Sigma J Eng Nat Sci, Vol. 42, No. 3, pp. 778−786, June, 2024

Sigma Journal of Engineering and Natural Sciences
Web page info: https://sigma.yildiz.edu.tr
DOI: 10.14744/sigma.2024.00000

Research Article

Rapid parameter estimation of four non-linear growth models for analyzing the growth of Escherichia Coli

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ARTICLE INFO

Article history
Received: 27 July 2022
Revised: 04 August 2022
Accepted: 27 February 2023

Keywords:
Kinetic Models; Microbial Growth; Parameter Estimation and Partial Sums

ABSTRACT

In this paper we develop five new methods of estimation to estimate the parameters of four widely used nonlinear models namely Haldane, Powell, Moser and Webb model. A standard growth data set of Escherichia Coli is considered for estimating the parameters. The estimated model parameters are analyzed by evaluating statistical parameters χ^2, Root Mean Square Error, R^2, R_a^2 and R_{pre}^2. As a result, the Powell model gives the best fit with estimation of R^2 as 99.7% with respect to method IV. Moreover, the other three models also provide remarkable fit along with the newly introduced methods. Method II gives R^2 value as 99% in case of the Haldane model. The method IV estimates with R^2 value as 99.6% in the Moser model and the method III estimates with R^2 value as 99.4% in case of the Webb model.

Cite this article as: Narayan Gogoi U, Saikia P, Mahanta DJ. Rapid parameter estimation of four non-linear growth models for analyzing the growth of Escherichia Coli. Sigma J Eng Nat Sci 2024;42(3):778−786.

INTRODUCTION

The growth kinetics of the microbial has been an area of vast potentiality for many scientific researches and it has many implications for our society. The combination of mathematical modeling with experimental works can provide a meaningful and quantitative interpretation of the experimental results and unveiling new windows of microbial physiology. The representation of a real-world phenomenon using mathematical tools is termed as Mathematical modeling. Biological phenomena are complex natural phenomena and mathematical modeling helps understanding these phenomena. Different mathematical models are applied to study the growth of microbials.

Microbial growth kinetics is the study of the relationship between the specific growth rate μ of a particular microbial population and the substrate concentration S. The first microbial growth equation was given by Blackman [1] in 1905. In 1913, Michaelis [2] derived a mathematical model to analyze the enzyme activity based on substrate concentration. In 1942 Monod [3] introduced a growth model based on specific growth rate. Contois [4] and Pfeffer [5] established that the Monod model is not adequate to explain the degradation of municipal waste. The Monod model cannot be applied when a substrate exhibit

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This paper was recommended for publication in revised form by Regional Editor Vildan Çetkin

inhibition [6]. Also, the Monod model does not adequately represent the lag phase and the death phase of the growth [7,8] process. To overcome these limitations Moser, Powell, Haldane, and Webb modified the Monod model and introduced their own models to study microbial growth. In 1958, Moser [9] modified the Monod model by introducing an adjustable parameter (m) which gives flexibility in fitting experimental data and describing the dynamic behavior in bioreactor [10]. At high substrate concentration the Moser model is capable of representing the lag phase [7] of microbial growth process. Krishnan [11] used the parameter (m) of the Moser model to describe substrate inhibition. The mathematical form of the Moser model is given by

$$\mu = \frac{\mu_{max} S^m}{k_s + S^m}, \tag{1}$$

where μ represents the specific growth rate, S represents the substrate concentration at time t and μ_{max} is the maximum growth rate. The constant k_s is called the half saturation constant as when $\mu = \frac{\mu_{max}}{2}$, $S = k_s$. The constant (m) represents the dynamic behavior in the bioreactor.

In 1930 Haldane [12] introduced a model and the mathematical form of the model is given by

$$\mu = \frac{\mu_{max} S}{k_s + S + \frac{S^2}{k_i}}, \tag{2}$$

where μ is the specific growth rate and S is the substrate concentration at time t and μ_{max} is the maximum growth rate. The constant k_s is the half saturation constant and k_i is called the inhibition constant. The Haldane model is capable of describing all the growth phases: lag, exponential, stationery and death phase [13]. This model is also capable of representing the growth rate at high and low substrate concentration [6,14].

In 1967 Powell [15] added a new parameter (p), to the Monod model which is known as maintenance parameter. The mathematical form of the Powell Model is given by

$$\mu = \frac{\mu_{max} + p}{\frac{k_s}{S} + 1} - p, \tag{3}$$

where μ represents the specific growth rate and S is the substrate concentration at time t. μ_{max} is the maximum growth rate. The constant k_s is the half saturation constant and p is called the Powell cell maintain parameter. The Powell model does not consider substrate inhibition, hence it finds difficulties in describing the lag phase and the death phase [16].

