Probabilistic Analysis of a Monod-type equation by use of a single chamber Microbial Fuel Cell

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Abstract

Renewable energy forms have become an increasing need for our society. Microbial fuel cells (MFCs) represent a new form of renewable energy by converting organic matter into electricity by using bacteria already present in wastewater while simultaneously treating the wastewater. Most of the current research on MFCs is concerned with increasing the power of the system with respect to the peripheral anode surface area; little research has been done on determining the effects of uncertainty associated with the power density. The power density produced in a MFC can be modeled as a function of substrate concentration using an empirical Monod-type equation. This particular study used a Monte Carlo simulation to demonstrate that the uncertainty intrinsic to the parameters of maximum power density and the half-saturation constant associated with the Monod-type equation by use of a single chamber Microbial Fuel Cell affect the power density produced in the Microbial Fuel Cell. The Monte Carlo simulation was used to justify the uncertainty associated with power density to be a continuous uniform distribution. The simulation determined that the maximum power density parameter from the Monod-type equation has a greater effect on power density, P, then the half-saturation constant parameter. Given the same probability range, the power density exhibited a range of 93.29 to 227.1 $\mathrm{mW/m^2}$ when the maximum power density was used in the Monte Carlo simulation in comparison to a range of 226.7 to 254.3 $\mathrm{mW/m^2}$ of the power density when the half-saturation constant was used in the Monte Carlo simulation. A derived distribution was determined for the power density assuming a normal population distribution. The Chebyshev inequality determined a probability of $P[P \leq (29720)] \geq 0.75$ corresponding to 2 sigma bounds. A Taylor series approximation of the mean and variance corresponded to values of 259.1 and 14720.

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$$
\begin{aligned}
c &= \text{mg} \\
e &= \text{mg} \\
E &= \text{mg} \\
E - S &= \text{mg} \\
K_s &= \text{mg/L} \\
K_m &= \text{mg/L} \\
k_{+1} &= \text{/s} \\
k_{-1} &= \text{/s} \\
k_{+2} &= \text{/s} \\
P &= \text{mW/m}^2 \\
P_{max} &= \text{mW/m}^2 \\
S &= \text{mg/L} \\
v &= \text{mg/s} \\
\mu &= \text{mg/s} \\
\mu_{max} &= \text{mg/s}
\end{aligned}
$$

1 Introduction

Renewable energy has become an increasing need to our society. Microbial fuel cell (MFC) technology represents a new form of renewable energy by generating electricity from what would otherwise be considered waste. This technology can use bacteria already present in wastewater as a catalyst to electricity generation while simultaneously treating wastewater (Lui et al., 2004, Min and Logan, 2004). Although MFCs generate a lower amount of energy than hydrogen fuel cells, a combination of both electricity production and wastewater treatment may help reduce the cost of treating primary effluent wastewater.

A typical MFC consists of two chambers separated by a Proton Exchange Membrane (PEM) such as Nafion (Oh et al. 2004). The disadvantage of the two chamber system is that the cathode chamber needs to be filled with a chemical liquid and aerated to provide oxygen to the cathode (Lui et al., 2004). In hydrogen fuel cells, the cathode is bonded to the PEM which allows oxygen from the air to directly react at the cathode. This same principle is used on single chamber MFCs where the anode chamber is separated from the air-cathode chamber by a gas diffusion layer (GDL) allowing oxygen from the air to transfer to the cathode (Lui et al., 2004). This eliminates the need for energy intensive air sparging of a chemical liquid such as ferrocyanide (Lui et al., 2004). Power generation of a single chamber MFC has been shown in the absence of a PEM decreasing the overall cost (Lui et al., 2004).

The power density produced in a single chamber MFC can be modeled as a function of substrate concentration using an empirical Monod-type equation (Lui et al. 2005). This algebraic equation exhibits power density as a state variable, substrate concentration as the independent variable, and maximum power density and the half-saturation constant as parameters (Lui et al. 2005). This particular equation uses empirical data of the power density and substrate concentration to solve for the parameters. The parameters are then used to develop a function of power density, the state variable, versus substrate concentration,

the independent variable following that of enzyme reaction kinetics (Aiba et al., 1965).

There exists uncertainty between the parameters within the Monod-type equation due to correlations between them (Liu, 2001). These uncertainties will effect the value of the power density. The probabilistic analysis of the this model will include a Monte Carlo simulation to develop histograms displaying frequency diagrams and cumulative frequency diagrams pertaining to power density. A better understanding of how these uncertainties effect the power density in this model will lead the way to a better understanding of how to improve the power density and, ultimately, the design of the MFC.

2 Problem Formulation

The objective of this study is to analyze data of the model variables from experimentation of a single chamber MFC to determine the range of values these parameters exhibit. Random numbers will then be generated by a random number generator intrinsic to the Microsoft Excel computer program to use as the population model. The population model will be validated by the chi-squared test, and K-S test. The population model of the random numbers will be computed according to the Monod-type equation for a Monte Carlo simulation. This simulation will be used to develop histograms displaying the frequency diagrams and cumulative frequency diagrams to determine how the effects of uncertainty change the value of the power density.

