Estimation of the microalgae growth using the optimization approach

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Abstract. This study estimates the parameters value of the microalgae growth kinetic model which are Monod, Tessier and modified Moser model using the Levenberg-Marquardt method, by minimizing the sum of squares error. The optimal control problem for microalgae growth in photobioreactor is formulated and solved by the optimal input design method and taking into account the parametric sensitivities in order to obtain the control function. Hence, the fourth-order Runge-Kutta method is implemented to predict the microalgae biomass concentration by solving the state equations of the optimal control problem. The result shows the Tessier model best describes the growth of microalgae with the produced biomass concentration of weight $1.813 \times 10^{10} \, \text{g}$.

1. Introduction

As the world population and economy are growing, global demand for energy is rapidly increasing, especially in fast-growing countries such as China and India. Therefore, the renewable energy such as biomass energy has to be explored to achieve environmental and economic sustainability. For example, the microalgae undergo photosynthesis to convert atmospheric carbon dioxide to biofuel. The microalgae have other advantages including as a source of nutrients for human and animals [1].

In the industrial sector, photobioreactor is used to control specific conditions needed for microalgae growth [2]. The common factors for microalgae growth include light intensity, nutrient availability, temperature and water pH [3]. There are many existing growth kinetic models such as Monod, Tessier and Moser model used to predict the microalgae growth with considering certain factors [4-6]. The biomass produced by microalgae in the photobioreactor can be optimized if the parameters of the growth model are optimal.

However, the optimal parameters of microalgae growth kinetic model such as maximum specific growth rate and half saturation constant for substrates are difficult to estimate based on the collected experimental data. In previous study, the parameters of microalgae growth model have been estimated by using the non-linear least squares method such as Nelder-Mead, Gauss-Newton and Levenberg-Marquardt method [7-10].

In this study, we estimate the parameters value of the microalgae growth kinetic model to fit the experimental data by applying Levenberg-Marquardt method. Meanwhile, the optimal control problem
for microalgae growth is solved by the optimal input design and the biomass concentration produced from microalgae is estimated using numerical method. In Section 2, the methodology implemented in this study is explained in detail. Next, the obtained results are presented and discussed, and finally is summarized in Section 3.

2. Methodology
In this research, Levenberg-Marquardt method which is a non-linear least squares method was used to minimize the sum of squares error ($SSE$) between experimental data and estimated data. As a result, the estimated parameters value of several kinetic models based on light intensity was obtained. One of the kinetic models that has the smallest $SSE$ value was chosen as the best fit model to the experimental data. Next, the optimal control problem for microalgae growth in photobioreactor was formulated and solved by optimal input design method. Lastly, the Runge-Kutta method was used to solve the state equations of the optimal control problem in order to predict the microalgae biomass concentration.

2.1. Growth kinetic models related to light intensity
This study considered the light intensity as the input parameter in the photobioreactor. Hence, three kinetic models based on light intensity were implemented which are Monod model, Tessier model and modified Moser model.

Tamiya et al. [11] applied the Monod model to describe the microalgae growth for light intensity, $I$ denoted as

$$
\mu = \mu_{\text{max}} \left( \frac{I}{K_I + I} \right),
$$

(1)

where $\mu$ is the specific growth rate, $\mu_{\text{max}}$ is the maximum specific growth rate and $K_I$ represents the half saturation constant for light.

On the other hand, van Oorschot [12] used the Tessier model as follows

$$
\mu = \mu_{\text{max}} \left[ 1 - \exp \left( -\frac{I}{K_I} \right) \right].
$$

(2)

Besides, Grima et al. [13] modified the Moser model by assuming the uptake of light energy depends hyperbolically on the light intensity as follows

$$
\mu = \mu_{\text{max}} \left( \frac{I}{I^* + K_I} \right),
$$

(3)

where $I^*$ represents the affinity of cells to light and whose significance is analogous to $K_I$ and $a$ is the ability of microalgae to uptake resources.

