Design and Simulation of Sensors to Detect Methanol

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Introduction: The Direct Methanol Fuel Cell (DMFC)has a high energy density when generating electrical power from fuel, and is an attractive power source for portable devices. A fundamental limitation in DMFC technology is methanol crossover. In this process methanol diffuses from the anode through the electrolyte to the cathode, where it reacts directly with the oxygen and produces no electrical current from the cell. Poisoning of the cathode catalysts is also another problem. The design and simulation would involve optimization of various parameters

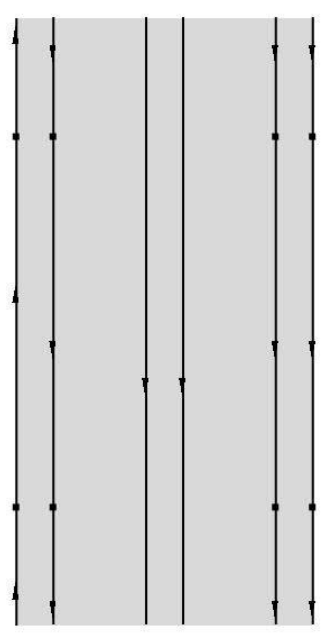


Figure 1. DMFC structure(1 mm^2)

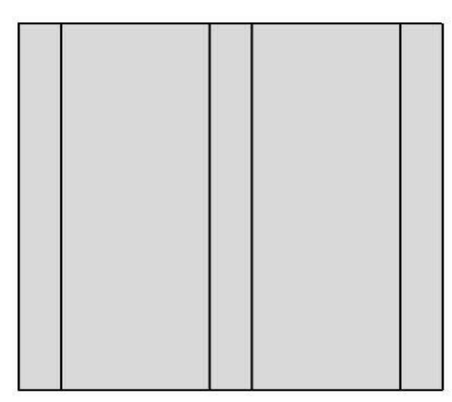


Figure 2. DMFC structure(1 cm^2)

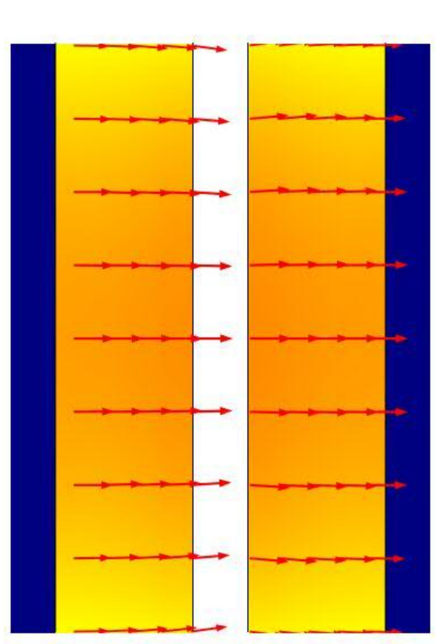
Computational Methods: A passive mode design, of about 1/10th of a cm area, using a single parameter function, is designed. Interfacing Darcy's law of fluidic flow through a porous medium under specific pressure and temperature.

$$Q = \frac{-kA}{\mu}\frac{(P_b - P_a)}{L}$$

$$q = \frac{-k}{\mu}\nabla P$$

The designing involves the construction of gas diffusion layers for anode and cathode, platinum electrodes as working and reference electrodes with different parameters of 1cm^2 area.

Methanol Inlet



Oxygen Inlet

Figure 2. Operation of DMFC

Redox reaction on electrodes (for 0.25 mol of methanol):

Anode: $$CH_3OH + H_2O \rightarrow 6\ H^+ + 6\ e^- + CO_2$$

Cathode: $$\frac{3}{2}O_2 + 6\ H^+ + 6\ e^- \rightarrow 3\ H_2O$$

Redox: $$CH_3OH + \frac{3}{2}O_2 \rightarrow 2\ H_2O + CO_2$$

Results: Platinum is used as a catalyst for both half-reactions. This contributes to the loss of cell voltage potential, as any methanol that is present in the cathode will be oxidized. The change in area of the working and counter electrodes, overlap length and porosity optimizes the power density of the cell.

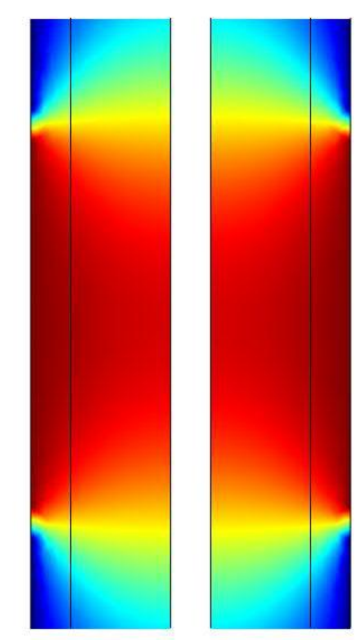


Figure 3. Surface pressure

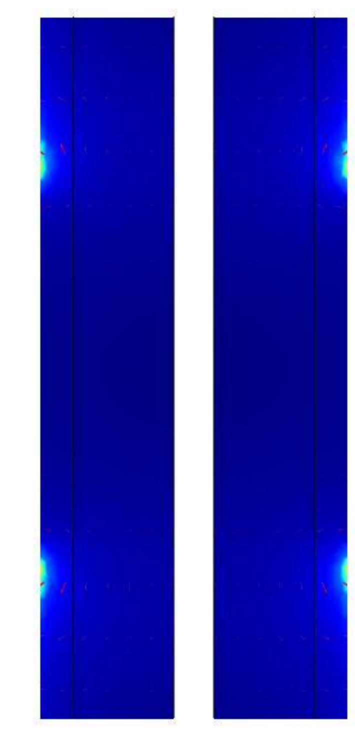


Figure 4. Velocity field

Variable	Value	Units
Electrode thickness	0.25	mm
Area of the cell	1	mm^2
Nafion thickness	0.1	mm
Diffusion coefficient(electrode)	1.6e-7	M^2/s