3 Literature Review

The purpose of this literature review is to organize relevent information to refer back to in an optimal fashion when applying principles of probablistic analysis to the Monod-type equation

used on a MFC. This section contains an overview of the Monod model and uncertainties within the parameters of the model.

3.1 The Monod Model

The Monod model can describe several important characteristics of microbial growth in a simple periodic culture of microorganisms (Dette et al., 2003). This model was first proposed by Nobel Laureate J. Monod more then 50 years ago and is one of the basic models for quantitative microbiology (Monod, 1949; Dette et al., 2003). This model is typically defined by a differential equation (Dette et al., 2003). Many limitations of this model as well as restrictions of its applications are well known (Pirt, 1975; Baranyi and Roberts, 1995; Ferenci, 1999; Dette et al., 2003). With these limitations, many modifications of the model have also been proposed within specific cases (Ellis et al., 1996; Fu and Mathews, 1999; Schirmer et al., 1999; Vanrolleghem et al., 1999; Dette et al., 2003). The Monod-type equation used in this analysis is in an algebraic form under the assumption of a steady state condition.

3.2 Parameter Uncertainty

Within one specific study on a single chamber MFC, a change in the experimental conditions varied the half-saturation constant from 9-141 mg/L and the maximum power density from 86-661mW/m^2 (Lui et al, 2005). One study suggested the Monod model parameters are correlated to each other linearly and are not to be considered statistically independent (Liu et al., 2001). However, this particular study will make the assumption of statistical independence between the models parameters. Since no distribution has ever been proposed on a specific case such as this, this study will assume the parameters of maximum power

density and the half-saturation constant within this model are random, uniformly distributed variables.

4 Model Formulation and Development

The Monod model was developed from the Michaelis-Menton equation. The formulation of the Michaelis-Menton equation begins with examining the reaction of an enzyme and a substrate (Aiba et al., 1965)

$$E + S \overset{k_{+1}\rightarrow}{\leftarrow k_{-1}} E\ S$$

$$E\ S \xrightarrow{k_{+2}} E + P$$

where

E	=	enzyme
S	=	substrate
$E\ S$	=	enzyme-substrate complex
P	=	product
k_{+1}	=	forward reaction rate constant
k_{-1}	=	reverse reaction rate
k_{+2}	=	reaction rate constant

If the variables e, S, and c are denoted as the concentrations of the total enzyme, substrate, and enzyme-substrate complex, the rate of change of the enzyme-substrate complex, $\frac{dc}{dt}$, can be expressed as (Aiba et al., 1965)

$$\frac{dc}{dt} = k_{+1}(e - c)S - k_{-1}c - k_{+2}c \tag{1}$$

This equation assumes the value of S is considerably greater then that of e. Assuming a steady state condition, the left hand side of the equation becomes zero and c can be solved

for and expressed as (Aiba et al., 1965)

$$c = \frac{eS}{\frac{k_{-1}+k_{+2}}{k_{+1}} + S} \tag{2}$$

From these enzyme reaction equations, the rate of product formation, v, can be expressed as (Aiba et al., 1965)

$$v = k_{+2}c = \frac{k_{+2}eS}{\frac{k_{-1}+k_{+2}}{k_{+1}} + S} = \frac{VS}{K_s + \frac{k_{+2}}{k_{+1}} + S} = \frac{VS}{K_m + S} \tag{3}$$

where

$$\begin{aligned} V &= ek_{+2} &&= \text{maximum rate of production} \\ K_s &= \tfrac{k_{-1}}{k_{+1}} &&= \text{equilibrium constant} \\ K_m &= K_s + \tfrac{k_{+2}}{k_{+1}} \end{aligned}$$

If the value of k_{+2} is considerably smaller than that of k_{+1}, K_m reduces to K_s. When $K_m = K_s$, the Michaelis-Menton equation becomes the Monod where the Monod-type equation replaces V and v with μ_{max} (maximum value of specific growth rate) and μ (specific growth rate). The Monod-type equation assumes only unicellular growth and can be expressed in the form (Aiba et al., 1965)

$$\mu = \mu_{max}\left(\frac{S}{K_s + S}\right) \tag{4}$$

The power density produced in a single chamber MFC can be modeled as a function of substrate concentration, S, using an empirical Monod-type equation (Lui et al., 2005)

$$P = \frac{P_{max}S}{K_S + S} \tag{5}$$

where

$$\begin{aligned} P &= \text{power density} \\ P_{max} &= \text{maximum power density} \\ S &= \text{substrate concentration} \\ K_s &= \text{half-saturation constant} \end{aligned}$$

4.1 Model Assumptions and Limitations

The progression from equation (1) to (2) assumes that substrate concentration will greatly exceed that of the total enzyme concentration. Equation (2) assumes a steady state condition. The later assumption suggests the model's state variable varies only with substrate concentration and not time. The progression of equation (3) to (4) assumes the forward reaction rate constant to be much greater then that of the reverse reaction rate, i.e. K_m is replaced with K_s (Aiba et al., 1965). The assumption of equation (4) is based on observations of unicellular growth limited by a single substrate type. Equation (5) replaces μ and μ_{max} with P and P_{max} suggesting power density to act according to the specific growth rate of microorganisms. The model used in this particular study will assume statistical independence of the parameters, P_{max} and K_s even though case studies of similar monod-type equations have stated these parameters are not statistically independent (Liu et al., 2001).

