

Numerical Modelling studies in Alkaline Fuel Cell

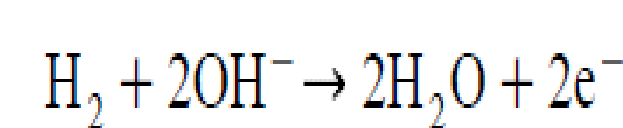
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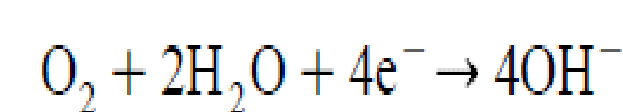
Introduction : Fuel cell converts chemical energy of fuel(Hydrogen) and oxidant (oxygen) to electrical energy. Fuel cells are classified on the basis of electrolyte used like Proton Exchange Membrane Fuel Cell (PEMFC), Alkaline Fuel Cell(AFC), Molten Carbonate Fuel Cell(MCFC), Solid Oxide Fuel Cell (SOFC) etc.

AFCs typically use alkali metal hydroxide like NaOH or KOH as electrolyte which makes the cell component susceptible to corrosion. Anion exchange membrane that can conduct OH⁻ anion is attractive alternative as it overcomes the problem of carbonate precipitation while offering low resistance.

Reaction at anode-



Reaction at Cathode



Overall reaction -

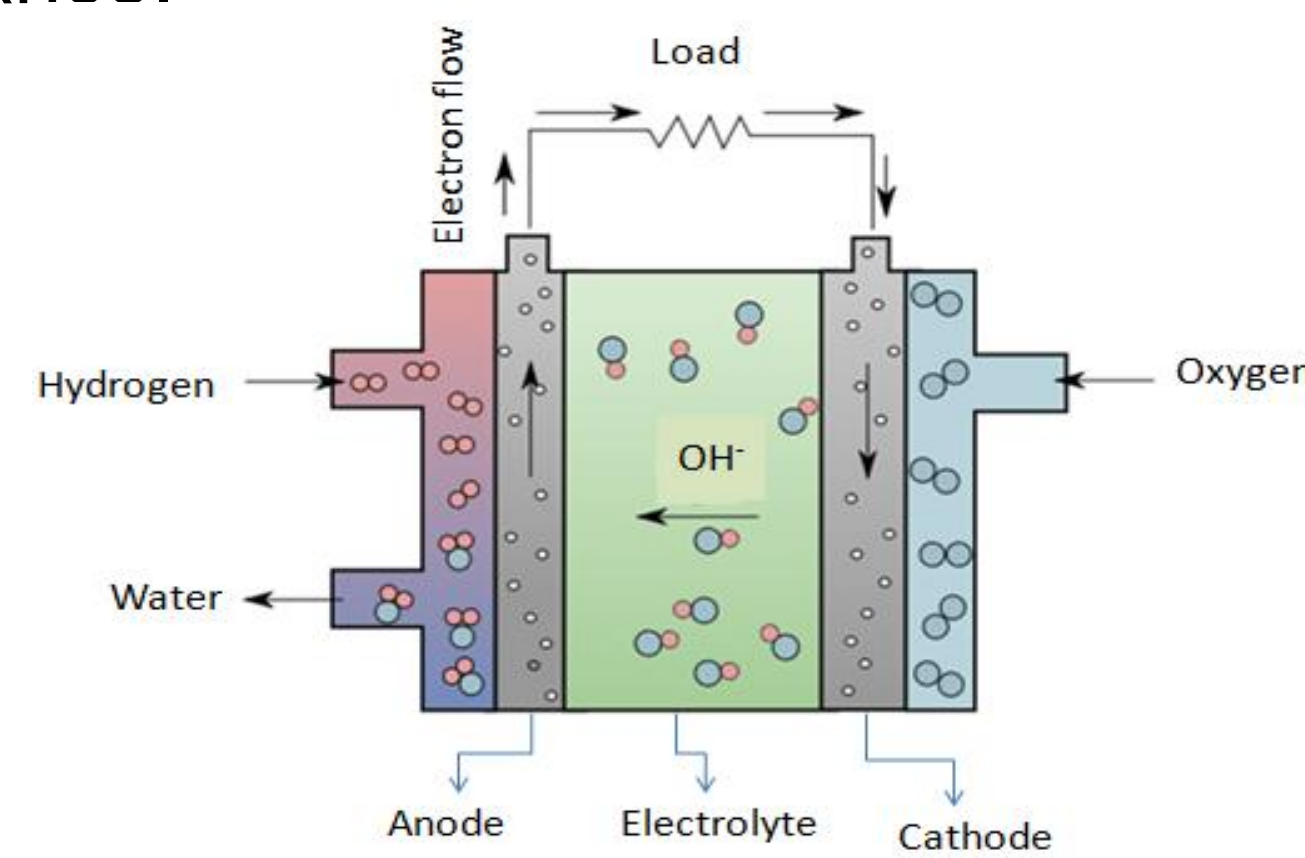
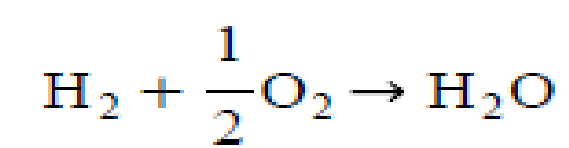