Webb [17] introduced a model in 1963 to study microbial growth. In this model the specific growth rate is represented as a function of substrate concentration. The characteristics of the Webb model is that it represents the inhibition effect properly. This model is an extension of the Haldane model. The mathematical form of the Webb model is given by

$$\mu = \frac{\mu_{max} S\left(1 + \frac{S}{k_i}\right)}{S + k_s + \frac{S^2}{k_i}}, \tag{4}$$

where μ is the specific growth rate, S is the substrate concentration, μ_{max} is the maximum growth rate, k_i is the inhibition constant and k_s is half saturation constant. Putting $\lambda = \frac{1}{k_i}$ the Webb model can be written in the form

$$\frac{1}{\mu} = \frac{k_S}{\mu_{\max}(S + \lambda S^2)} + \frac{1}{\mu_{max}}. \tag{5}$$

MATERIALS AND METHODS

The five new methods are based on arbitrary points and partial sums which are obtained from the data set. The idea is taken from Borah and Mahanta [18]. The mathematical formulation of the new methods is explained along with each model separately. The performance of the models is analyzed by using a selection criterion given in the section of Selection Criteria for the best fit model. A standard data set representing the growth of Escherichia coli [10] is used in this study. The data set contains bacterial growth rate and substrate concentration of a culture of Escherichia coli bacteria which is presented in Table

Methods of Estimation

Haldane model

Method I

Let S_1, S_2 and S_3 be three arbitrary data points representing substrate concentration and μ_1, μ_2 and μ_3 be the corresponding specific growth rate in the data set. Then from the Haldane model we can write the three equations,

$$\mu_1 = \frac{\mu_{max} S_1}{k_s + S_1 + \frac{S_1^2}{k_i}}, \tag{6}$$

Table 1. Bacterial growth rate data of Escherichia Coli.

S(1/h)	5.1	8.3	13.3	20.3	30.4	37	43.1	58	74.5	96.5	112	161	195	266	386
μ(mg/L)	.059	.091	.124	.177	.241	.302	.358	.425	.485	.546	61	.662	.725	.792	.852

$$\mu_2 = \frac{\mu_{max} S_2}{k_s + S_2 + \frac{S_2^2}{k_i}}, \tag{7}$$

$$\mu_3 = \frac{\mu_{max} S_3}{k_s + S_3 + \frac{S_3^2}{k_i}}. \tag{8}$$

By solving the equations (6), (7) and (8) the parameters are estimated as

$$\mu_{max} = \frac{\mu_1 S_1 \mu_2 \mu_3 (S_3^2 - S_2^2) + \mu_1 \mu_2 \mu_3 S_2 S_3 (S_2 - S_3) - \mu_1 S_1^2 \mu_2 \mu_3 (S_3 - S_2)}{S_1 \mu_2 \mu_3 (S_3^2 - S_2^2) + \mu_1 S_2 S_3 (\mu_2 S_2 - \mu_3 S_3) - \mu_1 S_1^2 (S_3 \mu_2 - S_2 \mu_3)},$$

$$k_s = \frac{S_1 \mu_2 \mu_3 S_2 S_3 (S_2 - S_3) - \mu_1 S_1 S_2 S_3 (S_2 \mu_2 - S_3 \mu_3) - \mu_1 S_1^2 S_2 S_3 (\mu_3 - \mu_2)}{S_1 \mu_2 \mu_3 (S_3^2 - S_2^2) + \mu_1 S_2 S_3 (\mu_2 S_2 - \mu_3 S_3) - \mu_1 S_1^2 (S_3 \mu_2 - S_2 \mu_3)},$$

$$k_i = \frac{S_1 \mu_2 \mu_3 (S_3^2 - S_2^2) + \mu_1 S_2 S_3 (\mu_2 S_2 - \mu_3 S_3) - \mu_1 S_1^2 (S_3 \mu_2 - S_2 \mu_3)}{S_1 \mu_2 \mu \mu_3 (S_2 - S_3) + \mu_1 S_2 S_3 (\mu_3 - \mu_2) + \mu_1 S_1 (\mu_2 \mu_3 - \mu_3 S_2)}.$$

Method II

Let us consider two arbitrary data points S_1 and S_2 representing substrate concentration of the data set. Suppose μ_1 and μ_2 be the corresponding specific growth rate in the data set. Form the Haldane model we can write the two equations,

$$\mu_1 = \frac{\mu_{max} S_1}{k_s + S_1 + \frac{S_1^2}{k_i}}, \tag{9}$$

$$\mu_2 = \frac{\mu_{m\mu ax} S_2}{k_s + S_2 + \frac{S_2^2}{k_i}}. \tag{10}$$

Assuming the parameter k_s as known from Method I. Then by solving the equations (9) and (10) we can estimate the other two parameters as

$$\mu_{max} = \frac{\mu_1 S_1^2 (k_s \mu_2 + \mu_2 S_2) - \mu_2 S_2^2 (k_s \mu_1 - \mu_1 S_1)}{S_2 \mu_1 S_1^2 - S_1 \mu_2 S_2^2},$$

$$k_i = \frac{S_2 \mu_1 S_1^2 - S_1 \mu_2 S_2^2}{S_1 (k_s \mu_2 + \mu_2 S_2) - S_2 (k_s \mu_1 - \mu_1 S_1)}.$$

Method III

Let the total n points of the data set be divided into three equal parts. Let $r = \left[\frac{n}{3}\right]$. The first partial sum is obtained from the data set which contains 1^{st} to r^{th} data point, the second partial sum is calculated from $(r+1)^{th}$ to $2r^{th}$ data point and the third partial sum is obtained from $(2r+1)^{th}$ to n^{th} observation of the data set. Then we can write the three equations from the Haldane model, as

$$\mu_{max} \sum_{i=1}^{r} S_i - k_s \sum_{i=1}^{r} \mu_i - \left(\frac{1}{k_i}\right) \sum_{i=1}^{r} \mu_i S_i^2 = \sum_{i=1}^{r} \mu_i S_i, \tag{11}$$

$$\mu_{max} \sum_{i=r+1}^{2r} S_i - k_s \sum_{i=r+1}^{2r} \mu_i - \left(\frac{1}{k_i}\right) \sum_{i=r+1}^{2r} \mu_i S_i^2 = \sum_{i=r+1}^{2r} \mu_i S_i, \tag{12}$$

$$\mu_{max} \sum_{i=2r+1}^{n} S_i - k_s \sum_{i=2r+1}^{n} \mu_i - \left(\frac{1}{K_i}\right) \sum_{i=2r+1}^{n} \mu_i S_i^2 = \sum_{i=2r+1}^{n} \mu_i S_i. \tag{13}$$