5 Model Application

This section details the primer process of the Monte Carlo method. This includes the characterization of uncertainty in the model parameters, random number generation and the validation of the random variable to each parameter K_s and P_{max}.

5.1 Characterizing Uncertainty in the Model Parameters

The probability density function and the mathematical expectation value and variance of the random variable are represented when characterizing the uncertainty of a probability distribution. For a continuous random variable, X, along the interval (a, b) the probability

distribution function can be expressed as,

$$f(x) = \begin{cases} 1/(b-a), & \text{if } a < x < b; \\ 0, & \text{otherwise.} \end{cases}$$

The mathematical expectation value and variance of the random variable, X, can be expressed as,

$$E(X) = \int_a^b \frac{x}{b-a} dx = \frac{a+b}{2}$$

and

$$Var(X) = \frac{1}{12}(b-a)^2$$

The expected value and variance of the random variable for maximum power density parameter with a sample space of 86-661 mW/m^2 is evaluated as,

$$E(X) = \int_{86}^{661} \frac{x}{661-86} dx = \frac{86+661}{2} = 373.5$$

$$Var(X) = \frac{1}{12}(661-86)^2 = 27550$$

For the half-saturation constant parameter with a sample space from 9-141 mg/L, the expected value and variance of the random variable is,

$$E(X) = \int_9^{141} \frac{x}{141-9} dx = \frac{9+141}{2} = 75$$

$$Var(X) = \frac{1}{12}(141-9)^2 = 1452$$

5.2 Random Number Generation

Random numbers play an important role in the Monte Carlo method (Manno, 1999). One hundred random numbers were generated by Microsoft Excel using a data analysis - random number generator add-on computer program corresponding to the sample space of each parameter. These random numbers were generated for both the parameters, K_s and P_{max}, corresponding the the range of the random variable. The mean and variance of the random numbers associated with each parameter can be compared to that of the sample space of each parameter assuming a uniform distribution (Table 1 and 2). A bin number for a histogram of each random variable is given by the equation,

$$k = 1 + 3.3log(n)$$

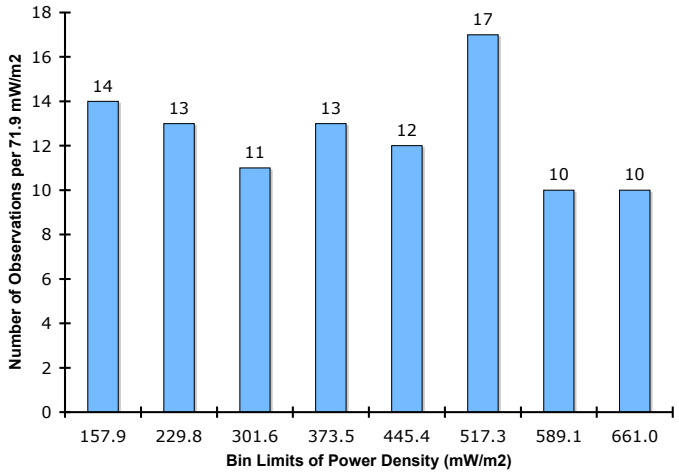
where

$$\begin{aligned} n &= \text{the number of observation} \\ k &= \text{the bin number} \end{aligned}$$

With 100 uniformly distributed, randomly generated numbers, a bin number of 7.6 was calculated and rounded up to 8 corresponding to bin size of each parameter (Figure 1(a) and 2(a)). A cumulative frequency distribution of each parameter is obtained by successively summing the number of observations from each bin by the total amount of observations (Figure 1(b) and 2(b)).

Table 1: Mean and Variance of the maximum Power Density (mW/m2)

	Sample Space	Population Model
Mean	373.5	366.0
Variance	27552	27491



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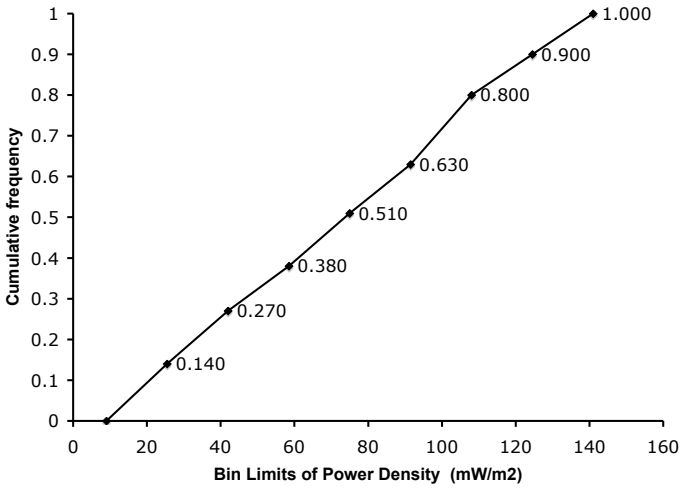