Figure 1. Schematic of alkaline fuel cell

The advantages of using alkaline fuel cells over proton exchange membrane fuel cells is that electrochemical kinetics is fast and non-noble metal based catalyst can be used.

Simulation can be used to predict behavior of the system for any given parameters and reduces the number of experiments for optimizing the performance.

An alkaline fuel cell was assembled with platinum based gas diffusion electrode and anion exchange membrane procured from Fujifilm.

Properties of the anion exchange membrane was studied using dynamic mechanical analysis, impedance spectroscopy and anion exchange capacity measurement. Performance of the cell was studied using polarization curve.

Computational Methods: The flow in open region(from flow field to GDL) is described by Navier-Stokes equations and in porous region(GDL to CL) by Brinkman equations.

Similarly, mass transfer in the model is defined by Maxwell-Stefan equations which account for diffusion of reactant species to catalyst layer at anode and cathode. This model takes into account two species in the anode—H₂ and H₂O—and three at the cathode—O₂, H₂O, and N₂. The model uses one instance of the transport of concentrated species interface for each electrode side.

The electrode kinetics for the charge transfer reactions are described by Butler-Volmer equation and current is defined as integral of the current density at anode.

$$i = i_0 \left[\prod_i \left(\frac{C_i}{C_i^0} \right)^{\alpha_i} \exp\left(\frac{\alpha_a F \eta}{RT}\right) - \prod_j \left(\frac{C_j}{C_j^0} \right)^{\alpha_j} \exp\left(-\frac{\alpha_c F \eta}{RT}\right) \right]$$

where $i_{loc,m}$ denotes the local charge transfer current density for reaction m , i_0 the exchange current density, α_a the anodic transfer coefficient, α_c the cathodic charge transfer coefficient, F the Faraday constant, and R the universal gas constant. The charge transfer current density can be included as a source or sink in the charge balances in porous electrodes or they can be included as boundary conditions in non-porous electrodes.

Current is defined as integral of the current density, at one of the electrode (anode in this case) as follows:

$$I = - \int_0^{L_{cl}} a^{\perp} i dz$$

Potential at one of the electrode is fixed in the model and potential at other electrode is varied using *parametric sweep* feature in COMSOL® i.e. cell voltage is varied and this gives current density. Thus cell potential is found out at a given current density.

