COMSOL Conference '08

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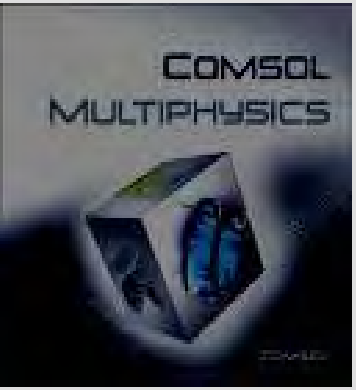
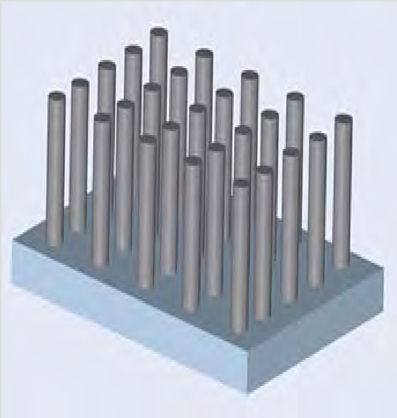
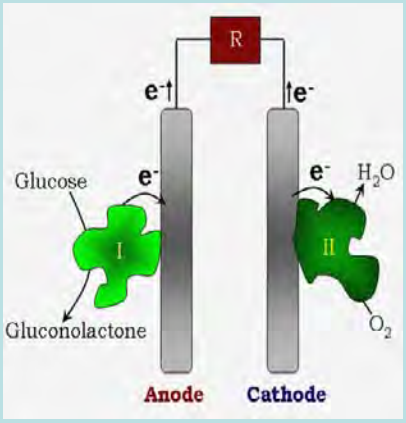
Simulation of C-MEMS based Enzymatic BioFuel Cell







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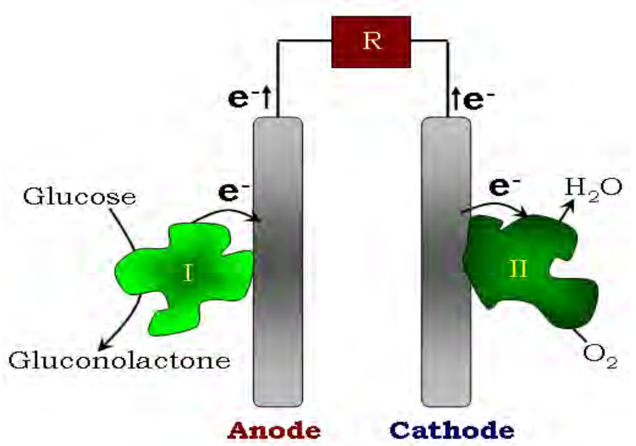
Introduction

- **Objective:** Derive the relationship between the Enzymatic Biofuel cell (EBFC) output response with respect to dimension (Height and width) of posts.



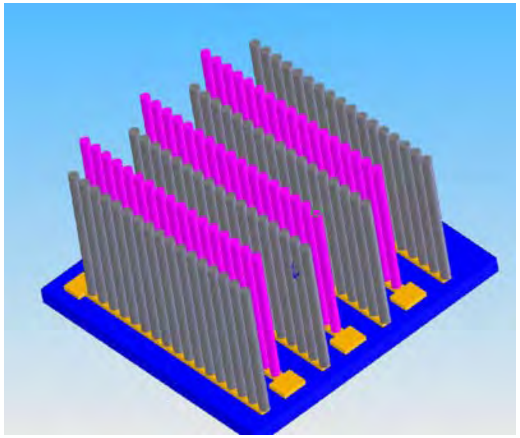
Biofuel cell configuration, with the electrons flowing from the anode to the cathode of the cell[1].

- **Applications:** Pacemakers, Defibrillators, Insulin pumps etc.
  (approx. 100-500uW power requirement)

[1]*B.Y.Park, R. Zaouk, C. Wang, M. Madou, Journal of the Electrochemical Society, vol 154, 2007*

Simulation

- Our model is dense 3-D micro array structure.