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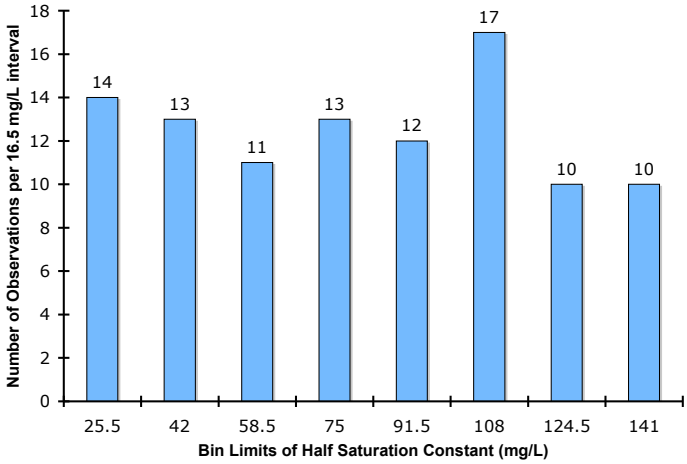
Figure 1: Graphical display of 100 randomly generated numbers. (a) Histogram of maximum power density data; (b) cumulative frequency distribution of maximum power density data.



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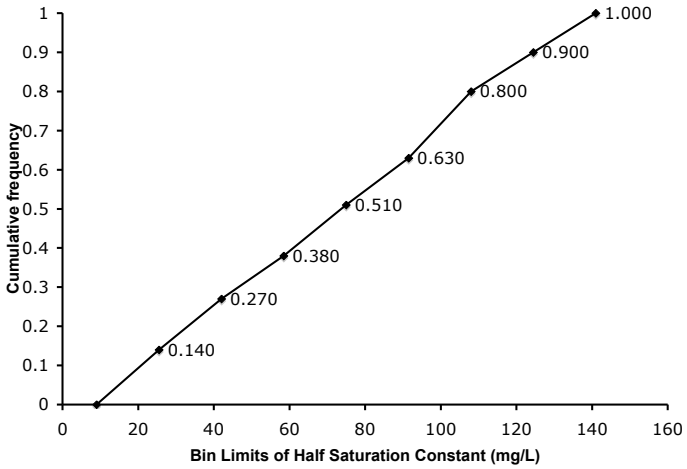


(b)

Figure 2: Graphical display of 100 randomly generated numbers. (a) Histogram of half-saturation constant data; (b) cumulative frequency distribution of half-saturation constant data.

Table 2: Mean and Variance of the Half-Saturation Constant (mg/L)

	Sample Space	Population Model
Mean	75.00	73.28
Variance	1452	1449

5.3 Validation of the Random Variable

Justification for the distribution type of each parameter is based on not only from case studies, but from validation of the random variable of each parameter. The goodness-of-fit tests are one way to validate a probability distribution. These goodness-of-fit tests include that will be performed on both the random numbers associated with the parameters, K_s and P_{max}, and the power density P_{max} include the chi-squared and Kolmogorov-Smirnov test. Due to the simplistic nature of the continuous uniform distribution, these tests were performed analytically.

5.3.1 Chi-Squared Test

The chi-squared test validates the distribution of the random variable by testing whether expected outcome frequencies follow a specified distribution; in this case a continuous uniform distribution for each parameter. Relative frequency is the first calculation required obtained by dividing the number of observations by the total number of observations. The distribution frequency is obtained by integrating the probability density function along the interval of a specific bin size,

$$\text{distribution frequency} = \int_i^j \frac{1}{b-a} dx$$

where

i = initial value of the specific bin size
j = ending value of the specific bin size
a = initial value of the sample space
b = ending value of the sample space

The distribution number (expected outcome frequency) is calculated by dividing the distribution frequency by the total number of observations. The chi-squared statistic is obtained by summing the differences between relative frequencies and expected outcome frequencies, each squared and divided by the expected outcome frequencies. A table was used to represent this process for each parameter (Table 3 and 4).

Table 3: Calculations of the Chi-Squared Methodology for the maximum Power Density random variable

Range (mW/m^2)	Obs. No.	Rel. Freq.(o)	Dist. Freq.	Dist. No.(e)	b-e	$(o-e)^2/e$
86-157.88	14	0.14	0.125	12.5	1.5	0.18
157.88-229.75	13	0.13	0.125	12.5	0.5	0.02
229.75-301.63	11	0.11	0.125	12.5	-0.5	0.02
301.63-373.5	13	0.13	0.125	12.5	0.5	0.02
373.5-445.38	12	0.12	0.125	12.5	-0.5	0.02
445.38-517.25	17	0.17	0.125	12.5	4.5	1.62
517.25-589.13	10	0.1	0.125	12.5	-1.5	0.18
589.13-661	10	0.1	0.125	12.5	-1.5	0.18
					sum =	2.24

Both parameters exhibit the same chi-squared statistic in which degrees of freedom, f, was calculated simultaneously for each parameter. Degrees of freedom is equal to the total number of bins less the number of parameter estimated less one (Willis, 2005),

$$f = 8 - 1 - 1 = 6$$

With 6 degrees of freedom and an alpha of 0.1, the maximum chi-squared statistic is 10.6 according to chi-squared tables (Ang and Tang, 1975). Since both random variables have a test statistic of 2.24 and it is less 10.6, the hypothesis of the random variable of each

Table 4: Calculations of the Chi-Squared Methodology for the Half-Saturation Constant random variable

Range (mg/L)	Obs. No.	Rel. Freq.(o)	Dist. Freq.	Dist. No.(e)	0-e	$(o-e)^2/e$
9-25.5	14	0.14	0.125	12.5	1.5	0.18
25.5-42	13	0.13	0.125	12.5	0.5	0.02
42-58.5	11	0.11	0.125	12.5	-0.5	0.02
58.5-75	13	0.13	0.125	12.5	0.5	0.02
75-91.5	12	0.12	0.125	12.5	-0.5	0.02
91.5-108	17	0.17	0.125	12.5	4.5	1.62
108-124.5	10	0.1	0.125	12.5	-1.5	0.18
124.5-141	10	0.1	0.125	12.5	-1.5	0.18
					sum=	2.24

parameter being uniformly distributed is accepted, i.e. the half saturation constant and maximum power density follow a uniform distribution.