Table 1. Design parameters

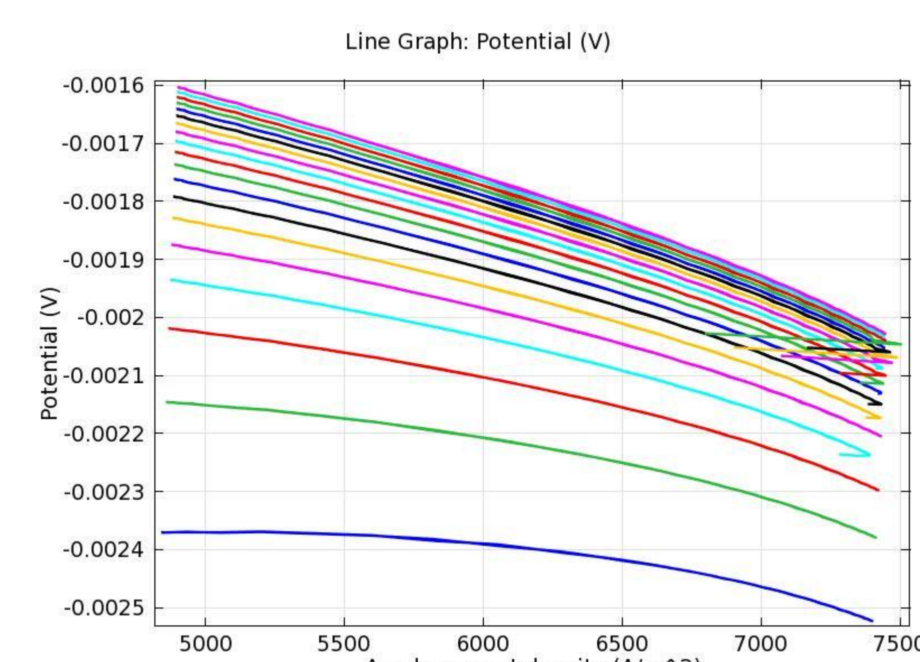


Figure 5. Polarization curve under various pressures

Variable	Value	Units
Electrode thickness	350	micron
Area of the cell	1	Cm^2
Nafion thickness	100	micron
Diffusion coefficient(electrode)	1.6e-7	M^2/s

Table 2. Design parameters

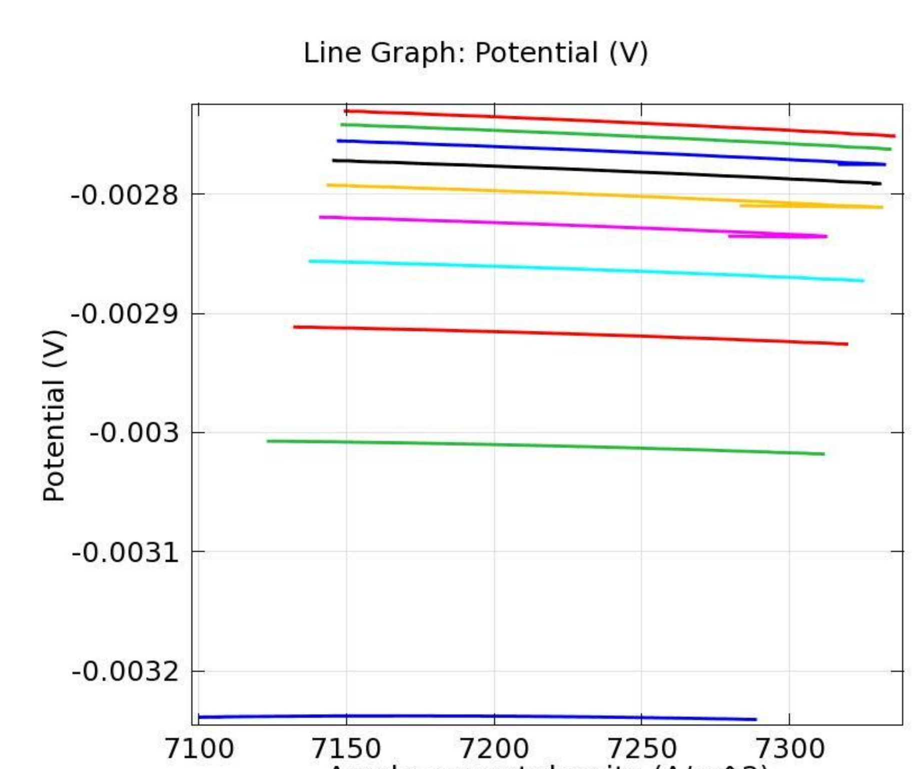


Figure 6. Polarization curve under various pressures

Conclusions: The design and simulation optimized the improved overall power density by the modification of various parameters like the area of the working electrodes and counter electrodes, separation distance and the area of the electrolyte.

References:

1.Brenda L.Garcia,Vijay A.Sethuraman, John W.Weidner, Mathematical model of a direct methanol fuel cell, Transactions of ASME, Vol 1,(Nov, 2004),43-48.
2. Hang guo, Chong-fang Ma, , 2D analytical model of a direct methanol fuel cell, Electrochemistry Communications 6 (2004) 306–312.
3.Chih-Hao chen,Tsung-Kuang Yeh, A mathematical model for simulating methanol permeation and the mixed potential effect in a direct methanol fuel cell, Journal of Power Sources 160 (2006) 1131–1141.