Pink - cathodes and Gray anodes

Advantages:

- High surface area of electrodes due to 3-D array
- More amount of enzymes immobilization per foot print area
- more interaction of glucose with posts
- Higher power density[1],

Issues:

- Less diffusion of glucose to the bottom of the micro scale posts.
- High reaction kinetics of enzymes[2].

What can be done to solve the issue?

- Optimized dimensions and geometry[3,4].

[1]Benjamin Y. Park, Rabih Zaouk, Chunlei Wang, Marc J. Madou, J. Electrochem. Soc., 154(2) (2007) P1-P5

[2]Min-Chol Shin, Hyun C. Yoon, Hak-Sung Kim, Analytical sciences, 597-604,August 1996, vol.12.

[3]Han Xu, Kartikeya Malladi, Chunlei Wang, Lawrence Kulinsky, Mingie Song, and Marc Madou, Biosensor and Bioelectronics, 1637–1644,2008, vol.23

[4]Venkataramani Anandan, Xiaoling Yang, euihyeon Kim, Yeswanth Rao, Guigen Zhang, Journal of Biological Engineering 2007,10.1186/1754-1611-1-5

Model-A

Two modules:

Conductive media DC (Potential distribution)

Diffusion (Glucose diffusion)

Overall Reaction:

$$\text{Glucose} + O_2 \xrightarrow{\text{Glucose Oxidase}} \text{Gluconolactone acid} + H_2O_2$$

Anode:

$$H_2O_2 \longrightarrow O_2 + 2H^+ + 2e^- \text{ (Oxidation)}$$

Cathode:

$$O_2 + 4H^+ + 4e^- \longrightarrow 2H_2O \text{ (Reduction)}$$

Nernst Planck's Equation

At anode:

$$E_{anode} = E^o_{anode} - (RxT/2xF) \ln ([H+]^2 \times pO2) \quad (V)$$

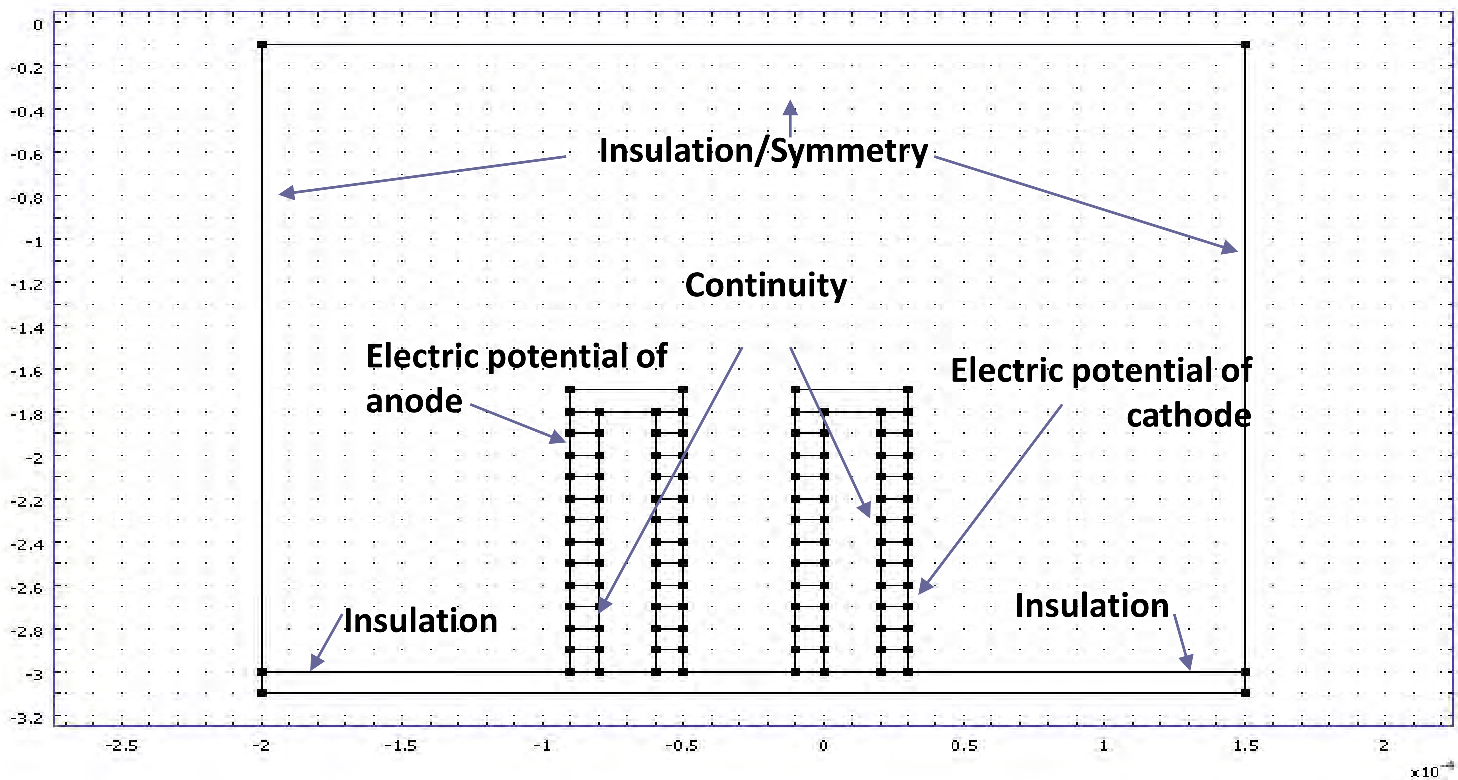
At cathode:

$$E_{cathode} = E^o_{cathode} - (RxT/4xF) \ln (1/ [H+]^4 \times pO2) \quad (V)$$

$$\text{Total cell voltage} = E_{cathode} - E_{anode} \text{ (V)}$$

* *Electrochemical methods, second edition, by allen J. Bard, Larry R. Faulkner, ISBN-0-471-04372-9 c*

Conductive Media DC Module



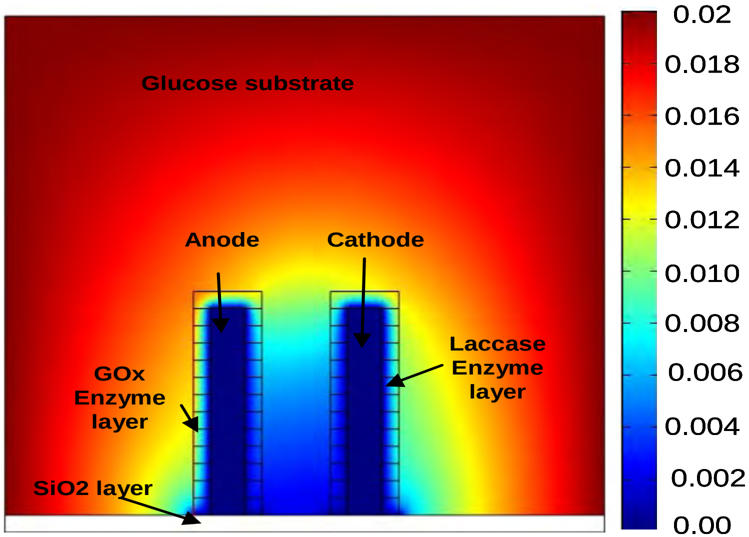
Height of posts= 120um,

Width of posts = 20um,

Boundary Conditions

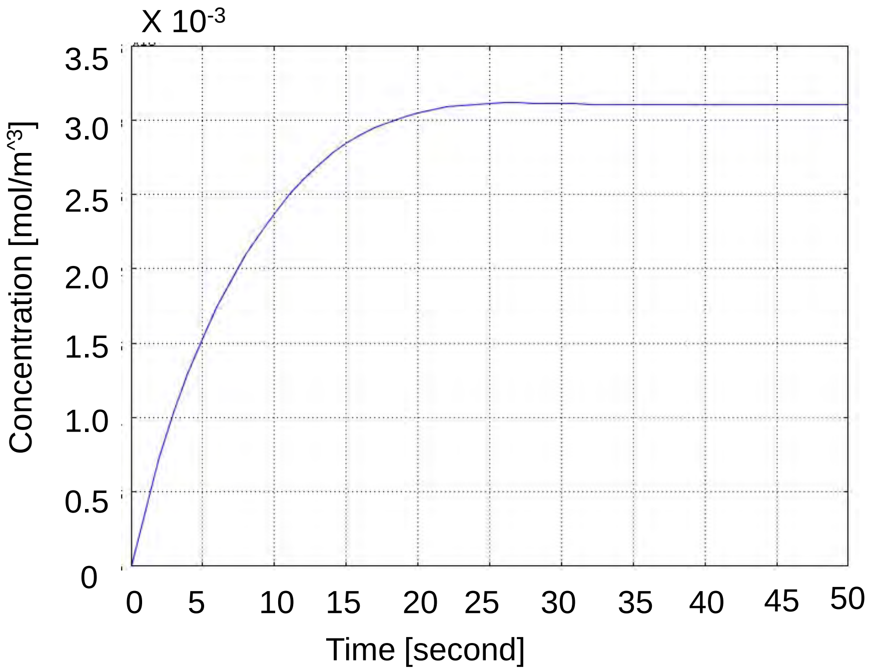
Well width= 40um

Thickness of enzyme layers= 10um



Surface plot for concentration [mol/m^3],

Time 50s

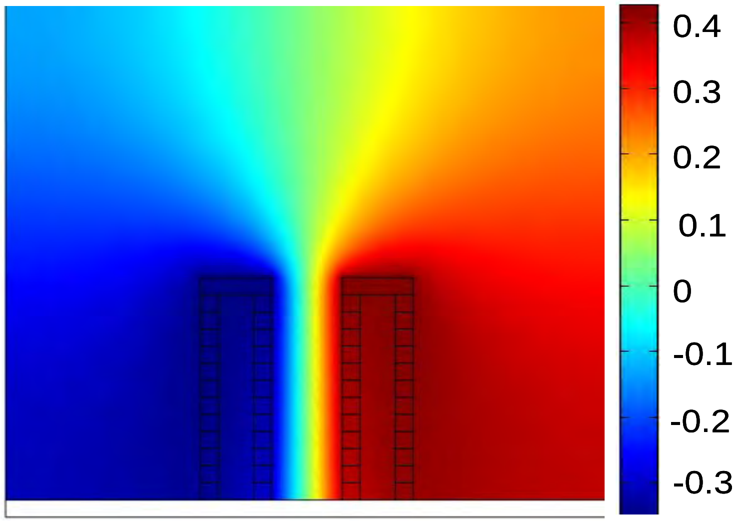


