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Mathematical Modeling for Determination of Correlation Between Current Density and Dissolved Oxygen in Yeast Microbial Fuel Cell-Based Biosensor

Marcelinus Christwardana*) and Linda Aliffia Yoshi

Department of Chemical Engineering, Institut Teknologi Indonesia, Jl. Raya Puspitek Serpong, South Tangerang, Indonesia 15320

*)Corresponding author: marcelinus@iti.ac.id; mchristwardana@gmail.com

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Abstract

Experiments were conducted to study the correlation between current density and dissolved oxygen (DO) and to develop a model for estimating the value of current density in yeast MFC based DO biosensors. A curve between current density and DO was made, and data analysis was performed using free-online data fitting, namely zunzun.com. One linear regression and nine different exponential models were used as an approach to determine the correlation between current density and DO. Current density increased rapidly as DO concentrations increased, where high DO concentration accelerated the Oxygen Reduction Reaction (ORR) in the cathode part. The exponential model shows a better fit compared to the linear line model, with R^2, SSQ_{ABS}, and RMSE values were 0.9975, 0.4745, and 0.3444, respectively. The exponential equation found in the correlation was $y = 1.532e^{0.320x}$. The results showed that exponential was the best model to describe the relationship between DO concentration and current density that occurred in the MFC-based DO biosensor yeast.

Keywords: *exponential equation, mathematical modeling, biosensor, yeast, dissolved oxygen*

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INTRODUCTION

Microbial Fuel Cell (MFC) is an electrochemical device that can convert chemical energy into electrical energy. Microorganisms are used as biocatalysts by consuming substrates to carry out metabolism, and then produce protons and electrons (Christwardana *et al*., 2017). Protons from the anode side move to the cathode side through the membrane separator, while electrons go away to the cathode side through an external circuit.

MFC can be widely used for various sectors, such as electricity generation, biohydrogen production, battery, wastewater treatment, or biosensors (Debabov, 2008; Yang *et al*., 2015; Zhao *et al*., 2017). In each use, microorganisms are located on the side of the anode along with the substrate. Each microorganism only consumes a specific substrate. Consumption of substrate by microorganisms will activate redox reactions, especially NAD/NADH and FAD/$FADH_2$ in the metabolism process as evidence of the Krebs Cycle process (Christwardana and Kwon, 2017; Christwardana *et al.*, 2018a). The electrons and protons produced then head out of the cell through the Electrons Transfer Chain (ETC) process. Then the electrons are carried by endogenous mediators (EM) to the electrode surface to be transferred to the cathode. At the cathode, an oxygen oxidation (ORR) reaction occurs where oxygen reacts with protons and electrons from the anode side to produce H_2O.

MFC-based biosensors are promising devices in the future. Several studies have been carried out related to the application of MFC into a biosensor device. Many previous researchers applied electrochemical-based biosensor, including from MFC, for detecting BOD, COD, oxygen content, microorganism activity, and corrosion (Chang *et al.*, 2004; Zhang *et al.*, 2011; Oh *et al.*, 2009; Kim *et al.*, 2007; Tront *et al.*, 2008; Xu and Gu, 2014). The MFC system used also varies both single and double chambers.

Yeast-MFC based biosensors, especially to find out dissolved oxygen levels, have never been studied before. In this system, yeast is used as a biocatalyst, where it consumes glucose as a substrate to produce protons and electrons. Whereas in the cathode, oxygen acts as an oxidant that is influential in the system. In full, the reactions that occur on the anode and cathode sides follow (Logan, 2008):

$$\text{An: } C_6H_{12}O_6 + 6H_2O \rightarrow 6CO_2 + 24e^- + 24H^+ \quad (1)$$

$$\text{Cat: } O_2 + 4e^- + 4H^+ \rightarrow 2H_2O \quad (2)$$

In yeast MFC-based biosensors, the cathode part is used as a sensor probe where the part is directly in contact with media that have varied oxygen levels. The variation of dissolved oxygen content will certainly affect the cathode potential, which also directly affects the cell potential. Therefore, the correlation between oxygen content and electrical energy needs to be studied. The cathode potential can be seen in the following equation (Logan, 2008):

$$E_{cat} = E_{cat}^0 - \frac{RT}{nF}\ln\frac{1}{[O_2]^{0.5}[H^+]^2} \quad (3)$$

where E_{cat} is cathode potential, E_{cat}^0 is initial cathode potential, R is the ideal gas constant, T is temperature, n is moles, and F is Faraday constant.

