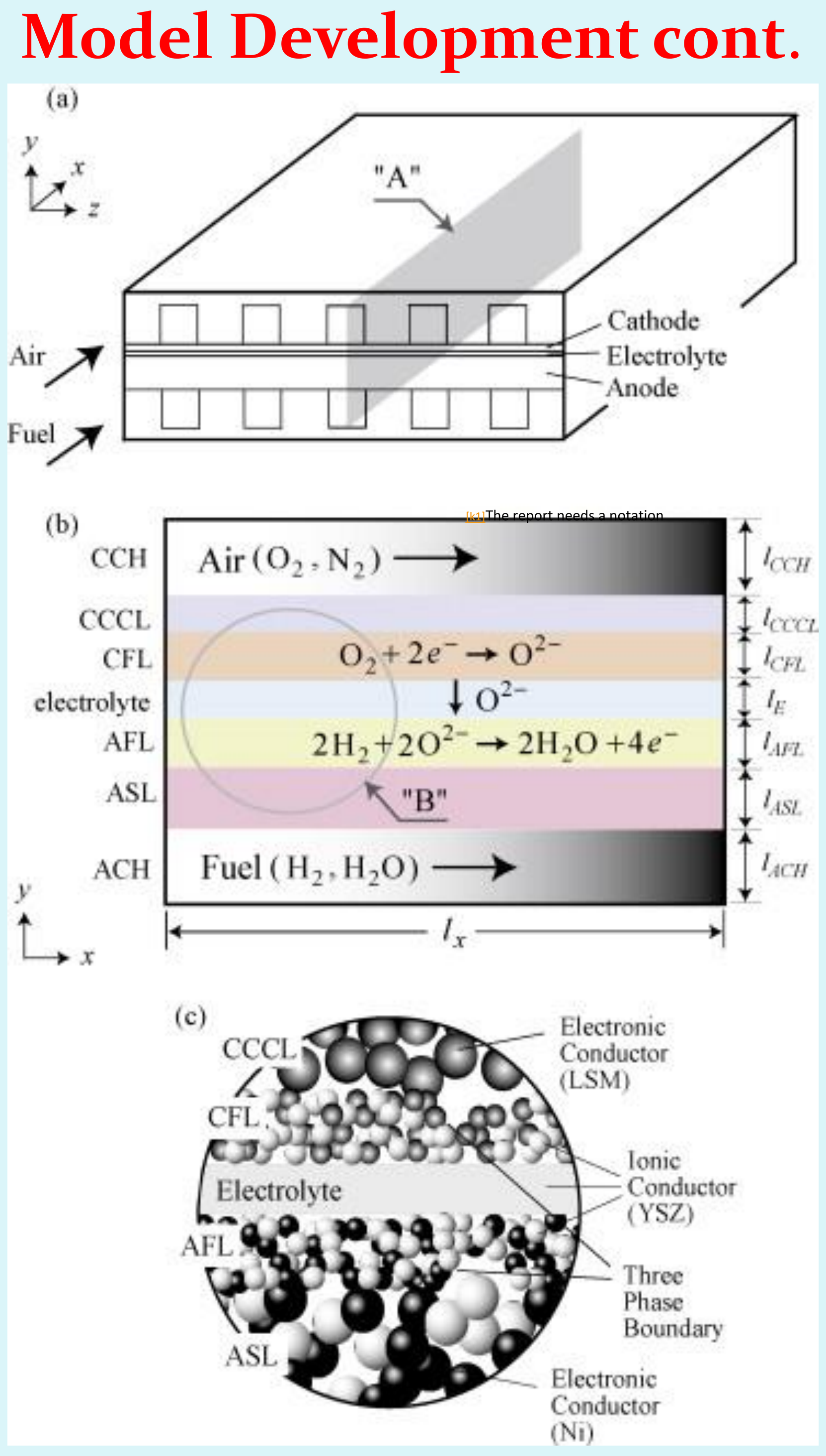
- Develop a 2D finite element SOFC model (COMSOL Multipysics) that is based on detailed electrochemical analysis and mass transfer calculations
- Verify the developed model using data from literature
- Conduct parametric studies on the model for optimisation
- Reactant gases are treated as ideal
- Temperature distribution is neglected
- Steady state condition is assumed