Considering,

$$\sum_{i=1}^{r} S_i = A_1;\ \sum_{i=r+1}^{2r} S_i = A_2;\ \sum_{i=2r+1}^{n} S_i = A_3,$$

$$\sum_{i=1}^{r} \mu_i = B_1;\ \sum_{i=r+1}^{2r} \mu_i = B_2;\ \sum_{i=2r+1}^{n} \mu_i = B_3,$$

$$\sum_{i=1}^{r} \mu_i S_i^2 = C_1;\quad \sum_{i=r+1}^{2r} \mu_i S_i^2 = C_2,$$

$$\sum_{i=2r+1}^{n} \mu_i S_i^2 = C_3;\ \sum_{i=1}^{r} \mu_i S_i = D_1,$$

$$\sum_{i=r+1}^{2r} \mu_i S_i = D_2;\quad \sum_{i=2r}^{n} \mu_i S_i = D_3.$$

Then the equations (11), (12) and (13) become

$$\mu_{max} A_1 - k_s B_1 - \left(\frac{1}{k_i}\right) C_1 = D_1, \tag{14}$$

$$\mu_{max} A_2 - k_s B_{21} - \left(\frac{1}{k_i}\right) C_2 = D_2, \tag{15}$$

$$\mu_{max} A_3 - k_s B_3 - \left(\frac{1}{k_i}\right) C_3 = D_3, \tag{16}$$

By solving the equations (14), (15) and (16) the parameters are estimated as

$$\mu_{max} = \frac{D_1 (B_2 C_3 - B_3 C_2) + B_1 (D_3 C_2 - D_2 C_3) - C_1 (D_3 B_2 - D_2 B_3)}{A_1 (B_2 C_3 - B_3 C_2) + B_1 (A_3 C_2 - A_2 C_3) - C_1 (A_3 B_2 - A_2 B_3)},$$

$$k_s = \frac{A_1 (D_3 C_2 - D_2 C_3) - D_1 (A_3 C_2 - A_2 C_3) - C_1 (A_2 D_3 - A_3 D_2)}{A_1 (B_2 C_3 - B_3 C_2) + B_1 (A_3 C_2 - A_2 C_3) - C_1 (A_3 B_2 - A_2 B_3)},$$

$$k_i = \frac{A_1 (B_2 C_3 - B_3 C_2) + B_1 (A_3 C_2 - A_2 C_3) - C_1 (A_3 B_2 - A_2 B_3)}{A_1 (D_2 B_2 - D_3 B_2) + B_1 (A_2 D_3 - A_3 D_2) + D_1 (A_3 B_2 - A_2 B_3)}.$$

Method IV

Let us divide the total n points of the data set into two equal parts. Let $r = \left[\frac{n}{2}\right]$. The first partial sum is calculated using the data points from 1^{st} to r^{th} observations, the second partial sum is calculated from $(r+1)^{th}$ to n^{th} observations of the data set. Then from the Haldane model we can have, the two equations,

$$\mu_{max} \sum_{i=1}^{r} S_i - \left(\frac{1}{k_i}\right) \sum_{i=1}^{r} \mu_i S_i^2 = k_s \sum_{i=1}^{r} \mu_i + \sum_{i=1}^{r} \mu_i S_i, \tag{17}$$

$$\mu_{max} \sum_{i=r+1}^{n} S_i - \left(\frac{1}{k_i}\right) \sum_{i=r+1}^{n} \mu_i S_i^2 = \sum_{i=r+1}^{n} \mu_i + \sum_{i=r+1}^{n} \mu_i S_i. \tag{18}$$

Considering,

$$\sum_{i=1}^{r} S_i = A_1;\quad \sum_{i=r+1}^{n} S_i = A_2,$$

$$\sum_{i=1}^{r} \mu_i = B_1;\quad \sum_{i=r+1}^{n} \mu_i = B_2,$$

$$\sum_{i=1}^{r} \mu_i S_i^2 = C_1 \quad \sum_{i=r+1}^{n} \mu_i S_i^2 = C_2,$$

$$\sum_{i=1}^{r} \mu_i S_i = D_1;\quad \sum_{i=r+1}^{n} \mu_i S_i = D_2.$$

Now assume that the parameter k_s as known from Method III. Then by solving the equations (17) and (18) the parameters are estimated as,

$$\mu_{max} = \frac{C_1(k_sB_2+D_2)-C_2(k_sB_1+D_1)}{A_2C_1-A_1C_2},$$

$$k_i = \frac{A_2C_1-A_1C_2}{A_1(k_sB_2+D_2)-A_2(k_sB_1+D_1)}\ .$$

Method V

In this method, the Haldane model is linearized with some suitable parameterization. After having the linear form, the method of least square [19] is used to estimate the parameters. The linear form of the Haldane model is given by, $y = (ax^2 + bx + c)$,

where $y = \frac{S}{\mu}, x = s, a = \frac{1}{k_i\mu_{max}}, b = \frac{1}{\mu_{max}}$ and $c = \frac{k_s}{\mu_{max}}$.