5.3.2 Kolmogorov-Smirnov Test

The Kolmogorov-Smirnov (K-S) Test is based on the maximum deviation between the theoretical cumulative density function and the empirical cumulative density function of the parameters. The maximum deviation can be expressed as,

$$D = max|F_X(x) - S_n(x)|$$

where

$$\begin{aligned} D &= \text{maximum deviation} \\ F_X(x) &= \text{theoretical cumulative frequency} \\ S_n(x) &= \text{emperical cumulative density function} \end{aligned}$$

A graphical display shows no difference between the cumulative distributions of the random variable associated with the maximum power density to that of the random variable associated with the half-saturation constant, i.e. both the empirical cumulative frequency and theoretical distribution function are the same for both parameters (Figure 3).

From these graphs, the maximum deviation was found to be 0.0258. Refering to a K-S table for a significance of 0.10 and 100 random numbers for each parameter, the critical statistic, S^*, is approximately 0.122 (Ang and Tang, 1975),

$$S^* = \frac{1.22}{\sqrt{n}} = \frac{1.22}{\sqrt{100}} = 0.122$$

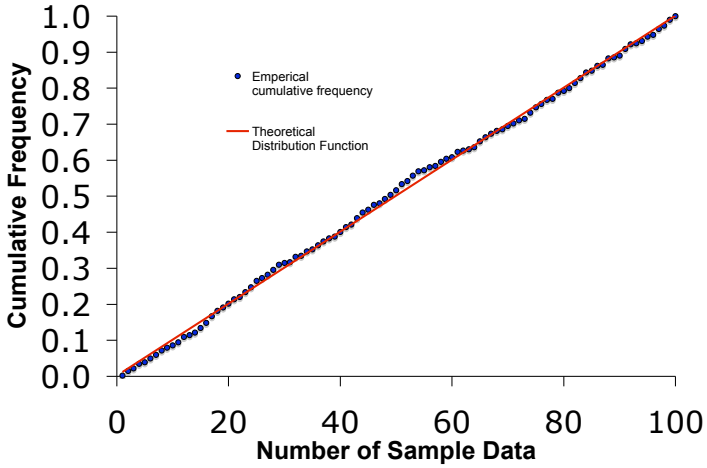
Since there is no exceedance of the maximum deviation observed to that which is allowed, the hypothesis of a uniform distribution for both parameters cannot be rejected.

5.4 Monte Carlo Application

With two random variables associated with the maximum power density and half-saturation constant justified as uniformly distributed, two separate runs generating 100 different values of the state variable, power density, will be used to construct a cumulative distribution function. Assuming statistical independence, one random variable is held constant at the average value while the other is evaluated by the model (both of which hold the substrate concentration at 200 mg/L) to produce the random variable of the state variable and vis versa.

6 Model Results

This section describes the results obtained from the Monte Carlo application. This includes: Monte Carlo results, validation of the monod model's state variable, calculating probabilities and random variables from the cumulative distributions, the derived distribution, the Chebyshev inequality and a Taylor series approximation of the expectation and variance of the random variable associated with power density, P.



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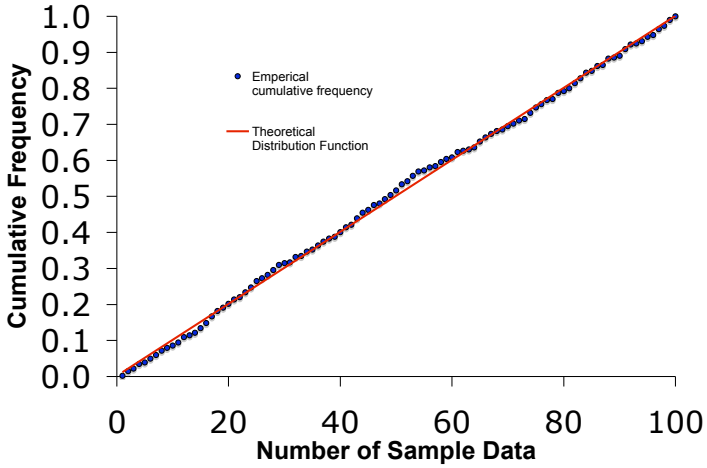


(b)

Figure 3: Empirical cumulative frequency vs. theoretical distribution function (a) Representative of maximum power density, P_{max} (mW/m^2); (b) representative of half-saturation constant, K_s (mg/L).

