DYNAMIC MODELLING OF BIOELECTROCHEMICAL ACTIVITY FOR ANODE MICROBIAL FUEL CELLS BY *GEOBACTER SULFURREDUCENS*

by

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Noor Fazliani Shoparwe, PhD Journey (2011-2016)

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LIST OF ABBREVIATIONS

HNQ	2-hydroxy-1,4 naphthoquinone
ATPs	Adenosine Triphosphate
ATCC	American Type Culture Collection
ANN	Artificial neural networks
BF	Biofilm compartment
BL	Bulk liquid compartment
Q	Charge transfer
COD	Chemical oxygen demand
CA	Chronoamperometry
CPE	Constant phase element
CI	Controlled inoculum
CE	Counter electrode
CV	Cyclic voltammetry
DCW	Dry cell weight
EIS	Electrochemical Impedance Spectroscopy
E	Electrode compartment
ETC	Electron transport chain
ECM	Equivalent Circuit model
EET	Extracellular electron transfer
FMN	Flavin mononucleotide
FTIR	Fourier transform infrared spectroscopy
FRA	Frequency-response analyzer
GC	Gas Chromatography

H_2O_2	Hydrogen peroxide
ADM1	IWA's anaerobic digestion model
LSV	Linear sweep voltammetry
MSE	Mean squared error
NR	Neutral red
OCV	Open circuit voltage
POME	Palm oil mill effluent
PDE	Partial differential equation
PEM	Proton exchange membrane
RE	Reference electrode
RVC	Reticulated vitrified carbon
SCE	Saturated calomel electrode
SEM	Scanning electron microscopy
TGA	Thermogravimetric analysis
WE	Working electrode
ODE	Ordinary differential equation

LIST OF SYMBOLS

k_{red}	Backward heterogeneous rate constants
L_L	Boundary layer thickness
X	Cell Biomass
C_o	Initial concentration of species in bulk solution
Q	Constant phase element
k_d	Deactivation rate constant for reduced redox protein
D	Diffusion coefficient
D_{SBF}	Diffusion coefficient of substrate at biofilm
C_{dl}	Double layer capacitance
i_o	Dynamic exchange electric current density rate
I	Electric current
A	Electrode surface area
R_{ext}	External resistance
F	Faradays constant
k_{ox}	Forward heterogeneous rate constants
R	Gas constant
L	Inductance
W	Infinite Warburg
K_I	Inhibition constant
R_{in}	Internal resistance
m_s	Maintenance coefficient
k_c	Mass transfer coefficient
X_m	Maximum biomass concentration

μ_{max}	Maximum specific growth rate
K_s	Monod saturation constant
n	Number of electron
R_Ω	Ohmic resistance
X_{ox}	Oxidized redox protein concentration
I_p	Peak of electric current
R_p	Polarization resistance
v	Potential scan rate
X_{red}	Reduced redox protein concentration
μ_o	Specific growth rate
R^2	Squared regression correlation coefficient
E^0	Standard potential of the redox couple
S	Substrate concentration
S_{BF}	Substrate concentration in biofilm
T	Temperature
t	Time
Y_{xs}	Total yield of cell biomass on substrate in bulk and biofilm
α	Transfer coefficient
V	Voltage
V	Volume of anode compartment
Y_M	Yield of oxidized redox protein

PERMODELAN DINAMIK BAGI AKTIVITI BIOELEKTROKIMIA UNTUK ANOD SEL BAHAN API MIKROB DARIPADA *GEOBACTER SULFURREDUCENS*

ABSTRAK

Sel bahan api mikrob merupakan teknologi baru yang berpotensi besar untuk menjana elektrik daripada substrat organik dengan menggunakan mikrob dan tindabalas bioeletrokimia. Projek penyelidikan ini telah dilaksanakan untuk meningkatkan lagi prestasi aktiviti bioeletrokimia bagi anod sel bahan api mikrob untuk penghasilan elektrik daripada *Geobacter sulfurreducens* sebagai biopemangkin. Dalam merealisasikan kajian ini, permodelan dinamik memfokuskan bahagian anod secara sistem berkelompok telah dibangunkan. Mekanisme bagi pemindahan elektron secara terus daripada sel ektrasellular kepada elektrod telah diberi penekanan. Penambahbaikan ke atas model telah dilakukan dengan mengambil kira kinetik bagi tindabalas biokimia dan elektrod serta menggabungkan kehilangan voltan bagi sistem tersebut. Penambahbaikan juga dilakukan dengan mengambil kira kadar penurunan bagi aktiviti enzim dalam tindakbalas biokimia. Model matematik yang dibangunkan membolehkan kajian dilakukan terhadap profil arus elektrik, penghasilan biojisim, penggunaan substrat dan penurunan voltan terhadap fungsi masa. Kerja-kerja eksperimen pada keadaan operasi yang berbeza telah dijalankan untuk mendapatkan parameter penting dan mengesahkan model matematik. Kaedah elektrokimia telah diaplikasikan untuk mengkaji aktiviti elektrokima bagi sistem tersebut. Lengkuk pengutuban telah digunakan untuk mendapatkan setiap jenis penurunan voltan seperti kehilangan pengaktifan, kehilangan Ohmic and kehilangan kepekatan. Kaedah impedans spektroskopi eletrokimia (EIS) telah diaplikasikan untuk mendapatkan

rintangan dalam dan rintangan pengutuban parameter. Selain itu juga, kaedah voltammetri berkitar telah digunakan untuk menjalankan kajian kinetik elektrod bagi sistem tersebut pada pengimbasan dan pemberian nilai voltan yang berbeza. Keputusan yang paling optimum diperolehi daripada eksperimen menggunakan reka bentuk kebuk tunggal, grafit lakan sebagai elektrod dan kepekatan asetat permulaan sebanyak 20 mM, iaitu menghasilkan penjanaan arus elektrik optimum iaitu 2.32 mA, rintangan dalam iaitu 85.24 Ω, kadar pertumbuhan spesifik iaitu 0.068 jam^{-1}, hasil biojisim sel iaitu 0.0098 g_{sel}/g_{asetat} dan kadar pemindahan elektron heterogen untuk anod iaitu 0.0018 $cm.s^{-1}$ telah digunakan untuk mengesahkan model yang dibangunkan. Model dinamik ini telah berjaya disahkan dengan data eksperimen yang memberikan min kuasa dua ralat kurang daripada 10%. Keseluruhan kerja dalam projek penyelidikan ini telah berjaya dilaksanakan dan membantu menangani sebahagian daripada cabaran dalam pembangunan teknologi sel bahan api mikrob. Gabungan proses bioelektrokimia dengan model matematik bukan sahaja telah memberi potensi yang besar untuk meningkatkan prestasi sel bahan api mikrob malah telah membantu kita memahami keseluruhan sistem sel bahan api mikrob.