Powell Model

Method I

Let S_1, S_2 and S_3 be three arbitrary data points representing substrate concentration and μ_1, μ_2 and μ_3 be the corresponding specific growth rate in the data set. Then from the Powell Model can be write the three equations,

$$\mu_{max}S_1 - k_s(p+\mu_1) = \mu_1S_1, \tag{19}$$

$$\mu_{max}S_2 - k_s(p+\mu_2) = \mu_2S_2\,, \tag{20}$$

$$\mu_{max}S_3 - k_s(p+\mu_3) = \mu_3S_3\,. \tag{21}$$

By solving the equations (19), (20) and (21) we estimate the parameters as

$$\mu_{max} = \frac{\mu_1S_1(\mu_3-\mu_2)+\mu_2\mu_3(S_3-S_2)-\mu_1(\mu_3S_3-\mu_2S_2)}{S_1(\mu_3-\mu_2)+(S_3\mu_2-S_2\mu_3)-\mu_1(S_3-S_2)},$$

$$k_s = \frac{S_1(\mu_2S_2-\mu_3S_3)+S_2S_3(\mu_3-\mu_2)+\mu_1S_1(S_3-S_2)}{S_1(\mu_3-\mu_2)+(S_3\mu_2-S_2\mu_3)-\mu_1(S_3-S_2)},$$

$$p = \frac{S_1\mu_2\mu_3(S_3-S_2)-\mu_1S_1(\mu_2S_3-\mu_3S_2)-\mu_1S_2S_3(\mu_3-\mu_2)}{S_1(\mu_2S_2-\mu_3S_3)+S_2S_3(\mu_3-\mu_2)+\mu_1S_1(S_3-S_2)}.$$

Method II

Let S_1 and S_2 be two arbitrary data points and μ_1 and μ_2 be the corresponding specific growth rate. Then from the Powell Model we can write the two equations

$$k_s(p+\mu_1) = \mu_{max}S_1 - \mu_1S_1, \tag{22}$$

$$k_s(p+\mu_2) = \mu_{max}S_2 - \mu_2S_2\,. \tag{23}$$

Assuming k_s as a known parameter from method I and solving the equations (22) and (23) the other parameters are estimated as

$$\mu_{max} = \frac{k_s\mu_1+\mu_1S_1-k_s\mu_2+\mu_2S_2}{S_1-S_2},$$

$$p = \frac{\mu_{max}S_1-\mu_1S_1-k_s\mu_1}{k_s}.$$

Method III

Suppose there are n points in the data set. Divide the data points into three equal parts. Let $r = \left[\frac{n}{3}\right]$. The first partial sum is obtained from the first part of the data set which contains 1^{st} to r^{th} data point, the second partial sum is calculated from the second part containing $(r+1)^{th}$ to $2r^{th}$ data point and the third partial sum is obtained from $(2r+1)^{th}$ to n^{th} observation of the data set. Then from the Powell model, we can write the three equations,

$$\mu_{max}\sum_{i=1}^{r} S_i - \sum_{i=1}^{r}(pk_s) - k_s\sum_{i=1}^{r}\mu_i = \sum_{i=1}^{r}\mu_iS_i, \tag{24}$$

$$\mu_{max}\sum_{i=r+1}^{2r} S_i - \sum_{i=r+1}^{2r}(pk_s) - k_s\sum_{i=r+1}^{2r}\mu_i = \sum_{i=r+1}^{2r}\mu_iS_i, \tag{25}$$

$$\mu_{max}\sum_{i=2r+1}^{n} S_i - \sum_{i=2r+1}^{n}(pk_s) - k_s\sum_{i=2r+1}^{n}\mu_i = \sum_{i=2r+1}^{n}\mu_iS_i. \tag{26}$$

Considering,

$$\sum_{i=1}^{r} S_i = A_1\ ;\ \sum_{i=r+1}^{2r} S_i = A_2\ ;\ \sum_{i=2r+1}^{n} S_i = A_3,$$

$$\sum_{i=1}^{r} \mu_i = B_1\ ;\ \sum_{i=r+1}^{2r} \mu_i = B_2\ ;\ \sum_{i=2r+1}^{n} \mu_i = B_3,$$

$$\sum_{i=1}^{r} \mu_iS_i = C_1;\ \sum_{i=r+1}^{2r} \mu_iS_i = C_2\ ;\ \sum_{i=2r}^{n} \mu_iS_i = C_3.$$

By solving the equations (24), (25) and (26) the parameters are estimated as

$$\mu_{max} = \frac{C_1(B_3-B_2)+(B_2-C_3)-B_1(C_3-C_2)}{A_1(B_3-B_2)+(A_3B_2-A_2B_3)-B_1(A_3-A_2)},$$

$$k_s = \frac{A_1(C_2-C_3)+(A_2C_3-A_3C_2)+C_1(A_3-A_2)}{A_1(B_3-B_2)+(A_3B_2-A_2B_3)-B_1(A_3-A_2)},$$

$$p = \frac{A_1(C_3B_2-C_2B_3)-C_1(A_1B_2-A_2B_3)-B_1(A_2C_3-A_3C_2)}{r\{A_1(C_2-C_3)+(A_2C_3-A_3C_2)+C_1(A_3-A_2)\}}.$$

Method IV

Let us first divide the given data n points into two equal parts. Let $r = \left[\frac{n}{2}\right]$. The first partial sum is calculated using the first part containing 1^{st} to r^{th} data point, the second partial sum is derived using second part containing $(r+1)^{th}$ to n^{th} observation of the data set. Then from the Powell model we can have the following two equations,

$$\mu_{max}\sum_{i=1}^{r} S_i - \sum_{i=1}^{r}(pk_s) - k_s\sum_{i=1}^{r}\mu_i = \sum_{i=1}^{r}\mu_i S_i, \quad (27)$$

$$\mu_{max}\sum_{i=r+1}^{n} S_i - \sum_{i=r+1}^{n}(pk_s) - k_s\sum_{i=r+1}^{n}\mu_i = \sum_{i=r+1}^{n}\mu_i S_i\ . \quad (28)$$