6.1 Monte Carlo results

The random numbers associated with the parameters of P_{max} and K_s were evaluated in the monod model separately. The mean and variance of the random numbers associated with each state variable distribution can be compared to that of the sample space of each state variable assuming a uniform distribution (Table 5 and 6). A histogram of the number of occurrences shows a difference between changing parameters of P_{max} than that of changing K_s in the random variable of the state variable, P (Figure 4).

Table 5: Mean and Variance of the Power Density (mW/m^2) by changing maximum Power Density (mW/m^2)

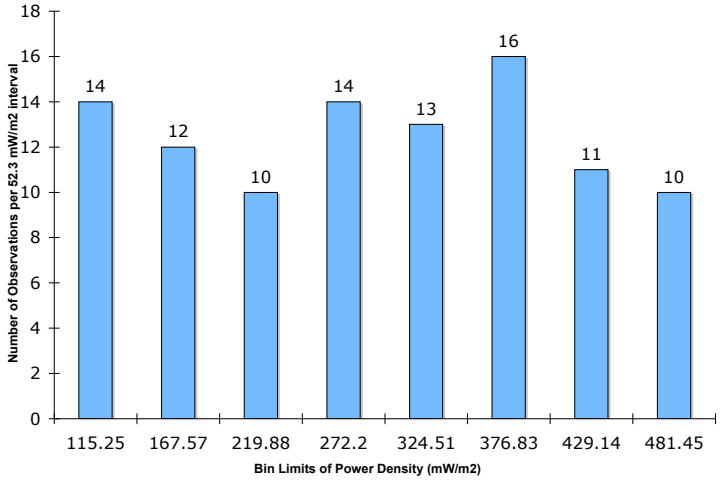
	Sample Space	Population Model
Mean	272.2	267.8
Variance	14596	14724

Table 6: Mean and Variance of the Power Density (mW/m^2) by changing Half-Saturation Constant (mg/L)

	Sample Space	Population Model
Mean	282.7	273.2
Variance	1521.5	1523.7

6.2 Validation of the Monod Model's State Variable

The goodness-of-fit tests were used to evaluated the distribution of the state variable, P_{max}, by changing both parameters P_{max} and K_s. A chi-squared test determining a uniform distribution was performed on the state variable P by changing the parameter P_{max} and resulted in a test statistic of 2.56 (Table 5). The chi-square test performed on the state variable P by



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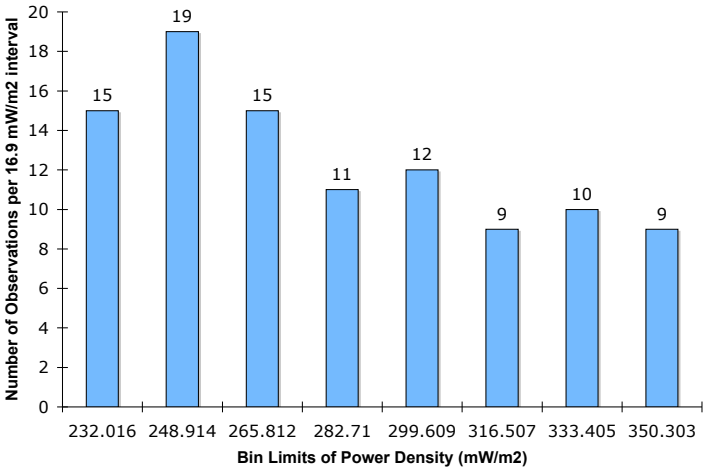


(b)

Figure 4: Histogram of evaluating the random variable associated with state variable P ($\mathrm{mW/m^2}$) (a) by changing P_{max} ($\mathrm{mW/m^2}$) while holding the parameter of K_s constant at the average value of randomly generated numbers; (b) by changing K_s (mg/L) while holding the parameter of P_{max} ($\mathrm{mW/m^2}$) constant at the average value of randomly generated numbers.

changing the parameter K_s resulted in a larger test statistic of 6.59 (Table 6). With an alpha of 0.1 and 6 degrees of freedom, both of these test statistics passed the maximum criteria of a 10.6 test statistic suggesting a uniform distribution as the distribution associated with the state variable.

Table 7: Calculations of the Chi-Squared Methodology for P by changing P_{max}

Range (mW/m^2)	Obs. No.	Rel. Freq.(o)	Dist. Freq.	Dist. No.(e)	b-e	$(o-e)^2/e$
62.94-115.25	14	0.14	0.125	12.5	1.5	0.18
115.25-167.57	12	0.12	0.125	12.5	-0.5	0.02
167.57-219.88	10	0.10	0.125	12.5	-2.5	0.5
219.88-272.20	14	0.14	0.125	12.5	1.5	0.18
272.20-324.51	13	0.13	0.125	12.5	0.5	0.02
324.51-376.85	16	0.16	0.125	12.5	3.5	0.98
376.85-429.14	11	0.11	0.125	12.5	-1.5	0.18
429.14-481.45	10	0.1	0.125	12.5	-2.5	0.5
					sum =	2.56