3. Model Development

Properties and conditions	Value
V_{cell}, T, P	0.7V, 800C, 1atm
x_{h2}, x_{o2}	0.7, 0.21
L_{asl}, (L_{afl}) L_e, L_{cfl}, (L_{cccl})	1000µm, 20µm, 10µm,20µm, 1000µm
ε_{sl} ε_{fl}	0.5, 0.25, 0.5, 0.25
τ	5
$d_{p,sl}$, $d_{p,fl}$	1µm, 0.5µm
U_{fuel}, U_{air}	5m/s, 13m/s

Geometry and operating conditions

Model Development cont.



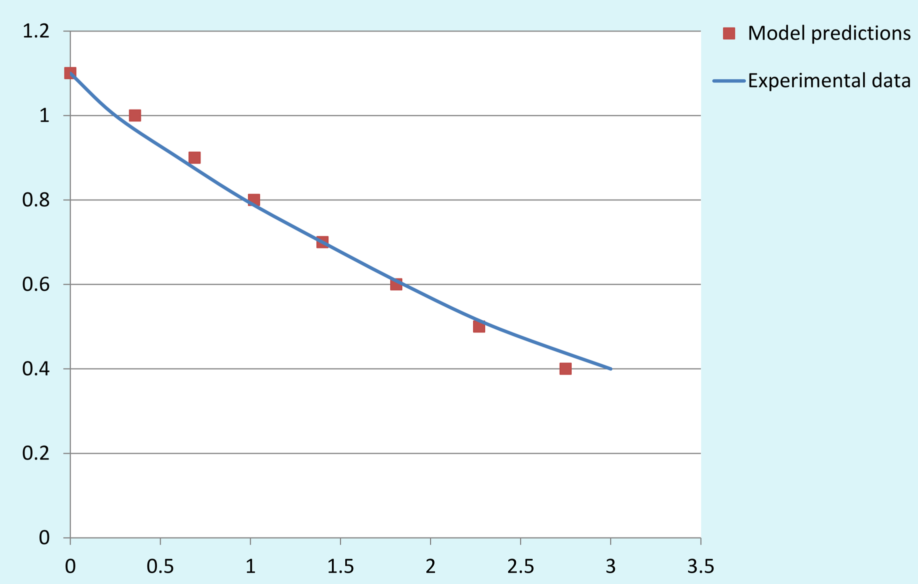
(a). Unit cell of planar sofc (b) Cross section of sofc © Micro scale description of sofc

Governing Equations	Mathematical Expressions
Conservation of electrons and ions	$\nabla . i_{el} = \nabla . (-\sigma_{el}^{eff} \nabla \varphi_{el}) = s_c$ $\nabla . i_{io} = \nabla . (-\sigma_{io}^{eff} \nabla \varphi_{io}) = -s_c$ Where $s_{c=A_v \sum i_{tpb}}$
Conservation of Momentum	$\frac{\rho}{\varepsilon_p}(\boldsymbol{u}.\nabla)\frac{\boldsymbol{u}}{\varepsilon_p} = \nabla.[-p+\mu(\nabla u+(\nabla \boldsymbol{u}^T)) - \frac{2}{3}\frac{\mu}{\varepsilon_p}(\nabla.\boldsymbol{u})] - \left(\frac{\mu}{k} + B_F\lvert\boldsymbol{u}\rvert + Q_{br}\right)\boldsymbol{u} + \boldsymbol{F}$
Conservation of Mass	$\nabla \cdot \left[-\rho w_i \sum_{j=1}^{N} D_{ij} \left\{\frac{M_n}{M_j}\left(\nabla w_j + w_j \frac{\nabla M_n}{M_n}\right) + (x_j - w_j)\frac{\nabla p}{p}\right\} + w_i \rho \mathbf{u} + D_i^T \frac{\nabla T}{T}\right] = R_i$ Where, $R_{h2} = -R_{h2o} = -\frac{i}{2F} M_{h2\,(or\,h2o)}$, $R_{o2} = -\frac{i}{4F} M_{o2}$