Considering,

$$\sum_{i=1}^{r} S_i = A_1\ ;\ \sum_{i=r+1}^{n} S_i = A_2,$$

$$\sum_{i=1}^{r}\mu_i = B_1\quad ;\quad \sum_{i=r+1}^{n}\mu_i = B_2,$$

$$\sum_{i=1}^{r}\mu_i S_i = C_1\quad ;\quad \sum_{i=r+1}^{2r}\mu_i S_i = C_2,$$

and assuming k_s as a known from Method III, and solving the equations (27) and (28) the parameters are estimated as

$$\mu_{max} = \frac{k_s(B_1-B_2)+C_1-C_2}{A_1-A_2},$$

$$p = \frac{\mu_{max}A_1-C_1-k_sB_1}{rk_s}\ .$$

Method V

The Powell model can be linearized in the form $y = (cx + d)$ by assuming k_s as known from Method III and by putting $y = \mu$, $\frac{k_s}{S} = \frac{1}{x}$, $c = (\mu_{max} + p)$ and $d = -p$. After having the linear form, the method of least square [19] is used to estimate the parameters.

Moser Model

Method I

Consider two arbitrary data points S_1 and S_2 representing substrate concentrations with corresponding specific growth rate μ_1 and μ_2 of the used data set. Taking the natural log on both sides of the Moser model we have the two equations

$$\log k_s - m\log S_1\ = \log(\mu_{max}-\mu_1)\log\mu_1, \quad (29)$$

$$\log k_s - m\log S_2 = \log(\mu_{max}-\mu_2)\log\mu_2. \quad (30)$$

From the properties of the parameters of Moser Model, we come to know that the parameter μ_{max}defines the maximum specific growth rate. So, in this method we are considering the value of the parameter μ_{max} is the largest value of μ in the data set. Then by solving the equations (29) and (30), the other two parameters can be estimated as

$$m = \frac{\log(\mu_{max}-\mu_1)-\log\mu_1-\log(\mu_{max}-\mu_2)+\log\mu_2}{\log S_2-\log S_1},$$

$$k_s = \frac{\mu_{max}S_1^m-\mu_1S_1^m}{\mu_1}.$$

Method II

Let S_1 and S_2 be two arbitrary data points and μ_1 and μ_2 be the corresponding specific growth rate. The Moser model can be written as

$$\mu_{max}S_1^m - k_s\mu_1 = \mu_1S_1^m, \quad (31)$$

$$\mu_{max}S_2^m - k_s\mu_2 = \mu_2S_2^m. \quad (32)$$

Assuming m as a known parameters from Method I and then by solving (31) and (32) we can estimate μ_{max} and k_s as

$$\mu_{max} = \frac{\mu_1\mu_2S_2^m-\mu_1\mu_2S_1^m}{\mu_1S_2^m-\mu_2S_1^m},$$

$$k_s = \frac{S_1^mS_2^m\mu_2-S_1^mS_2^m\mu_1}{\mu_1S_2^m-\mu_2S_1^m}.$$

Method III

Let the total observations n of the data set be divided into two equal groups. Let $r = \left[\frac{n}{2}\right]$. The first partial sums contain 1^{st} to r^{th} observation, the second partial sums contain $(r+1)^{th}$ to n^{th} observation. Taking the natural log on both sides of the Moser model we get the following three equations,

$$\log k_s - m\log S\ = \log(\mu_{max}-\mu) - \log\mu, \quad (33)$$

$$\sum_1^r\log k_s - m\sum_1^r\log S_i = \sum_1^r\log(\mu_{max}-\mu_i) - \sum_1^r\log\mu_i, \quad (34)$$

$$\sum_{r+1}^n\log k_s - m\sum_{r+1}^n\log S_i = \sum_{r+1}^n\log(\mu_{max}-\mu_i) - \sum_{r+1}^n\log\mu_i. \quad (35)$$

Assuming μ_{max} as a known parameter from Method II, and solving the equations (34) and (35) we can estimate the parameters as

$$m = \frac{\sum_1^r\log(\mu_{max}-\mu_i)-\sum_1^r\log\mu_i-\sum_{r+1}^n\log(\mu_{max}-\mu_i)+\sum_{r+1}^n\log\mu_i}{\sum_{r+1}^n\log S_i-\sum_1^r\log S_i},$$

$$k_s = \exp\left(\frac{\sum_1^r\log(\mu_{max}-\mu_i)-\sum_1^r\log\mu_i+m\sum_1^r\log S_i}{r}\right).$$

Method IV

Suppose there are n points in the data set.