Constants name	Values (unit)	Description
RR	3.3e-6[mol/dm^3][1]	Reaction rate
Diff_laccase	7.6e-7[cm^2/s][2]	diffusion coefficient inside laccase layer
Diff_GOx	4e-7[cm^2/s][3]	diffusion coefficient inside glucose layer

[1]*Han Xu, Kartikeya Malladi, Chunlei Wang, Lawrence Kulinsky, Mingie Song, and Marc Madou, Biosensor and Bioelectronics, 23 (2008) 1637–1644*

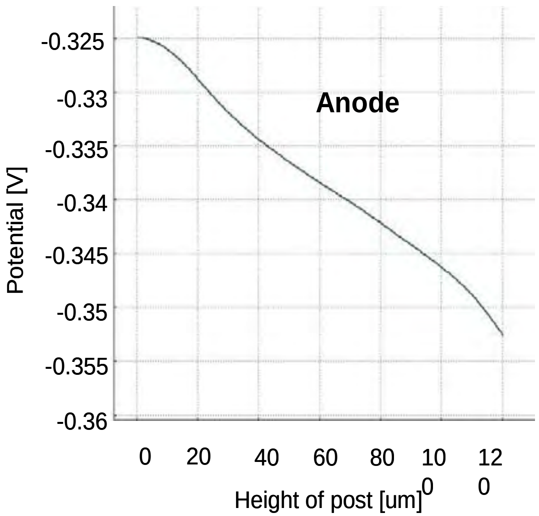
[2]*Nicolas Mano, Valentine Soukharev, and Adam Heller, A Laccase-Wiring Redox Hydrogel for Efficient Catalysis of O2 Electroreduction, J. Phys. Chem. B 2006, 110, 11180-11187*