Constitutive Equations	Mathematical Expressions
Open circuit voltage	$v^{ocv} = E_O + \frac{RT}{2F} In \left[\frac{p_{h2} p_{o2}^{1/2}}{p_{h2o}}\right]$
TPB length transfer current density	$i_{tpb}^e = i_{o,e} \frac{c_i}{c_{i,ref}} \left(exp\left(\frac{\alpha F \Psi}{RT}\right) - exp\left(\frac{-\alpha F \Psi}{RT}\right)\right)$
Exchange current density	$i_{o,e} = \frac{RT}{n_e F} A_{i,e} . exp\left(\frac{-E_{i,e}}{RT}\right)$
Binary Diffusivity	$D_{ij} = \frac{0.00143 T^{1.75}}{p M_{ij}^{1/2} \left(v_i^{1/3} + v_j^{1/3}\right)^2}$
Knudsen Diffusivity	$D_{ik} = \frac{4r}{3}\left(\frac{2RT}{\pi M_i}\right)^{1/2}$
Effective Diffusion coefficient	$D_i^{eff} = \frac{\varepsilon}{\tau}\left(\frac{1}{D_{ij}} + \frac{1}{D_{ik}}\right)^{-1}$
Anode electronic conductivity	$\sigma_{s,a} = \frac{9.5 * 10^7}{T} . exp\left(\frac{-1150}{T}\right)$
Cathode electronic conductivity	$\sigma_{s,c} = \frac{4.2 * 10^7}{T} . exp\left(\frac{-1200}{T}\right)$
Electrolyte ionic conductivity	$\sigma_{l,el} = 33.4 * 10^3 . exp\left(\frac{-10300}{T}\right)$
Effective conductivity	$\sigma_i^{eff} = \frac{1-\varepsilon}{\tau}\sigma_i$

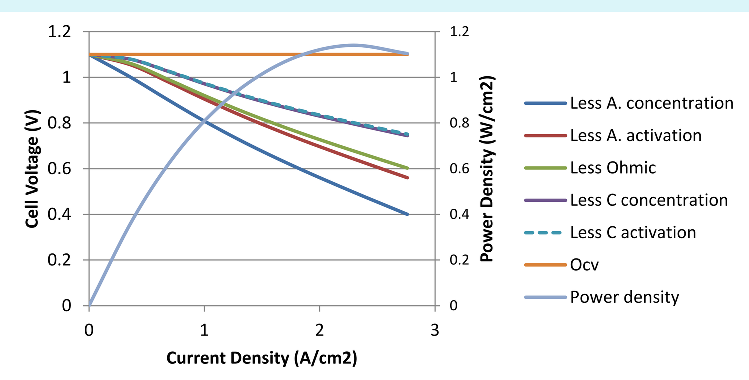
Key equations and expressions.