2.2. Levenberg-Marquardt method for parameter estimation
Table 1 shows the experimental data set for specific growth rate of microalgae Botryococcus sp. for different light intensity [14]. In this research, parameters of the three models are estimated by using Levenberg-Marquardt (LM) method to fit the experimental data. LM method is a non-linear least squares method which blends the Gauss Newton and gradient-descent method.
Table 1. Specific growth rate versus light intensity.

| Light intensity (μmolm⁻²s⁻¹) | Specific growth rate (day⁻¹) |
|--------------------------------|----------------------------|
| 2.7                           | 0.412                      |
| 48.6                          | 0.461                      |
| 94.5                          | 0.959                      |
| 176.0                         | 1.026                      |
| 243.0                         | 1.307                      |
| 324.0                         | 1.160                      |

Since LM method is an iteration method, initial guess for each parameter is significant. Good initial guess can be determined by observing the value from the experimental data that corresponds to the definition of the parameter [9]. Thus, the initial guess for \( \mu_{\text{max}} \) is 1.307 \( \text{day}^{-1} \). Meanwhile, \( K_r \) and \( I_k \) are set as 70 \( \mu\text{molm}^{-2}\text{s}^{-1} \), which is the value of \( I \) when \( \mu \) reached half of \( \mu_{\text{max}} \) in the experimental data. Initial guess for \( a \) is arbitrary choose as 0 due to difficulty estimate from the data.

To fit the model to the data, LM method minimizes the sum of squares error (SSE) to obtain the optimal parameters. Therefore, SSE is the objective function, \( f \) which can be defined as [15]

\[
\min f = SSE = \sum_{i=1}^{n} r_i^2,
\]

where \( r \) is the different between error calculated from the experimental and the estimated data.

Hence, the Jacobian matrix, \( J \) is defined as

\[
J = \begin{bmatrix}
\frac{\partial r_i}{\partial p_1} & \ldots & \frac{\partial r_i}{\partial p_p} \\
\vdots & \ddots & \vdots \\
\frac{\partial r_i}{\partial p_1} & \ldots & \frac{\partial r_i}{\partial p_p}
\end{bmatrix},
\]

where \( p \) is the parameter of the kinetic model.

The updated value of the parameter \( p \) is computed using

\[
p_{i+1} = p_i - \left(J^T J + k \mathbf{I}\right)^{-1} J^T r_i,
\]

where \( k \) is the damping parameter and \( \mathbf{I} \) is identity matrix. The initial value of \( k \) is 0.001.

For each iteration, the \( SSE_{i+1} \) was compared with the \( SSE_i \) value. If the value of \( SSE_{i+1} \) is higher compared to \( SSE_i \), the step is retracted by recalculating the parameter value of \( p_{i+1} \) and its \( SSE_i \). Then \( k \) is multiplied by 10 and \( p_{i+1} \) is computed using equation (6). If the value of \( SSE_{i+1} \) is lower compared to \( SSE_i \), the step is continued by dividing the value of \( k \) with 10 and \( p_{i+1} \) is computed using equation (6) [16]. The parameters values and their \( SSE \) are iterated until \( SSE \) achieves the desired tolerance of 0.000001. The process flow of the algorithm for LM method can be described as shown in figure 1.
2.3. Photobioreactor model

The microalgae photobioreactor system is described as in figure 2 [17]. In this figure, $L_{in}$ and $L_{out}$ are the incoming and outgoing liquid flow of photobioreactor, respectively. Meanwhile, $V$ represents the volume capacity of photobioreactor, $C$ is concentration of microalgae in photobioreactor, $C_{in}$ is incoming concentration of microalgae and $C_{out}$ is outgoing concentration of microalgae.

Figure 1. Flowchart of algorithm for Levenberg-Marquardt method.

Figure 2. Microalgae photobioreactor system.
The mass balance in the photobioreactor system is given by

\[
\text{mass accumulation} = \text{mass flow in} - \text{mass flow out} + \text{mass production}
\]  

(7)

\[
\frac{d[VC]}{dt} = L_{in} C_{in} - L_{out} C_{out} + \mu CV.
\]  

(8)

By applying the product rule, equation (8) becomes

\[
V \frac{dC}{dt} + C \frac{dV}{dt} = L_{in} C_{in} - L_{out} C_{out} + \mu CV.
\]  

(9)

The change of volume is the difference of the incoming and outgoing liquid flow, hence

\[
\frac{dV}{dt} = L_{in} - L_{out}.
\]  

(10)

By substituting equation (10) to equation (9) gives

\[
V \frac{dC}{dt} + C (L_{in} - L_{out}) = L_{in} C_{in} - L_{out} C_{out} + \mu CV.
\]  

(11)

Assume that no microalgae coming into the system, \( C_{in} = 0 \), then, \( C_{out} = C \). Therefore, equation (11) becomes

\[
V \frac{dC}{dt} + C L_{in} = \mu CV.
\]  

(12)

Assume that the microalgae with dilution rate, \( D = \frac{L_{in}}{V} \) is equal to 0, then photobioreactor model is defined as

\[
\frac{dC}{dt} = \mu C.
\]  

(13)

2.4. Optimal input design method

In parametric models, the output sensitivity with respect to a parameter, \( p \) can be determined by the accuracy of a parameter estimation from the input data. The general dynamic equation is

\[
\dot{x}(t) = f(x(t), u(t), p, t),
\]  

(14)

where \( t \) is time, \( x(t) \) is the state vector, \( \dot{x}(t) \) is first order derivative function with respect to \( t \), \( u(t) \) is the control vector and \( f \) is a nonlinear vector function [18].