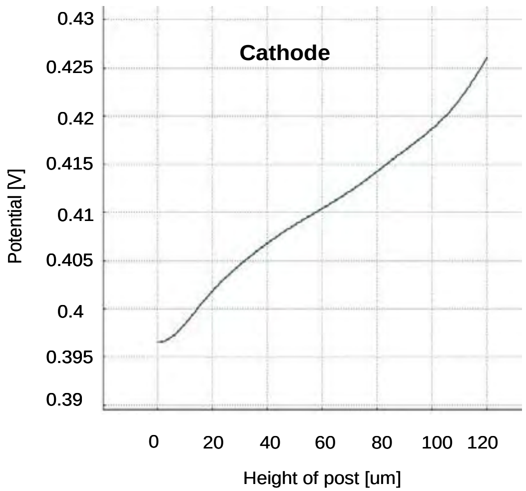
[3]*Guoliang Tao, Eugenii Katz and Itamar Willner,. Chem. Commun. 1997*



Surface plot for Potential [V],

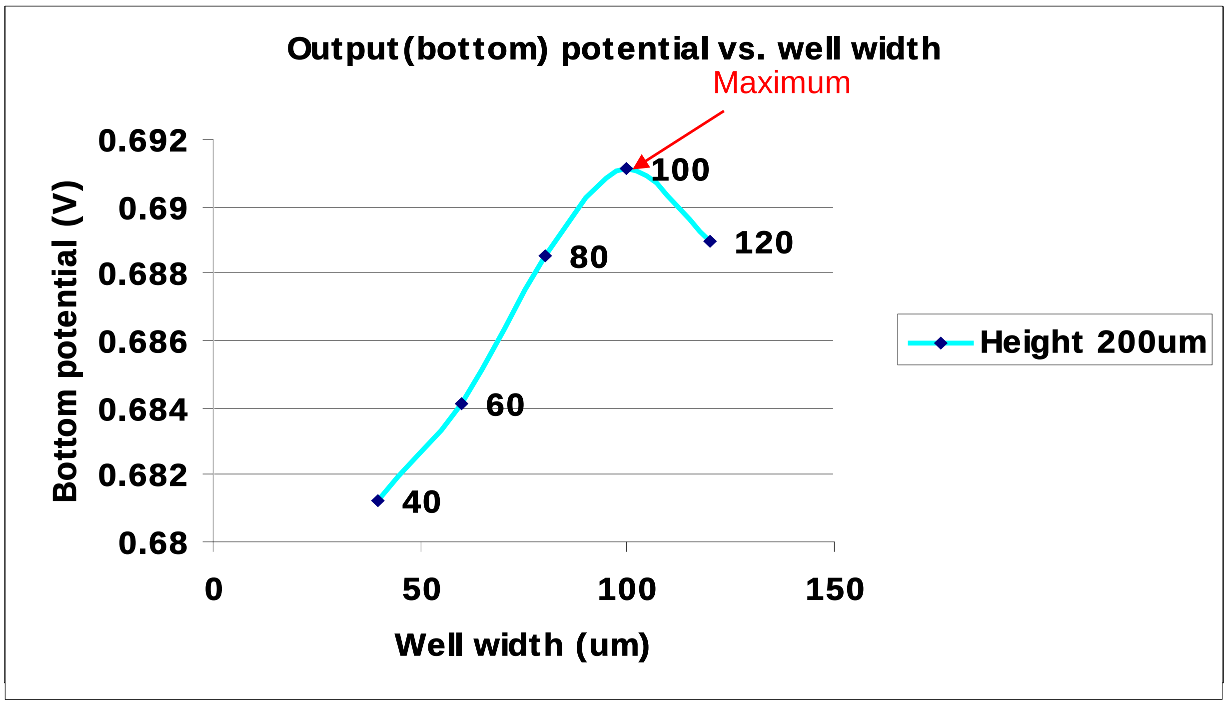
Time 50s





External load[2] (kΩ)	O/P potential (V)	Current (uA)	O/P Power (uW)
5	0.7132	142.64	200
10	0.7132	71.32	100
15	0.7132	47.547	67
20	0.7132	35.66	50
25	0.7132	28.528	40