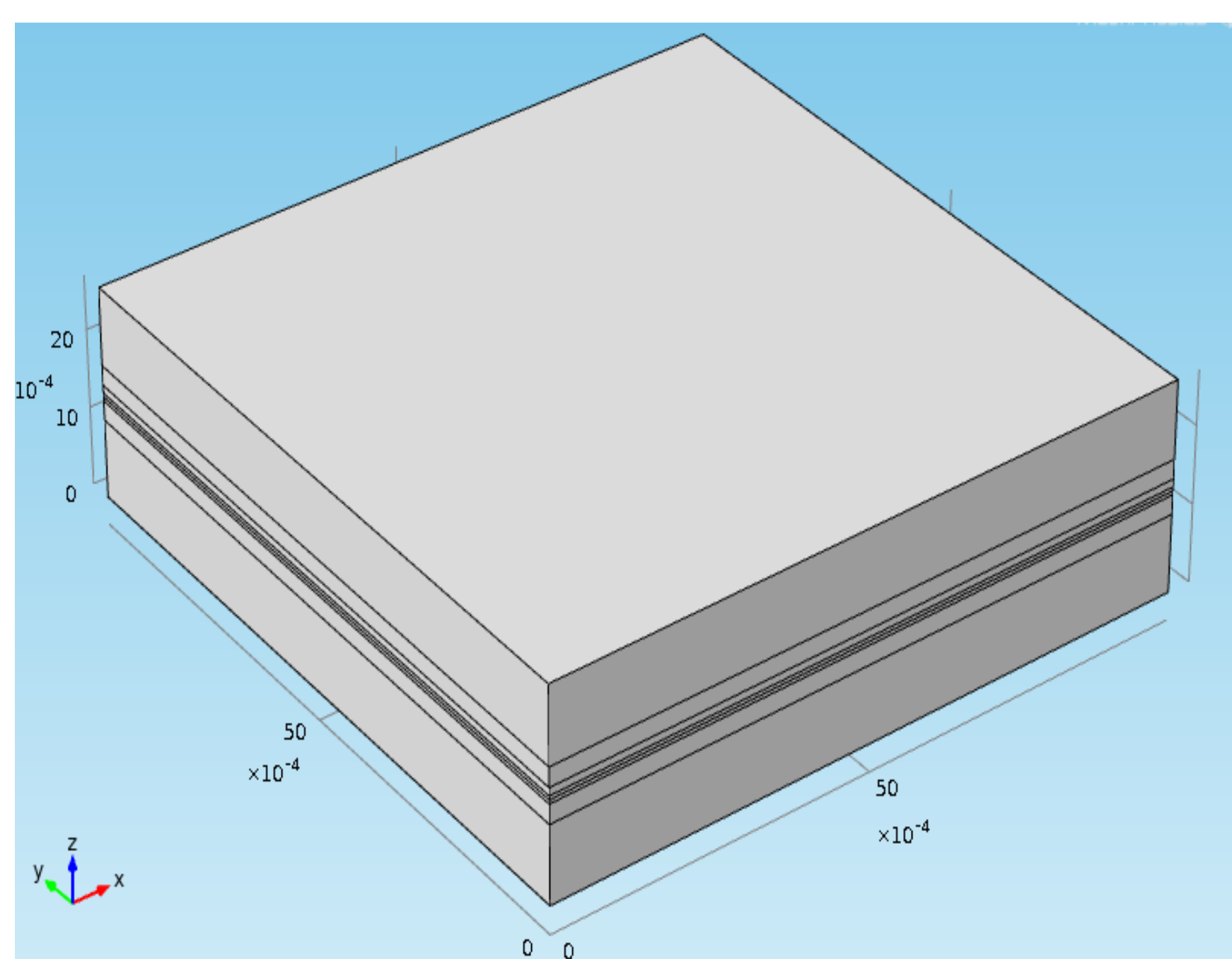


Figure 2. 3D view of fuel cell model

Assumptions:

- Electrons move in the direction opposite of potential applied hence current flows in the direction of potential applied. Movement of electrons in any other directions are neglected
- There is no mechanical or chemical degradation in the system
- There is no temperature variation in the system i.e. no heat generation in the system or loss in the surrounding.

Results: Mass transport and velocity profile across cross-section of flow field plate, gas diffusion layer and catalyst layer were simulated using the parameters specified in the table given below.

Mass fraction of the inlet gases decreases as distance from the flow channel increases and as the distance from gas inlet increases.

From inlet to outlet there is not much variations in the velocity of the gases. However variations were observed across the cross-sections of the cell. Mixing of the gases across the membrane was also not observed.

As we can see from figure 5 that the performance of cell increases with increase in mole fraction of the inlet gas. A stable OCP of 1.02V was obtained for the cell. Experimental results suggested that maximum power of 24mW was obtained using the AFC cell assembled. At low current densities the simulated and the experimental curves were comparable. At high current densities there was deviation between the two curves.