In Closed Circuit Voltage (CCV), the current density will be formed due to external resistance following the equation:

$$J = (V/R)/A \quad (4)$$

where J is current density, V is cell potential, R is external resistance, and A is electrode area.

In this work, we want to find a correlation between current density and dissolved oxygen concentration under CCV conditions with simple mathematical modeling. The results of the current density in various dissolved oxygen concentrations are related to each other, and several mathematical models' approach is carried out to obtain a near-perfect regression coefficient (close to 1).

MATERIALS AND METHODS

Biosensor Preparation and Electrochemical Analysis

The one-chamber cubic MFC reactor, which is the anode chamber, is made of acrylic with an active volume of 28 mL. Carbon felt with a projected active area of 7 cm^2 is used as an anode and cathode. While Nafion 117, which was treated with 3% wt. H_2O_2, 0.5M H_2SO_4, and DI water, acted as a membrane separator that was placed between the anode and the cathode. The broth solution acts as an anolyte consisting of yeast (Lessafre, Marcq-en-Baroeul, France), yeast extract (Merck, Darmstadt, Germany), peptone (Himedia, Mumbai, India), and D-glucose (Merck, Darmstadt, Germany) (Christwardana *et al.*, 2018b; 2019). The anode and cathode are connected to a 1000 Ω resistor as an external resistance and the UNI-T UT61E multimeter (Dongguan, China) for voltage reading. On the other hand, the value of the current density is calculated following the ohm law following equation (4).

The MFC reactor was put into a container containing 1.5 L distilled water and was operated in batch mode. Air-gas containing 21% oxygen was used to control DO levels in the container during the test period, while inert nitrogen gas was used to create close to anaerobes condition. As a comparison, DO readings from the Lutron WA-2015 commercial sensor (Taipei, Taiwan) was used. The configuration of the yeast MFC-based DO sensor shown in Figure 1. All experiments were carried out at room temperature, around 27 °C. Since oxygen saturation in the water at 27 °C is around 8 ppm (Truesdale *et al.* 1955), the DO value of 8 ppm becomes the maximum independent variable value for this modeling study.

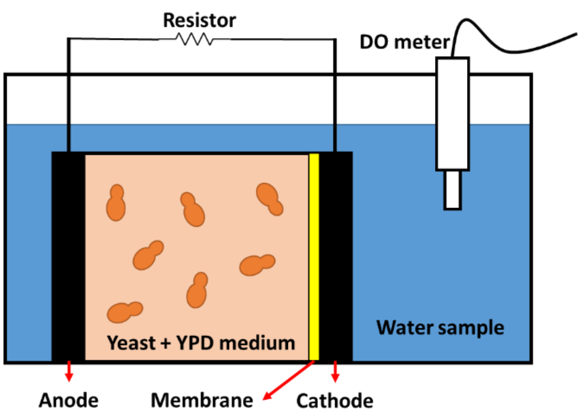

Figure 1. Configuration of yeast MFC-based DO biosensor

The correlation approach between current density and DO using various models

The correlation between current density and DO is installed in several models using linear and non-linear regression analysis, as shown in Table 1. The model for non-linear regression analysis uses the exponential equation approach where the resulting line approaches the linear line. The coefficient of determination (R^2), the absolute sum of square (SSQ_{ABS}), and root mean square error (RMSE) are some of the main criteria for choosing the best model to compare with experimental data. The best model that describes the correlation between current density and DO was chosen as the model with the highest R^2 value, and the lowest SSQ_{ABS} and RSME values.