200um post height



Maximum output when Height = 2x Wellwidth

Model-B

Diffusion coefficient of substrate into polymer film, (cm2/s)

$$D_s^{*\wedge} = \frac{A_k^{2} \times K_{cat} \times e_0}{K_M}$$

Reaction rate inside polymer layer

$$K = \frac{V_{max} \times [C]}{[C] + K_M}$$

K_M = Michaelis-Menten constant (mmol/l)
e_0 = Concentration of total enzyme, (mmol/l)
k_{cat} = catalytic reaction rate(s^{-1})
n= number of electron taking place in reaction
I_0 = exchange current density, A/m^2
alpha= electron transfer constant

Potential losses:

1. **Activation overpotential** (related to the rates of electrode reactions),

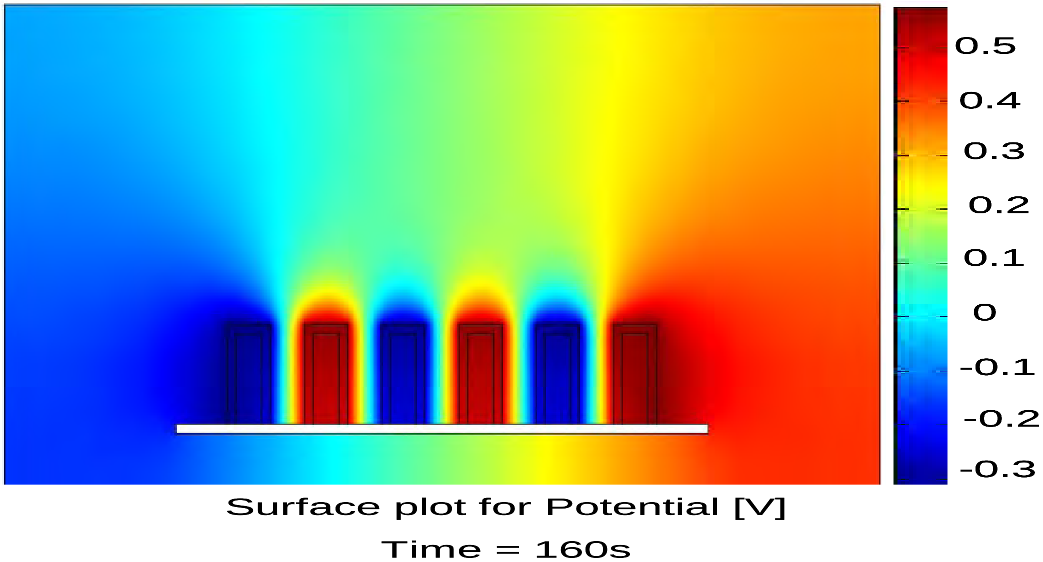
   Butler-Volmer equation & Taefl equation: $$E_{act} = \frac{R \times T \ln(i / i_0)}{alpha \times n \times F}$$

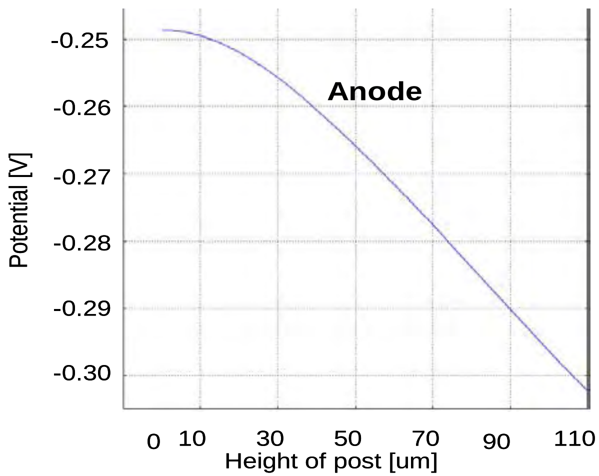
2. **Ohmic overpotential** (related to the resistance)