Input parameters for the simulation are being modified to include the effect of transport number for the hydroxyl ions through the membrane, membrane permeability parameters to gases, membrane conductivity variation as a function of temperature etc.

K_GDL	1.01×10 ⁵ S/cm
k_ACL	0.94×10 ⁵ S/cm
k_CCL	4.87×10 ⁵ S/cm
K_graphite	6×10 ⁴ S/cm
K_membrane	9.825 S/cm

Table 1. Permeability values

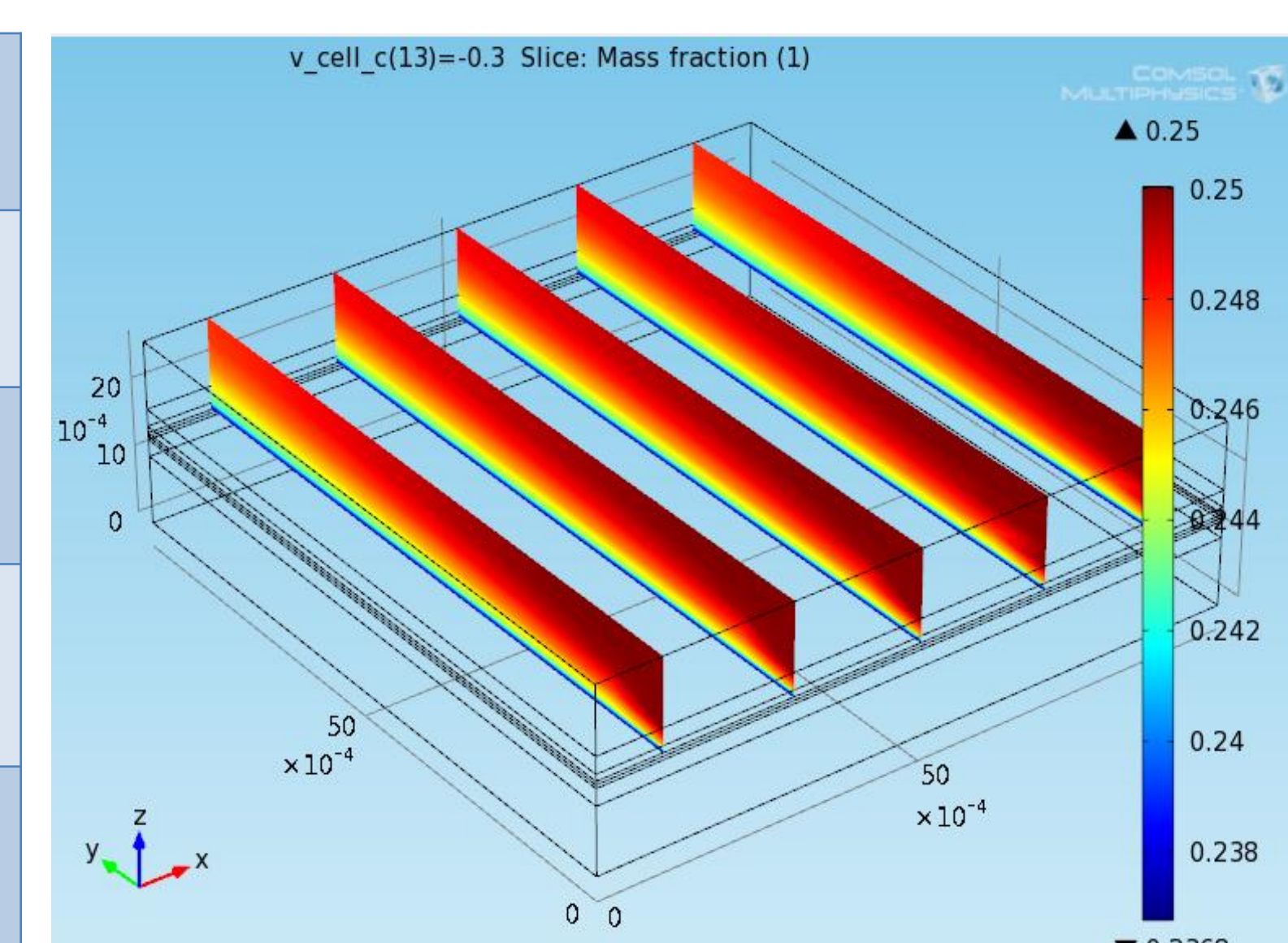


Figure 3. Mass fraction of oxygen

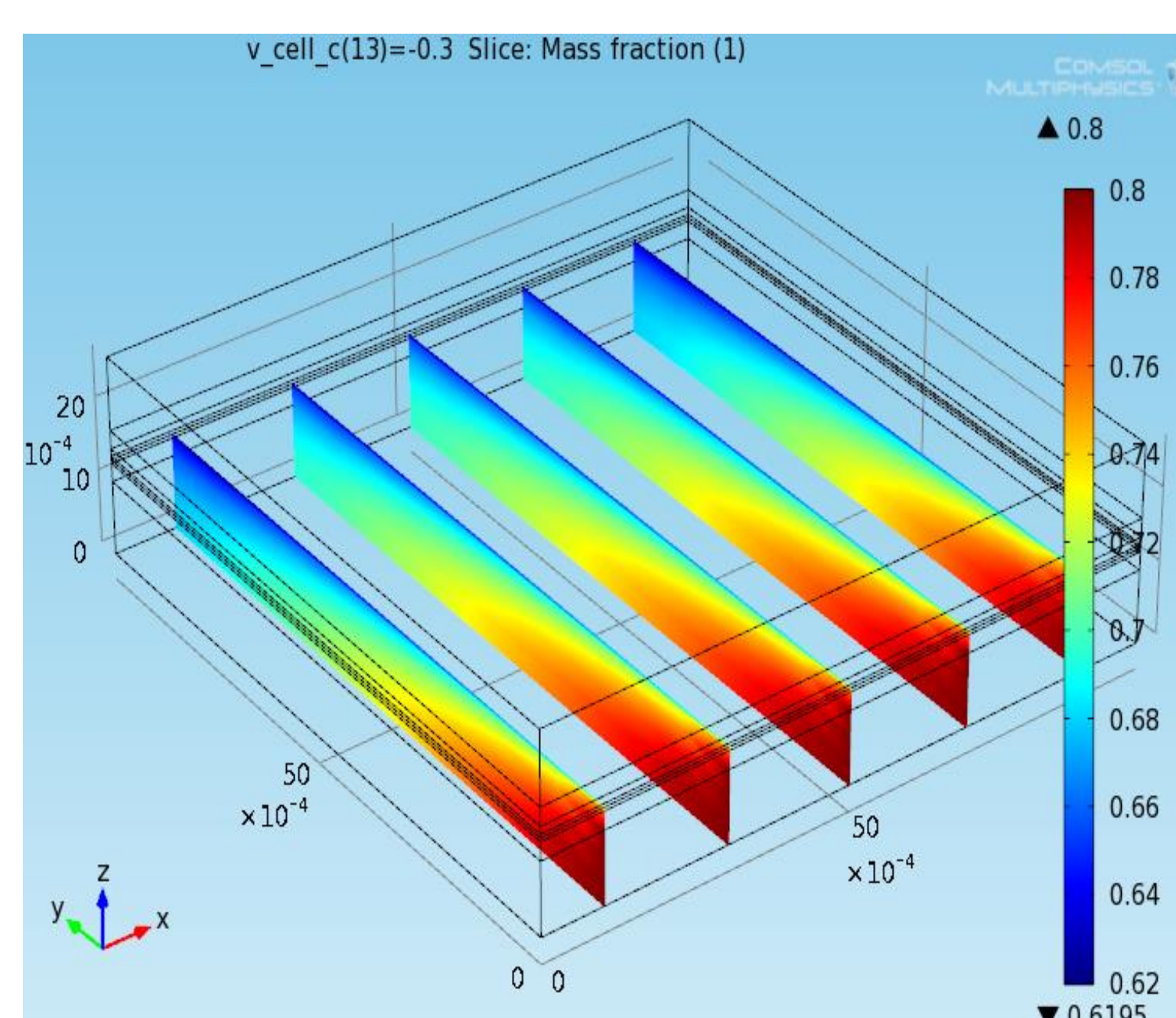


Figure 4. Mass fraction of hydrogen

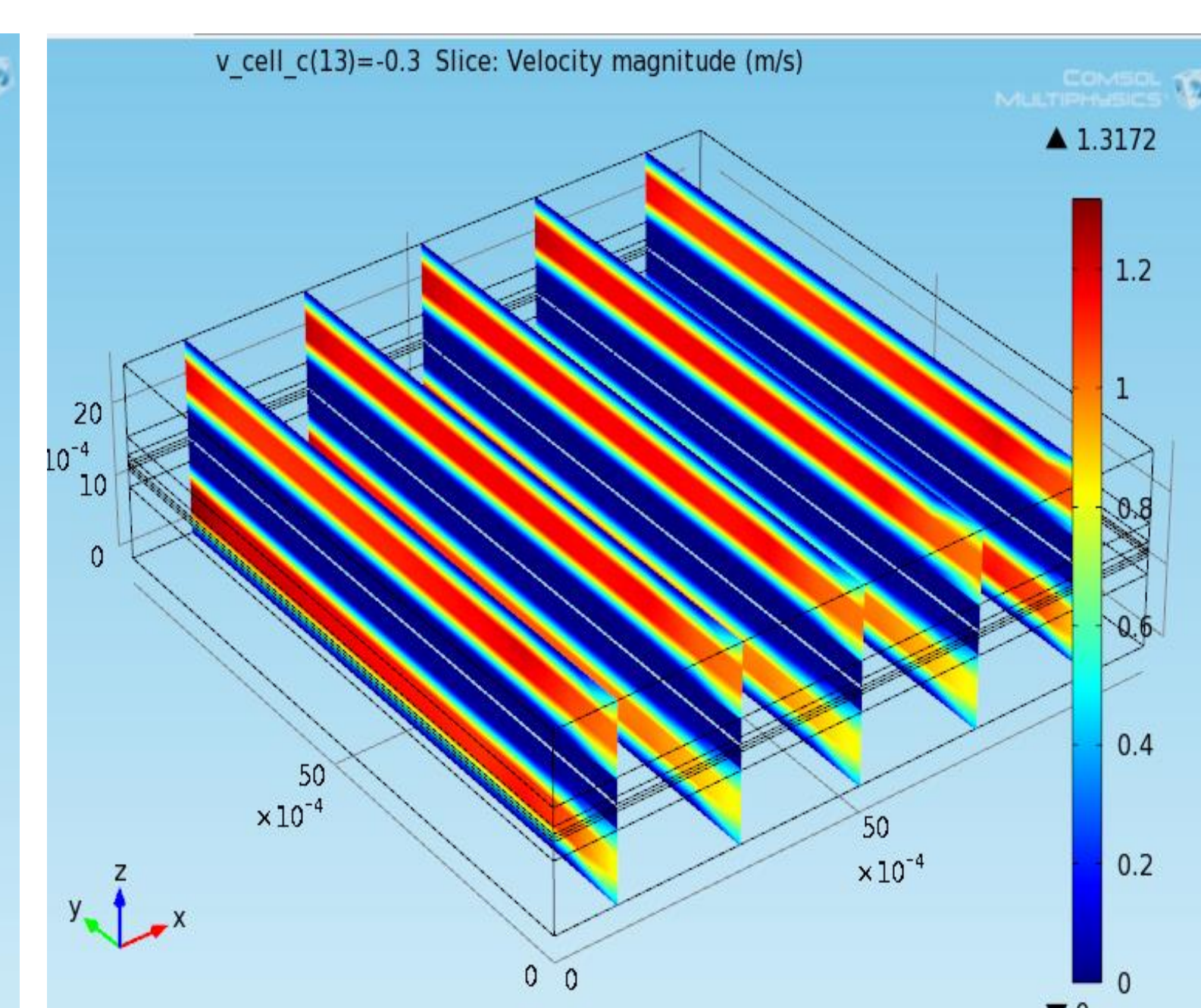