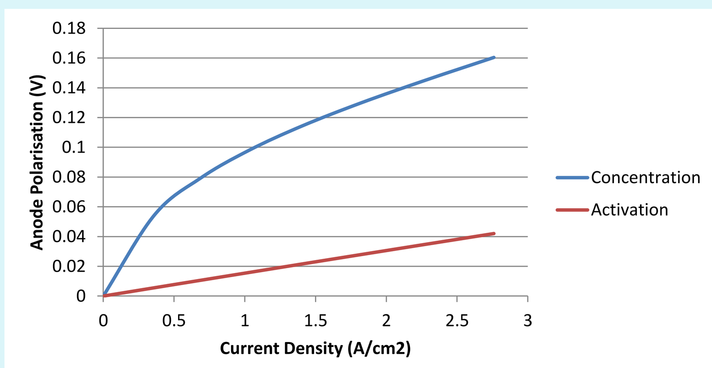
4. Model Validation

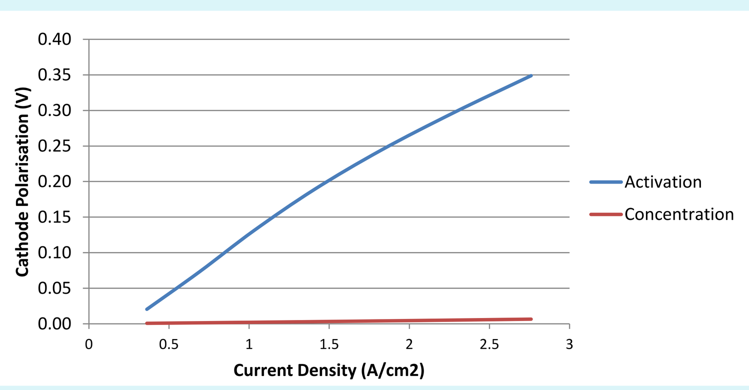


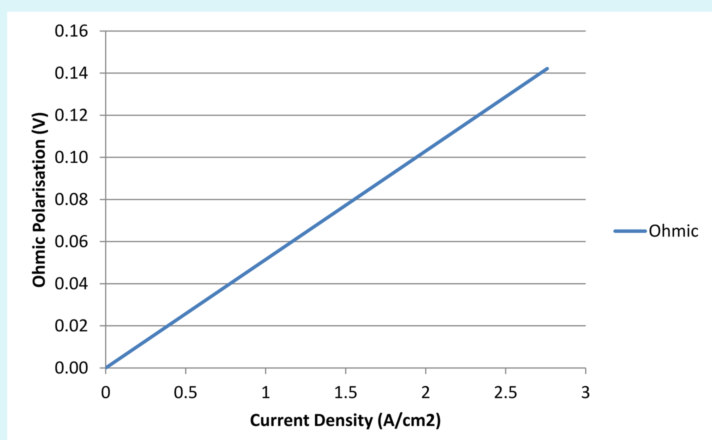
Model predictions agree will with zhoa et al (2004)