Let us divide the n points of data set into two equal parts. Let $r = \left[\frac{n}{2}\right]$. The first partial sum is obtained from the first part which contains first r^{th} observations and the second partial sum is obtained from the second part which contains $(r+1)^{th}$ to n^{th} observations of the data set. Then from the Moser model we can write the two equations,

$$\mu_{max}\sum_{i=1}^{r} S_i^m - K_s\sum_{i=1}^{r}\mu_i = \sum_{i=1}^{r}\mu_i S_i^m, \quad (36)$$

$$\mu_{max}\sum_{i=r+1}^{n} S_i^m - K_s\sum_{i=r+1}^{n}\mu_i = \sum_{i=r+1}^{n}\mu_i S_i^m. \quad (37)$$

Considering,

$$\sum_{i=1}^{r} S_i^m = A_1\,,\ \sum_{i=r+1}^{n} S_i^m = A_2\,, \sum_{i=1}^{r}\mu_i = B_1$$

$$\sum_{i=r+1}^{n}\mu_i = B_2\,.,\sum_{i=1}^{r}\mu_i S_i^m = C_1\,, \sum_{i=1}^{n}\mu_i S_i^m = C_2,$$

and assuming the parameter m as a known parameter from Method I and by solving the equations (36) and (37), we estimate the parameters

$$k_s = \frac{C_1A_2 - C_2A_1}{B_2A_1 - B_1A_2}\,,$$

$$\mu_{max} = \frac{k_sB_1 + C_1}{A_1}.$$

Method V

The Moser model can be linearized in the form $y = (ax + b)$ by considering the parameter m known from Method III and by substituting $y = \frac{1}{\mu}, x = \frac{1}{S^m}, a = \frac{k_s}{\mu_{max}}, b = \frac{1}{\mu_{max}}$. After having the linear form, the method of least square [10] is used to estimate the parameters.

Webb Model

Method I

Let S_1, S_2 and S_3 be three arbitrary data points representing substrate concentration and μ_1, μ_2 and μ_3 be the corresponding specific growth rate in the data set. Then from the Webb model we can have the three equations,

$$\frac{1}{\mu_1} = \frac{k_s}{\mu_{max}(S_1+\lambda S_1^2)} + \frac{1}{\mu_{max}}\,, \quad (38)$$

$$\frac{1}{\mu_2} = \frac{k_s}{\mu_{max}(S_2+\lambda S_2^2)} + \frac{1}{\mu_{max}}\,, \quad (39)$$

$$\frac{1}{\mu_3} = \frac{k_s}{\mu_{max}(S_3+\lambda S_3^2)} + \frac{1}{\mu_{max}}\,. \quad (40)$$

After simplification the above equations we have a quadratic equation in λ, which is

$$A\lambda^2 + B\lambda + C = 0, \quad (41)$$

Where,

$$A = \mu_3(\mu_2 - \mu_1)S_1^2(S_3^2 - S_2^2) - \mu_1(\mu_3 - \mu_2)S_3^2(S_2^2 - S_1^2),$$

$$B = \mu_3(\mu_2 - \mu_1)\{S_1^2(S_3^2 - S_2^2) + S_1^2(S_3 - S_2)\} - \mu_1(\mu_3 - \mu_2)\{S_3^2(S_2^2 - S_1^2) + S_3^2(S_2 - S_1)\}\,,$$

$$C = \mu_3(\mu_2 - \mu_1)S_1(S_3 - S_2) - \mu_1(\mu_3 - \mu_2)S_3(S_2 - S_1).$$

The real positive root of the quadratic equation (41) is considered as the estimated parameter $k_i = \frac{1}{\lambda}$.

To estimate the parameter k_s rewrite the equations (38) and (39) in the form

$$\mu_1(S_1 + k_s + \lambda S_1^2) = \mu_{max}(S_1 + \lambda S_1^2)\,, \quad (42)$$

$$\mu_2(S_2 + k_s + \lambda S_2^2) = \mu_{max}(S_2 + \lambda S_2^2)\,. \quad (43)$$

After simplification of the equations (42) and (43) the parameters are estimated as

$$k_s = \frac{\mu_2(S_2+\lambda S_2^2)(S_1+\lambda S_1^2) - \mu_1(S_1+\lambda S_1^2)(S_2+\lambda S_2^2)}{\mu_1(S_2+\lambda S_2^2) - \mu_2(S_1+\lambda S_1^2)}\,,$$

$$\mu_{max} = \frac{\mu_1(S_1 + k_s + \lambda S_1^2)}{S_1 + \lambda S_1^2}.$$

Method II

Let S_1 and S_2 be two arbitrary points of the data set which represent substrate concentration and μ_1, μ_2 the corresponding specific growth rate. Then from the Webb model we have,

$$\left(\frac{\mu_{max}}{\mu_1} - 1\right)(S_1 + \lambda S_1^2) = k_s, \quad (44)$$

$$\left(\frac{\mu_{max}}{\mu_2} - 1\right)(S_2 + \lambda S_2^2) = k_s. \quad (45)$$