Table 1. Several of the model for fitting the curve between current density and DO

No.	Model Name	Formula
1.	Expontential	$y = ae^{bx}$
2.	Simple Exponential	$y = a^x$
3.	Inverted Exponential	$y = ae^{b/x}$
4.	Shifted Exponential	$y = ae^{x+b}$
5.	Asymptotic Exponential A	$y = 1\text{-}a^x$
6.	Asymptotic Exponential B	$y = a(1\text{-}e^{bx})$
7.	Scaled Exponential	$y = ae^x$
8.	Stirling	$y = a(e^{bx}\text{-}1)/b$
9.	Hoerl	$y = x^a e^x$
10.	Linear	$y = mx+c$

RESULTS AND DISCUSSION

Experimental data as current density versus dissolved oxygen (DO) concentration were first tried using linear regression, as shown in Figure 2a. Using that approach, the resulting R^2 value is 0.9179, while the SSQ_{ABS} and RMSE values are 15.1464 and 2.7519, respectively. Based on the result, it is still possible to have an approach using other models so that the R^2 value close to 1. For that, the exponential equation is more suitable to be used.

After that, the correlation between current density and DO data were mounted on nine models with an exponential model approach, as shown in Table 2. Table 2 shows the results of regression analyzes conducted on current density in various variations of DO levels. Non-linear regression analysis was performed using free online fitting data (zunzun.com). Statistical parameter estimation shows that the regression coefficient (R^2) ranges from 0.0000 to 0.9975, with the lowest value being the Asymptotic Exponential A model, and the highest value was the exponential model. The R^2 value in the Hoerl model was not detected (n.d.) because the resulting regression line deviates too far from the points resulted. Whereas SSQ_{ABS} and RSME values have a range between 0.4745 to 4458457.5822 and 0.3444 to 1055.7530, respectively. The value of SSQ_{ABS} and RSME is inversely proportional to R^2, where an increase in the value of SSQ_{ABS} and RSME can decrease the value of R^2.

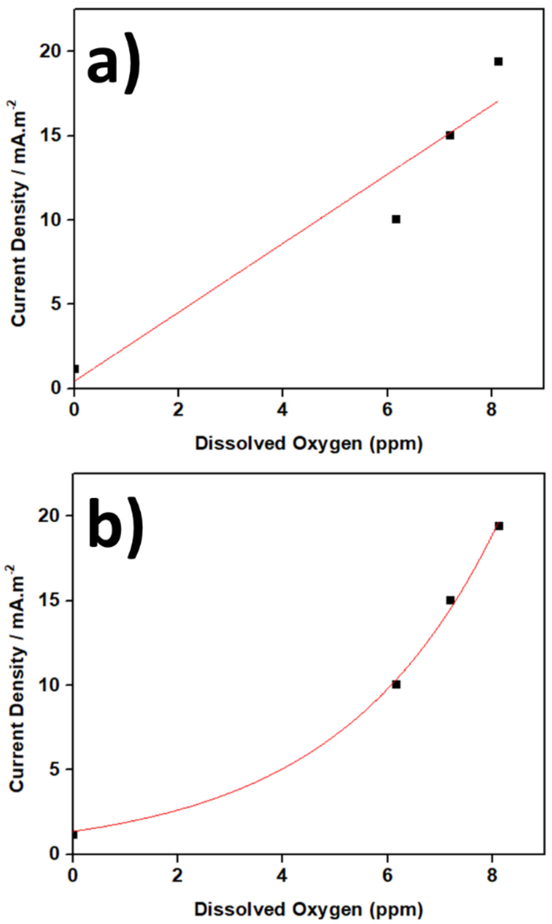

Figure 2. The plot between DO level vs. Current Density with a) Linear regression and b) Exponential model approach

From the results obtained, based on the values of R^2, SSQ_{ABS}, and RSME, the exponential equation ($y = ae^{bx}$) is the most appropriate model to describe the correlation between DO and current density in the yeast MFC-based DO biosensor. The approach with an exponential model produces R^2, SSQ_{ABS}, and RSME of 0.9975, 0.4745, and 0.3444, respectively.