Table 8: Calculations of the Chi-Squared Methodology for P by changing K_s

Range (mW/m^2)	Obs. No.	Rel. Freq.(o)	Dist. Freq.	Dist. No.(e)	b-e	$(o-e)^2/e$
215.12-232.02	15	0.15	0.125	12.5	2.5	0.5
232.02-248.91	19	0.19	0.125	12.5	6.5	3.38
248.91-265.81	15	0.15	0.125	12.5	2.5	0.5
265.81-282.71	11	0.11	0.125	12.5	-1.5	0.18
282.71-299.61	12	0.12	0.125	12.5	-0.5	0.02
299.61-316.51	9	0.09	0.125	12.5	-3.5	0.98
316.51-333.41	10	0.10	0.125	12.5	-2.5	0.05
333.41-350.30	9	0.09	0.125	12.5	-3.5	0.98
					sum =	6.59

A K-S test was performed on both the random variable of the state variable when changing the maximum power density (mW/m^2) and when changing the half-saturation constant (mg/L). A maximum deviation between the theoretical cumulative density function and the empirical cumulative frequencies of the state variable P when changing the parameter P_{max} was found to be 0.0403. A maximum deviation associated with changing

the parameter K_s was found to be 0.0871. Although both these deviations are larger then the previous deviations found for the random variables associated for the parameters, both of these deviations associated with the state variable are of lesser value then the critical statistic of 0.122, i.e. pass the test (Ang and Tang, 1975). Both of these distributions were passed through a FORTRAN 90 computer program named FA1NEW after compiling the source code named FA1NEW.f. The results from FA1NEW of the state variable when changing the maximum power density, P_{max} passed both the chi-squared and K-S test for a normal distribution. For the state variable associated with changing the half-saturation constant, K_s, FA1NEW results suggested either a Type I Extremal distribution or a Log-Pearson Type III distribution. Since the uniform distribution is the most simplistic distribution that passed for both random variables associated with the state variable, the continuous uniform distribution is chosen as the distribution of power density.

6.3 Calculating Probabilities and Random Variables from the Cumulative Distributions

Both the cumulative frequencies and the cumulative density function can be used to determine the probability of occurrence of a random variable. They can also be used to determine a particular probability given a random variable. The examples described in this particular study use the empirical cumulative frequencies. For example, the probability of a random variable being less than or equal to 227.1 mW/m^2 of power density is equal to 0.41,

$$P(x \leq 227.1) = 0.41$$

A graphical representation of this problem can be seen by drawing a line parallel to the y-axis above the point 227.1 mW/m^2 of power density until a data point is reached, and then left running perpendicular to the y-axis until it reaches the y-axis containing the probability

value (Figure 5 (a)). This can also be done in reverse, i.e. given a probability of 0.41, what is the value of the random variable?

Interestingly, because the cumulative frequencies of the state variable differ depending on which random variable corresponding to a particular parameter is evaluated by the model to produce the state variable; the probability of 0.41 of power density P occurrence by a change in P_{max} does not equal the same random variable associated with power density P occurrance by a change in K_s (Figure 5 (a) and (b)).

$$P(x \leq 254.3) = 0.41$$

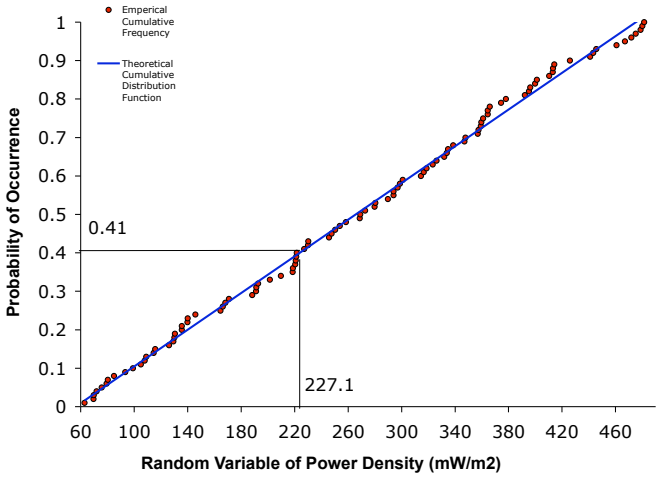
In fact, when the state variable is determined to be 226.7 mW/m^2 (relatively close to 227.1 mW/m^2) from a change in the random variable corresponding to the parameter of K_s, the probability is 0.1, i.e. less likely to occur (Figure 5 (b)). This would suggest that a change in the parameter of K_s would effect the state variable in larger magnitude then a change in the parameter of P_{max}, but this is not the case. With closer inspection, a range of values,

$$P(0.11 < x < 0.41) = 93.29 to 227.1$$

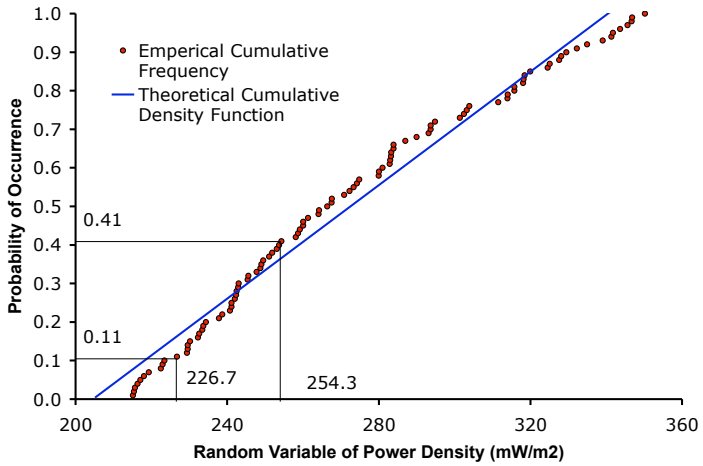
corresponding to the state variable cumulative frequencies with a change in P_{max} is greater then the range of values,

$$P(0.11 < x < 0.41) = 226.7 to 254.3$$

corresponding to the state variable cumulative frequencies with a change in K_s. Thus, a change in P_{max} has a greater effect in magnitude on the state variable then K_s (Figure 5 (a) and (b)).