From the properties of the parameters of Webb Model, we come to know that the parameter μ_{max} defines the maximum specific growth rate. So, in this method we are considering the value of the parameter μ_{max} is the largest value of μ in the data set. Also, by considering, $\left(\frac{\mu_{max}}{\mu_1} - 1\right) = A_1$, $\left(\frac{\mu_{max}}{\mu_2} - 1\right) = A_2$, the parameters λ and k_s are estimated as

$$\lambda = \frac{A_2S_2 - A_1S_1}{A_1S_1^2 - A_2S_2^2},$$

$$k_s = A_1(S_1 + \lambda S_1^2).$$

Method III

Let the total observations n of the data set be divided into two equal groups. Let $r = \left[\frac{n}{2}\right]$. The first partial sums contain 1^{st} to r^{th} observation, the second partial sums contain $(r + 1)^{th}$ to n^{th} observation of the data set. Then we have from the Webb model the two equations,

$$k_s\sum_{i=1}^{r}\mu_i = \mu_{max}\sum_{i=1}^{r}(S_i + \lambda S_i^2) - \sum_{i=1}^{r}\mu_i(S_i + \lambda S_i^2), \quad (46)$$

$$k_s\sum_{i=r+1}^{n}\mu_i = \mu_{max}\sum_{i=r+1}^{n}(S_i + \lambda S_i^2) - \sum_{i=r+1}^{n}\mu_i(S_i + \lambda S_i^2) \quad (47)$$

Considering,

$$\sum_{i=1}^{r} \mu_i = A_1, \sum_{i=r+1}^{2r} \mu_i = A_2$$

$$\sum_{i=1}^{r} \sum_{i=1}^{r} (S_i + \lambda S_i^2) = B_1,$$

$$\sum_{i=r+1}^{2r} (S_i + \lambda S_i^2) = B_2$$

$$\sum_{i=1}^{r} \sum_{i=1}^{r} \mu_i (S_i + \lambda S_i^2) = C_1,$$

$$\sum_{i=r+1}^{2r} \mu_i (S_i + \lambda S_i^2) = C_2 .$$

Then equations (46) and (47) reduce to

$$k_s A_1 = \mu_{max} B_1 - C_1, \quad (48)$$

$$k_s A_2 = \mu_{max} B_2 - C_2. \quad (49)$$

Assuming $k_i = \frac{1}{\lambda}$ as a known parameter from method II and solving equations (48) and (49) the parameters k_s and μ_{max} are estimated as

$$\mu_{max} = \frac{C_1 A_2 - C_2 A_1}{A_2 B_1 - B_2 A_1},$$

$$k_s = \frac{\mu_{max} B_1 - C_1}{A_1}.$$

Method IV

Let the total observations n of the data set be divided in to two equal parts. Let $r = \left[\frac{n}{2}\right]$. The first partial sums contain the 1^{st} to r^{th} observations, the second partial sums contain $(r + 1)^{th}$ to n^{th} point of the data set. Then from the Webb model we can write the two equations,

$$k_s \sum_{i=1}^{r} \mu_i + \lambda\left(\sum_{i=1}^{r} \mu_i S_i^2 - \mu_{max} S_i^2\right) = \mu_{max} \sum_{i=1}^{r} S_i - \sum_{i=1}^{r} \mu_i S_i, \quad (50)$$

$$k_s \sum_{i=r+1}^{n} \mu_i + \lambda\left(\sum_{i=r+1}^{n} \mu_i S_i^2 - \mu_{max} S_i^2\right) = \mu_{max} \sum_{i=r+1}^{n} S_i - \sum_{i=r+1}^{n} \mu_i S_i . \quad (51)$$

From the properties of the parameters of Webb Model, we come to know that the parameter μ_{max} defines the maximum specific growth rate. So, in this method we are considering the value of the parameter μ_{max} is the largest value of μ in the data set. Also, by considering

$$\sum_{i=1}^{r} \mu_i = A_1, \ \sum_{i=r+1}^{n} \mu_i = A_2,$$

$$\left(\sum_{i=1}^{r} \mu_i S_i^2 - \mu_{max} S_i^2\right) = B_1,$$

$$\left(\sum_{i=r+1}^{n} \mu_i S_i^2 - \mu_{max} S_i^2\right) = B_2,$$

$$\mu_{max} \sum_{i=1}^{r} S_i - \sum_{i=1}^{r} \mu_i S_i = C_1,$$

$$\mu_{max} \sum_{i=r+1}^{n} S_i - \sum_{i=r+1}^{n} \mu_i S_i = C_2,$$

and solving (50) and (51) we can estimate k_s and $\lambda = \frac{1}{K_i}$ as

$$k_s = \frac{C_1 B_2 - C_2 B_1}{A_1 B_2 - A_1 B_1},$$

$$k_i = \frac{A_1 B_2 - A_1 B_1}{A_1 C_2 - A_2 C_1}.$$

Method V

The Webb model is linearized in the form

$y = (px + q)$ by considering the parameter k_i known from Method II and by substituting $y = \frac{1}{\mu}, x = \frac{1}{S\left(1+\frac{S}{k_i}\right)}, p = \frac{k_s}{\mu_{max}}$, $q = \frac{1}{\mu_{max}}$. After having the linear form, the method of least square [19] is used to estimate the parameters.

SELECTION CRITERIA FOR THE BEST FIT MODEL

After fitting the growth models using the new methods of estimation, the best fit model is selected based on a selection criterion. The selection criteria are adopted from the paper [20] which consists of five distinct steps.

Step I: Logical Consistency test.

Step II: Chi-Square (χ^2) test.

Step III: Root Mean Square Error (RMSE) test.

Step IV: Coefficient of Determination (R^2) and Adjusted Coefficient of Determination (R_a^2) test.

Step V: Approximate R^2 for prediction (R_{pre}^2) test.

RESULTS AND DISCUSSION

The estimated parameters of the models and the values of χ^2, RMSE (Root Mean Square Error), R^2, R_a^2 and R_{pre}^2 for the five new methods are given in the Table 2.