The correlation between current density and DO concentration with the exponential equation model approach can be seen in Figure 2b. The value of the current density increased non-linearly with an increase in DO, so the approach using linear regression is not suitable to be applied here. From that figure, the non-linear regression line precisely touches the correlation points between current density and DO. The relationship between DO and current density in this study is different from the work done by Zhang and Angelidaki (2012), where linear lines are obtained with the majority of R^2 values greater than 0.99. DO concentration limited the cathode ORR activity in MFCs (Rismani-Yazdi *et al.*, 2008). This relationship curve was also influenced by the architecture of MFCs and microorganisms used on the anode side, which indirectly affects the correlation profile between current density and DO level.

Table 2. The value R^2, SSQ_{ABS}, and RSME after an approach using several models

No.	Model Name	Formula with Parameters Coefficient	R^2	SSQ_{ABS}	RMSE
1.	Expontential	$y = 1.532e^{0.320x}$	0.9975	0.4745	0.3444
2.	Simple Exponential	$y = 1.457^x$	0.9941	1.1973	0.5471
3.	Inverted Exponential	$y = 133.995e^{-15.411/x}$	0.9942	1.4022	0.5921
4.	Shifted Exponential	$y = 0.035e^{x-1.525}$	0.3645	96.0211	4.8995
5.	Asymptotic Exponential A	$y = 1\text{-}0.036^x$	0.0000	619.9004	12.4489
6.	Asymptotic Exponential B	$y = -2.802(1-e^{0.260x})$	0.9925	1.7163	0.6550
7.	Scaled Exponential	$y = 0.008e^x$	0.6345	96.0211	4.8995
8.	Stirling	$y = 0.728(e^{0.260x}-1)/0.260$	0.9925	1.7163	0.6550
9.	Hoerl	$y = x^{-0.273}e^x$	n.d.	4458457.5822	1055.7530
10	Linear	$y = 2.092x+0.469$	0.9179	15.1464	2.7519

SSQ_{ABS}: Sum of Square Absolute; RMSE: Root Mean Square Error

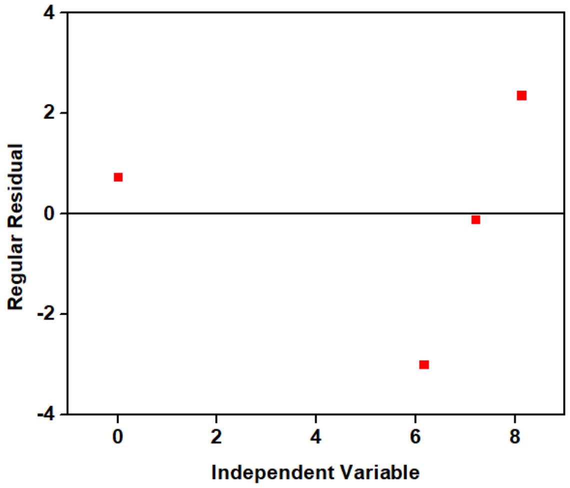

Figure 3. Error plot between DO level vs. Current Density with Exponential model approach

While Figure 3 is an error plot showing how much deviation has occurred in this exponential model approach. From that figure, there are 2 points deviate more than y = 0, and two points deviate less than y = 0. However, the deviation of all points was not too far from the y-axis = 0.

CONCLUSION

Current density at various concentration of dissolved oxygen was measured under 27 °C, and the correlation was sought. The correlation model curve between current density and DO level showed that the resulting line was a non-linear regression. The results demonstrated that the exponential model had the highest R^2 value with a value of 0.9975, and the SSQ_{ABS} and RMSE values were 0.4745 and 0.3444, respectively, the lowest compared to the other models. The obtained exponential equation was $y = 1.532e^{0.320x}$. So, the exponential model is the most appropriate correlation between current density and DO level.

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