Assuming that \( p \) is the time invariant, differentiate equation (14) with respect to \( p \) and gives the additional state equation as follows

\[
\dot{x}_p(t) = \frac{\partial f}{\partial x} \dot{x}(t) + \frac{\partial f}{\partial p},
\]  

(15)

where \( x_p(t) \) is the additional state variable.

The number of additional state equations are depending on the number of parameters of the model that will be estimated.

The optimal control problem to optimize the cost function, \( F \) is defined as

\[
F = \phi[x(t_f)] + \int_0^T L(x, u, t) \, dt,
\]  

(16)
where \( \phi(x(t_f)) \) is the terminal condition and \( L \) is the operating cost.

Meanwhile, the additional state variables of parametric sensitivity in optimal input design problem are computed in time by the operating cost, \( L \), which can be defined as [17]

\[
L(x,u,t) = q_s \dot{s}^1 + q_s \dot{s}^2 + \ldots + q_s \dot{s}^z,
\]

(17)

where \( z \) is the number of the additional state variables, \( s \) is the parametric sensitivity and \( q \) is the weighting factors for the parametric sensitivity.

The scalar Hamiltonian function for this problem, \( H(t) \) is defined as [17]

\[
H(t) = L(x,u,t) + \lambda'(t) f(x,u,t),
\]

(18)

where \( \lambda'(t) \) is Lagrange multiplier vector.

In this study, the following conditions must be satisfied in order to solve the optimal control problem for the microalgae growth and to obtain \( u(t) \).

State equation : \( \dot{x} = f(x,u,t) \) (19)

Co-state equation : \( \dot{\lambda} = -H^T \) (20)

Stationary equation : \( H^T_u = 0 \) (21)

Boundary condition : \( x(t_0) = x_0 \) and \( \lambda(t_f) = \phi^T(t_f) \) (22)

2.5. Runge-Kutta method for solving state equations

A study by See and Jamaian [19] successfully solved the state equations of optimal control problem for microalgae growth by the first order Runge-Kutta method, which also called the Euler method. The higher the order of Runge-Kutta method, the more accurate the numerical solutions obtained when using fixed step size for most cases [20]. To increase the accuracy of the numerical solution, the fourth-order Runge-Kutta (RK4) method is applied to solve the system of the state equations in this research.

The RK4 formula [21] is described as

\[
y_{\text{m},i+1} = y_{\text{m},i} + \frac{h}{6} \left( k_1 + 2k_2 + 2k_3 + k_4 \right), \quad 1 \leq m \leq n
\]

(23)

where

\[
k_1 = f_u \left( t_i, y_{\text{m},i}, y_{\text{m},i}, \ldots, y_{\text{m},i} \right),
\]

\[
k_2 = f_u \left( t_i + \frac{h}{2}, y_{\text{m},i} + \frac{h}{2} k_1, y_{\text{m},i} + \frac{h}{2} k_1, \ldots, y_{\text{m},i} + \frac{h}{2} k_1 \right),
\]

\[
k_3 = f_u \left( t_i + \frac{h}{2}, y_{\text{m},i} + \frac{h}{2} k_2, y_{\text{m},i} + \frac{h}{2} k_2, \ldots, y_{\text{m},i} + \frac{h}{2} k_2 \right),
\]

\[
k_4 = f_u \left( t_i + h, y_{\text{m},i} + h k_1, y_{\text{m},i} + h k_1, \ldots, y_{\text{m},i} + h k_1 \right),
\]

and \( f_u = y'_{\text{m}} \), \( n \) represents the number of first order differential equations, \( h \) is the step size and \( i \) is the iteration number.
3. Results and discussion

3.1. Parameter estimation for microalgae growth kinetic model

The iterative results of the parameters for the Tamiya, van Oorschot and Grima model by applying the LM method and solved by the Matlab software are shown in table 2, table 3 and table 4, respectively. The optimal parameters and the corresponding values for the three microalgae growth kinetic models are summarized as in table 5. The comparison between experimental and estimated data for each kinetic model is also visualized graphically as in figure 3.