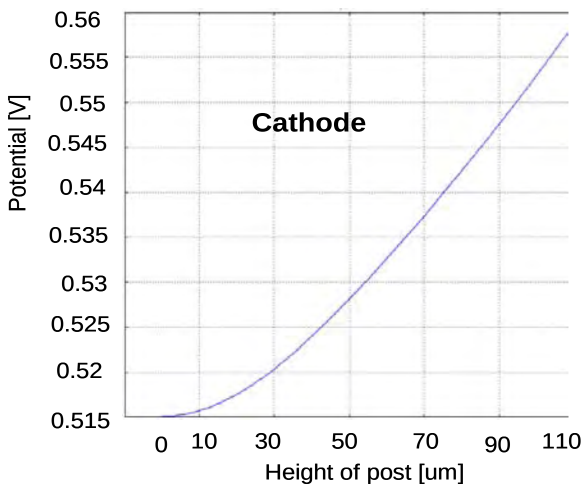
3. **Concentration overpotential** (related to mass transfer limitations)

   Nernst Planck's equation: $$E_{conc} = \frac{R \times T \ln(c_s / c_b)}{n \times F}$$

*P. N. Bartlett, and R. G. Whitaker, Electrochemical Immobilisation of Enzymes Part-I. Theory. J. Electroanal. Chem., **224**: p. 27-35, (1987).
^P. N. Bartlett, P. Tebbutt and R. G. Whitaker, Kinetics Aspects of the Use of Modified Electrodes and Mediators in Bioelectrochemistry. Prog. Reaction Kinetics, **16**: p. 55-155, (1991)







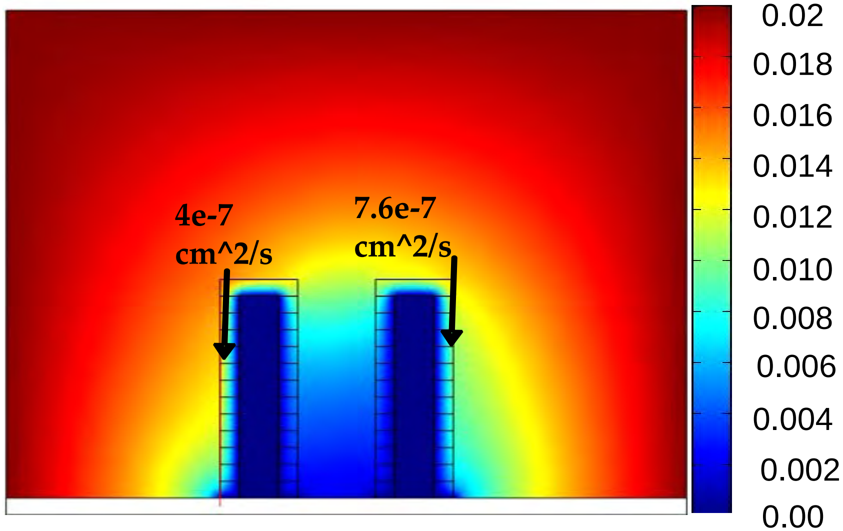
Output potential is around 725mV

Conclusions

Model – A:

1. Higher reaction rate of enzymes can make less deeper diffusion in between posts.

2. Height of the post should be kept twice than that of well width to provide enough space for the diffusion.



Surface plot for concentration [mol/m ^3], Time 50s

Model – B:

For this model, we will incorporate Fluid parameters and find out the relationship between dimensions of posts and output potential to optimize the geometry.

Acknowledgement

Collaborators:

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- Dr. Sylvia Daunert@ UK
- Leonidas@ UK

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National Science Foundation
WHERE DISCOVERIES BEGIN


Thank you!