(a)



(b)

Figure 5: Empirical cumulative frequency vs. theoretical distribution function (a) Representative of power density, P, by changing the maximum power density, P_{max} (mW/m^2); (b) representative of power density, P, by changing the half-saturation constant, K_s (mg/L).

6.4 Derived Probability Distribution

Since the parameter P_{max} has the greatest effect on the state variable, it was chosen to be used as the inverse. The random variable of the state variable, P, associated with a change in P_{max} was determined to have a normal distribution with the computer program FA1NEW so the parameter can be assumed a normal distributed random variable. The inverse function of the monod equation can be expressed as,

$$P_{max} = \frac{P(K_s + S)}{S}$$

The derived density function can then be expressed as,

$$f_P(p) = \frac{1}{\sqrt{2\pi}\sigma} e^{\left[-\frac{1}{2}\left(\frac{\frac{P(K_s+S)}{S}-\mu}{\sigma}\right)^2\right]\frac{(K_s+S)}{S}}$$

which can be simplified and expressed as,

$$f_P(p) = \frac{1}{\sqrt{2\pi}\sigma\frac{S}{(K_s+S)}} e^{\left[-\frac{1}{2}\left(\frac{P-\frac{S}{(K_s+S)}\mu}{\sigma\frac{S}{(K_s+S)}}\right)^2\right]}$$

6.5 Chebyshev inequality

The Chebyshev inequality can show that the mean and standard deviation alone can determine a probability of a random variable lying within any given bound. The expression can be denoted as,

$$P[(m_X - h\sigma_X) \leq X \leq (m_X + h\sigma_X)] \geq 1 - \frac{1}{h^2}$$

corresponding to one, two and three sigma bounds; h equals 1, 2 and 3. Using P as the random variable associated with a change in P_{max} and with a mean of 267.8 and a standard deviation of 14724, the expression can be expressed as,

$$P[(267.8 - 14724h) \leq P \leq (267.8 + 14724h)] \geq 1 - \frac{1}{h^2}$$

if $h = 2$ corresponding to 2 sigma bounds

$$P[(-29180) \leq P \leq (29716)] \geq 0.75$$

and assuming non-negativity of power density

$$P[P \leq (29716)] \geq 0.75$$

In this case, due to the very large magnitude of variance, the bounds are much larger than the exact bounds. This suggests that the variance associated with the maximum power density is much larger then what may be thought of as a typical magnitude of variance.

6.6 Taylor Series Approximation

The Taylor series can be used to approximate the mean and variance of the state variable given empirical data of the state variable. From one case study, twenty seven data points of the maximum power density correspond to a mean of 356.3 and a variance of 23987 (Lui, 2005). The expected value can then be computed (assuming substrate concentration of 200 mg/L and K_s at the average of the random variable),

$$E(P) \simeq g(\mu_{P_{max}}) = \frac{356.3 * 200}{75 + 200} = 259.1$$

The variance can be computed as,

$$Var(P) \simeq Var(P)\left(\frac{dg}{dP_{max}}\right)^2 = Var(P)\frac{S}{K_s + S} = 23987\frac{200}{75 + 200} = 17445$$

The mean and variance from the approximations can compared to the mean and variance from the state variable from the Monte Carlo simulation (Table 7). Although they are not the same, the mean is a fairly close figure to that of the Monte Carlo simulation. With more data of the power density, perhaps the results would have had less of a difference.

Table 9: Mean and Variance of the Power Density (mW/m^2)

	Taylor Series Approx.	Monte Carlo simulation
Mean	259.1	267.8
Variance	17445	14724

7 Conclusions

The results of the Monte Carlo simulation demonstrate that the uncertainty intrinsic to the parameters associated with the Monod-type equation by use of a single chamber Microbial Fuel Cell, affect the power density produced in the Microbial Fuel Cell. Specifically, the investigation shows the following:

1. The Monte Carlo simulation demonstrates a difference in uncertainty of the state variable between the parameters.

2. Probabilities of power density in a Microbial Fuel Cell can be determined by use of a cumulative frequency diagram obtained from the Monte Carlo simulation, i.e. the value of the probability or the value of the power density.

3. The maximum power density parameter associated with the Monod-type equation has a greater effect on power density, P, then the half-saturation constant parameter.

4. The Taylor series approximation of the mean and variance associated with the power density is a close approximation to that of the random variable determined in the Monte Carlo simulation.

5. The variance associated with the maximum power density in a Microbial Fuel Cell is large.

8 Further Research

There is suspicion as to a joint distribution associated with the parameters in the Monod-type equation. Further research might show this relationship.

9 References

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10 Appendix