Table 2. The iterative result of parameters values for Tamiya model.

| i  | $\mu_{\max}$ | $K_i$ | $SSE$   |
|----|--------------|-------|---------|
| 0  | 1.307000     | 70.00000 | 0.281965 |
| 1  | 1.508991     | 70.00373 | 0.187728 |
| 2  | 1.510204     | 70.05820 | 0.187720 |
| 3  | 1.513063     | 70.53120 | 0.187672 |
| 4  | 1.524475     | 72.42140 | 0.187545 |
| 5  | 1.532258     | 73.71701 | 0.187517 |
| 6  | 1.533127     | 73.86302 | 0.187517 |

Table 3. The iterative result of parameters values for van Oorschot model.

| i  | $\mu_{\max}$ | $K_i$ | $SSE$   |
|----|--------------|-------|---------|
| 0  | 1.307000     | 70.00000 | 0.219243 |
| 1  | 1.210798     | 70.03692 | 0.185938 |
| 2  | 1.211736     | 70.36231 | 0.185723 |
| 3  | 1.220454     | 72.68546 | 0.184455 |
| 4  | 1.238663     | 77.46902 | 0.183199 |
| 5  | 1.244104     | 78.81671 | 0.183138 |
| 6  | 1.244142     | 78.82171 | 0.183138 |

Table 4. The iterative result of parameters values for Grima model.

| i  | $\mu_{\max}$ | $I_i$   | $a$     | $SSE$   |
|----|--------------|---------|---------|---------|
| 0  | 1.307000     | 70.00000 | 0.00000 | 1.011069 |
| 1  | 1.749498     | 70.00000 | 0.546630 | 0.880697 |
| 2  | 1.179702     | 70.10079 | 1.500466 | 0.787273 |
| 3  | 1.179702     | 70.10079 | 1.500466 | 0.787273 |
Table 5. Optimal parameters and the corresponding $SSE$.

| Model     | $\mu_{\text{max}}$ | $K_I$     | $I_k$     | $a$   | $SSE$   |
|-----------|---------------------|-----------|-----------|-------|---------|
| Tamiya    | 1.533127            | 73.863027 | -         | -     | 0.187517|
| van Oorschot | 1.244142        | 78.821711 | -         | -     | 0.183138|
| Grima     | 1.179702            |           | 70.100794 | 1.500466 | 0.787273|

Figure 3. Comparison of the experimental data versus the estimated data using the kinetic models.

From figure 3, the results show that the estimated data by Tamiya and van Oorschot model are very close to the experimental data, while the Grima model is not. This result is consistent with the numerical results in table 5 where the minimum $SSE$ for Tamiya and van Oorschot model are approximate to zero. This indicate that the parameters computed by Tamiya and van Oorschot model are optimal. Therefore, it can be concluded that among the three kinetic models, the van Oorschot model is the best fit kinetic model to the experimental data with the smallest $SSE$ value of 0.183138. Meanwhile, the smallest $SSE$ value for Tamiya and Grima models is 0.187517 and 0.787273, respectively.

3.2. Optimal control problem for microalgae growth

The optimal control problem for the microalgae growth in photobioreactor is formulated based on van Oorschot model which gives the best fit kinetic model to the experimental data. The optimal control problem is solved using the optimal input design and also taking into account the parametric sensitivities.

Let the concentration of microalgae in photobioreactor, $C$ by $x_1$ and the light intensity, $I$ by $x_2$. Then, substituting the van Oorschot model (equation (2)) into the microalgae photobioreactor model (equation (13)), the dynamic state equation can be denoted as

$$\dot{x}_1 = \mu_{\text{max}} \left[ 1 - \exp \left( - \frac{x_2}{K_I} \right) \right] x_1.$$  

(24)
Since the light intensity, $I$ is the only input factor considered in the photobioreactor, the state equation for $x_1$ is equal to the control function, $u(t)$.

$$x_1 = u$$ (25)

Besides, in this study we only maximize the parametric sensitivity of $K_i$. Equation (15) is used to generate the additional state equation for parametric sensitivity of $K_i$. Thus, the state equation for the additional state variable $x_3 = \frac{\partial x_3}{\partial K_i}$ is defined as the following equation.

$$x_3 = \frac{\partial f}{\partial x_1}x_1 + \frac{\partial f}{\partial K_i} = \mu_{\max} \left[ 1 - \exp \left( \frac{x_2}{K_i} \right) \right] x_3 - \frac{H_{\max} x_1 x_3}{K_i^2} \exp \left( - \frac{x_2}{K_i} \right)$$ (26)