Figure 5. velocity profile in the cell

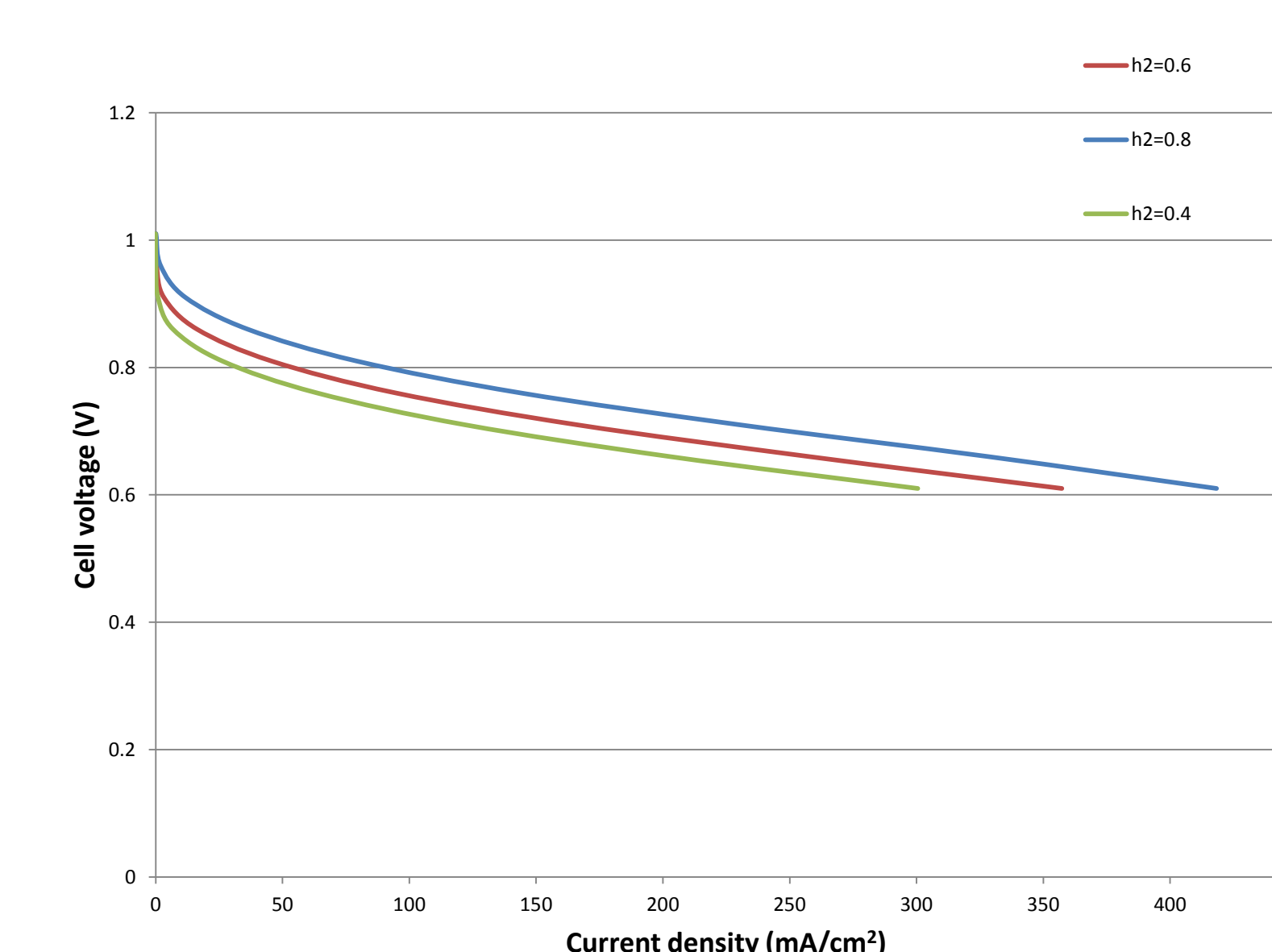


Figure 7. Polarisation curve for different mole fraction of h₂

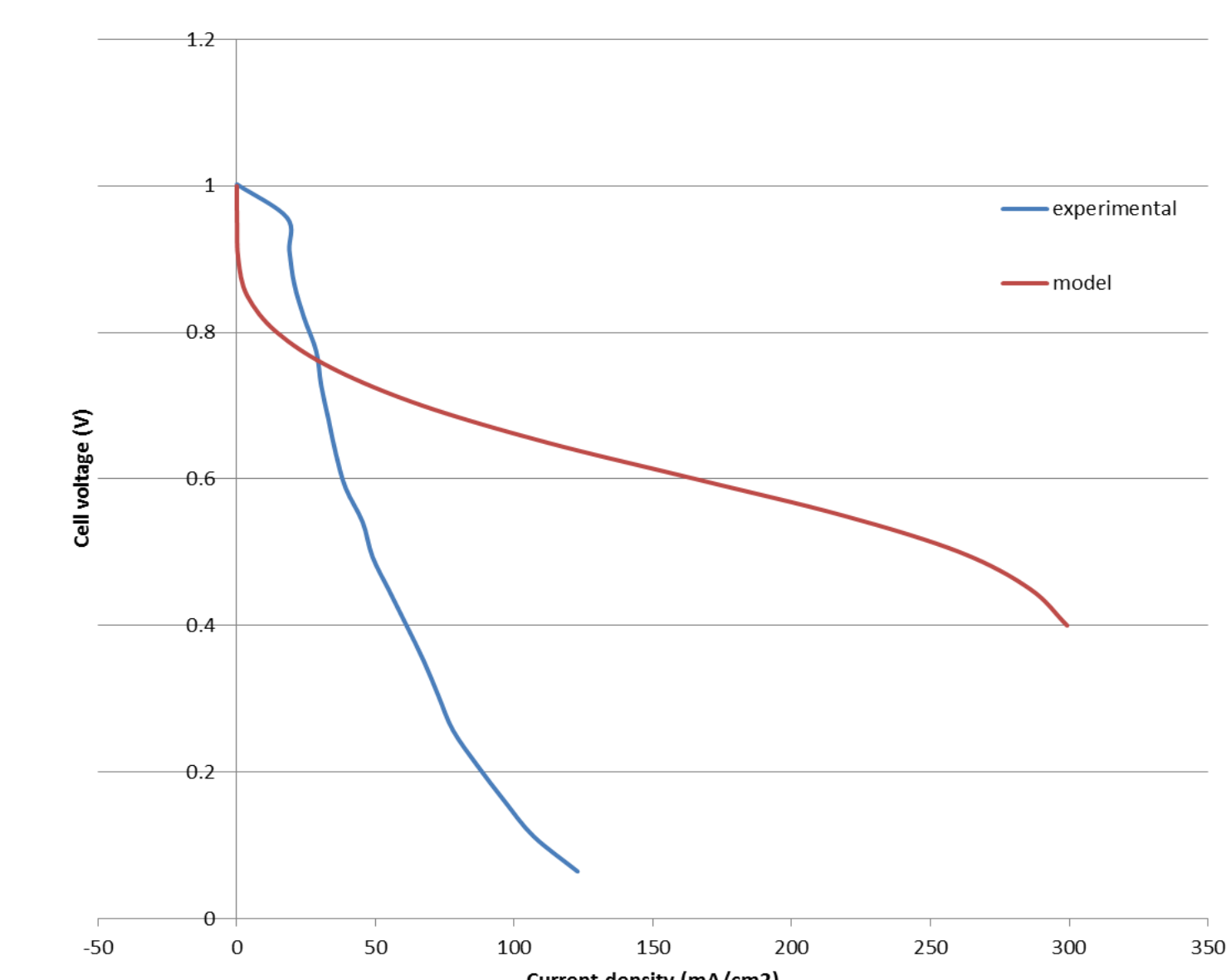


Figure 8. Polarisation curve for experiment & simulated model

Conclusions: simulated model provides valuable information about spatial concentration variation at anode and cathode, velocity and pressure profile in alkaline fuel cell in 3D which are not available from experimental measurements. The dynamic behaviors observed in this study are of significant importance to the future development of AAEM fuel cells for portable and automotive applications.

References:

- Jang-Ho Jo, Sung-Chul Yi (1999), A computational simulation of an alkaline fuel cell, Journal of Power Sources 84,87–106
- Hao Deng, Sen Huo, Yafei Chang, Transient analysis of alkaline anion exchange membrane fuel cell anode, Hydrogen Energy 38 (2013) 6509-6525