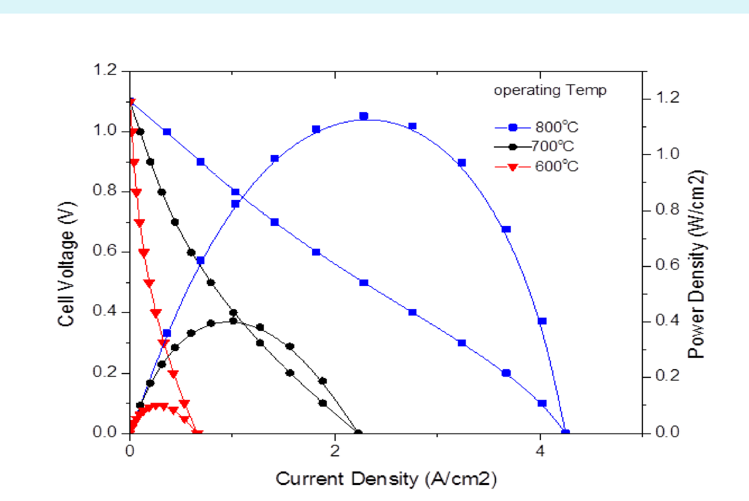
5. Results

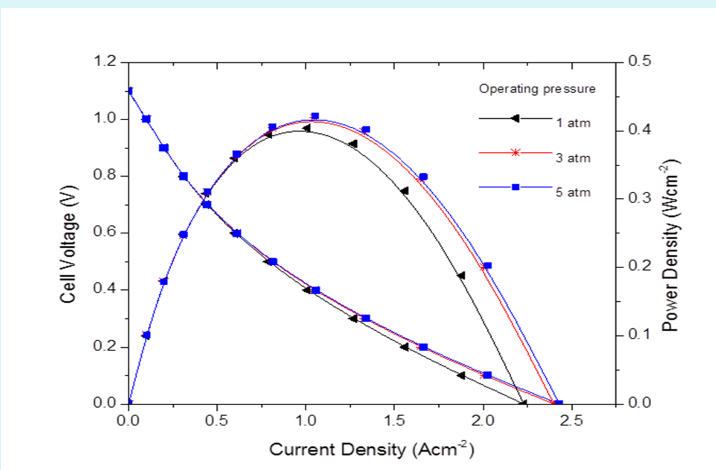


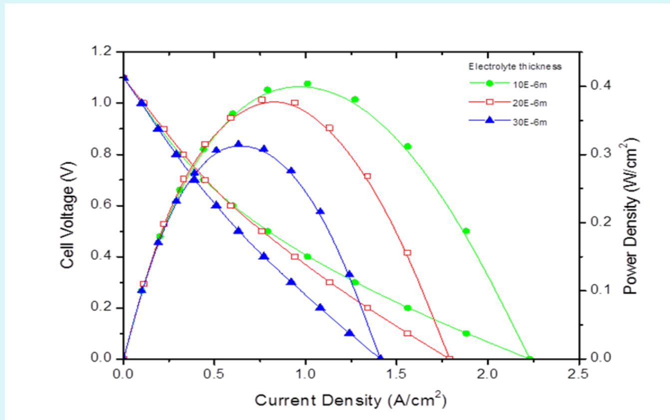


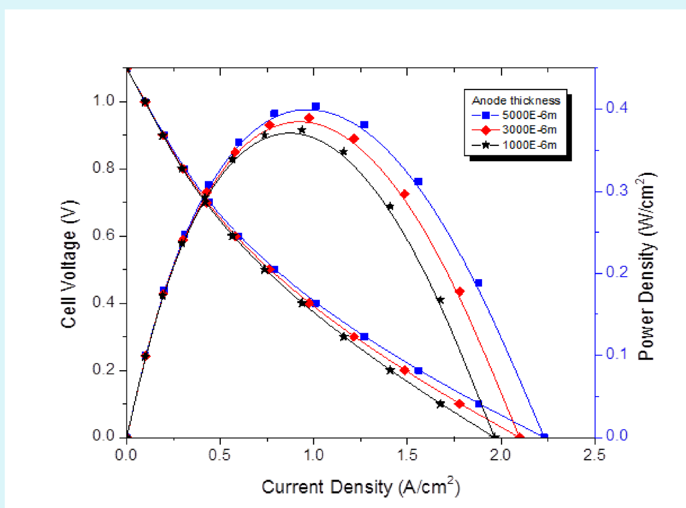












6. Major Findings

- Mpd is 1.14W cm^{-2} at current density of 2.28A cm-2 at cell voltage of 0.5V, largest contributor to losses are cathode activation, anode concentration and ohmic losses
- Cell performance increases with increase in temperature and increase in pressure as a result of enhanced electrochemical reaction rate (temperature) and reduced concentration losses (pressure)
- Cell performance increases with reduced electrolyte thickness as a result of reduced ohmic losses
- Cell performance increases with reduced anode thickness as a result of reduced concentration losses

7. Conclusions

- A 2-D isothermal Sofc model has been developed and verified
- A numerical investigation of the performance of the Sofc with different operation conditions and support structures has been carried out
- Results demonstrate that increasing the operating temperature and pressure can increase cell performance, also decreasing the electrolyte thickness and anode thickness improves cell performance

8. References

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