Furthermore, it is required to maximize the operating cost in order to maximize the parametric sensitivity. Since the good choice for the weighting factors of $x_3$ is equal to 1, the maximum operating cost, $L$ is defined as the following equation [17].

$$\max L(x(t), u(t), t) = x_3^2$$ (27)

Pontryagin’s minimum principle states that the control function, $u(t)$ is optimal when Hamiltonian function, $H(t)$ is minimized [22]. Since maximizing $L$ is equal to minimizing $-L$, the minimum $H(t)$ can be defined as

$$\min H(t) = -x_3^2 + \lambda_1 x_1 + \lambda_2 x_2 + \lambda_3 x_3$$

$$= -x_3^2 + \lambda_1 \mu_{\max} \left[ 1 - \exp \left( - \frac{x_2}{K_i} \right) \right] x_3 + \lambda_2 u + \lambda_3 \left[ \mu_{\max} \left[ 1 - \exp \left( - \frac{x_2}{K_i} \right) \right] x_3 - \frac{H_{\max} x_1 x_3}{K_i^2} \exp \left( - \frac{x_2}{K_i} \right) \right]$$. (28)

Next, the co-state equations, $\dot{\lambda}_1$, $\dot{\lambda}_2$ and $\dot{\lambda}_3$ are computed using the equation (20) based on the defined $H(t)$ . Moreover, the stationary equation is obtained by differentiating $H(t)$ with respect to $u(t)$ which shown below.

$$H_s = \dot{\lambda}_i$$ (29)

Since $u$ does not exist in equation (29), this optimal control problem becomes a singular optimal control problem. Thus, equation (29) is differentiated repeatedly with respect to $t$ until $u$ appears explicitly in the equation. Then, arranging the differential equations into the form of matrix $A \dot{\lambda} = 0$. Since $A \dot{\lambda}$ cannot be zero, the matrix $A$ must be singular in order to solve the system [23]. Therefore, the determinant of matrix $A$ which is shown in the equation below is equal to zero [24]. As a result, control function, $u(t)$ is equal to zero.

$$\det(A) = -\frac{\mu_{\max} x_1^2 u}{K_i} \exp \left( - \frac{2x_2}{K_i} \right) = 0$$ (30)

$$u(t) = 0$$ (31)
3.3. Prediction of microalgae biomass concentration

In this study, the system of the state equations is solved by RK4 method using Matlab software. The period for the microalgae growth, \( t \) is set for 14 days and the step size is set as 0.5. Whereas, the values of the parameters of van Oorschot model are set as \( \mu_{\text{max}} = 1.244142 \) and \( K_I = 78.821711 \), which generated by the Levenberg-Marquardt method.

As denoted in equation (31), the control function is equal to zero which indicates that the light intensity, \( I \) does not change with respect to time. Therefore, the initial value of \( I \) gives the large impact to the iterative result. After trial and error, solving the system of state equations with different initial \( I \) in the range of \( 250 \leq I \leq 324 \), \( x_3 \) is maximized if \( x_2 = 254 \). Hence, the initial value of \( x_1, x_2 \) and \( x_3 \) are set as 1000, 254 and 0, respectively. The predicted biomass concentration of microalgae Botryococcus sp. for 14 days by the RK4 method are shown numerically in table 6 and graphically in figure 4.

| Table 6. Prediction of biomass concentration of microalgae for 14 days by the fourth-order Runge-Kutta method. |
|---------------------------------------------------------------|
| Time (day) | Biomass Concentration (g L⁻¹) |
|-------------|-------------------------------|
| 0           | 1000.000000                   |
| 1           | 3299.534445                   |
| 2           | 10886.927556                  |
| 3           | 35921.792475                  |
| 4           | 118525.191611                 |
| 5           | 391077.952363                 |
| 6           | 1290375.174638                |
| 7           | 4257637.336147                |
| 8           | 14048221.046436               |
| 9           | 46352589.238640               |
| 10          | 152941964.824165              |
| 11          | 504637281.077207              |
| 12          | 1665068091.323224             |
| 13          | 5493949521.178147             |
| 14          | 18127475686.154606            |
From Figure 4, we can observe that the biomass concentration for microalgae slowly increases from day 1 until day 9. This is known as the lag phase when the microalgae culture is transferred from a plate to liquid culture due to the physiological adaptation of the cell metabolism to growth [25]. After the lag phase, the microalgae grew exponentially beginning from day 9 as they are undergoing the exponential phase and produce the biomass concentration of weight $1.813 \times 10^{10} \text{ g}$.

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