In this study it is observed that the parameters of the Haldane model produce some unexpectedly large estimates for the methods I, II, and IV. Also, it is observed that, the method V for both the Powell and the Webb model produce unexpectedly small estimates of μ_{max} than the highest tabulated value of μ_{max}. Therefore, these methods are eliminated in step -1. Due to logically and biologically consistent values of the estimated parameters, the other methods for their respective growth models are promoted to the next step.

In step -2, it is observed that the calculated Chi-square (χ^2) are above 99.5% level of significance for all the methods with respect to the corresponding degrees of freedom associated with each candidate model.

In step-3, the top five methods are selected from all the methods and the candidate models by comparing the RMSE. The RMSE of the methods whose estimated values are less than or equal to 0.0170 (up to four digits after decimal sign) are considered in our study.

Table 2. Estimated parameters with the statistical analysis

Model	Method	Parameters					χ^2	$RMSE$	R_a^2	R^2 (In %)	R_{pre}^2 (In %)
		k_s	μ_{max}	k_i	m	p					
Haldane	I	92.7081	1.1316	4388.229			0.0166	0.0197	0.9929	99.3950	99.3036
	II	92.7081	1.2018	2496.271			0.0245	0.0262	0.9875	98.9313	98.9313
	III	145.3654	1.5251	771.468			0.0166	0.0248	0.9887	99.0383	98.7600
	IV	145.3654	0.9782	732.029			1.2154	0.1747	0.4468	52.5889	37.6748
	V	98.7702	1.1150	7100.315			0.0068	0.0122	0.9972	99.7662	99.7341
Powell	I	80.2710	1.0297			0.0027	0.0156	0.0170	0.9947	99.5506	99.5116
	II	80.2710	1.0297			0.0027	0.0156	0.0170	0.9947	99.5506	99.5116
	III	78.9884	1.0312			0.0292	0.0262	0.0133	0.9967	99.7220	99.6960
	IV	78.9884	1.0320			0.0245	0.0195	0.0128	0.9970	99.7430	99.7170
	V	78.9884	0.0206			1.0291	0.0148	0.0127	0.9970	99.7489	99.7219
Moser	I	103.6765	0.8520		1.1896		0.0556	0.0387	0.9727	97.6679	97.2094
	II	76.2564	1.1753		1.1896		0.01545	0.0185	0.9937	99.4669	99.3772
	III	60.8693	0.8520		0.9060		0.1335	0.0699	0.9113	92.4007	89.9835
	IV	146.833	0.9337		1.1896		0.01767	0.0155	0.9959	99.6246	99.5538
	V	95.6606	1.3428		0.9060		0.02325	0.0312	0.9823	98.4839	97.9424
Webb	I	34.9998	2.0518	27.5899			0.07374	0.0383	0.9733	97.7183	97.4991
	II	90.7722	0.8520	117.6560			0.01301	0.0174	0.9945	99.5296	99.3785
	III	89.3791	0.8771	117.6560			0.01260	0.0184	0.9938	99.4703	99.3418
	IV	96.1564	0.8520	75.3356			0.02299	0.0252	0.9893	99.0079	98.7717
	V	58.6506	0.6898	117.6560			0.1291	0.0724	0.9048	91.8434	88.5318

If the value of $R^2_{prediction}$ is r and the value of R^2 is m, then about r% of the variability could be expected from the model to explain in prediction of new observations. In step-4 in our study we considered only those methods having R^2 greater than 99%, R_a^2 above 0.99 and R_{pre}^2 above 99.7%.

After following all the steps of the selection criteria, it is concluded that the Powell model in case of method IV is the best fit among all the candidate models in our study.

All the eliminated methods along with the results are displayed through the shaded area in Table 2.

Several applications of the Haldane, Moser, Powell and the Webb model are available in the literature. Some of the application of these models using traditional parameter estimation methods and results obtained are highlighted and compared with our study.

The Haldane model was fitted satisfactorily by Mohanty [21] for a mixed microbial culture and estimated R^2 value as 74.4%. Krishnan [11] observed satisfactory fit of the Haldane model on his study of biodegradation kinetics of Azo dye mixture with estimated R^2 as 94.7%. The Moser model was fitted satisfactorily by Choi and Lee [22] on micro algal biomass production and estimated R^2 value as 95.7%. Ardestani [23] fitted the Moser model on growth of Pseudomonas putida and calculated R^2 as 91.3%. The Powell model was fitted satisfactorily by Mahanta [10] on Escherichia Coli with estimated R^2 value as 99.6%. Dutta [13] reported satisfactory fit of the Webb model on growth kinetics of Pseudomonas cepacian and estimated R^2 value as 93.3%.

In our study we have observed that these models are fitted satisfactorily to the growth data of Escherichia Coli while using the newly introduced estimation methods.

CONCLUSION

In general, the traditional estimation methods require more calculations and time. The newly developed methods are simple and require lesser amount of time to estimate the parameters and better results can be obtained.

In this study it is found that all the newly developed methods produce satisfactory results. The Powell model produces the best results with respect to method IV compared to the other models with estimated (χ^2) value 0.0195, RMSE value 0.0128, R^2 value 99.75%, R_a^2 value 0.9970 and R_{pre}^2 value as 99.72% . On the basis of the findings of this study we conclude that all these models as well as these new methods can be applied to study any microbial growth phenomenon in a comprehensive way.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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