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Transformations of some growth models widely used in gas production measurements

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Abstract A mathematical model is a tool used to obtain information about the behavior of a system. The mathematical models can be used to have a preliminary knowledge about the functioning of a system, reducing the product costs and improving the performance. In this study, the modified models of several existing models, Gompertz, Orskov, Logistic and Monomolecular were developed that basically divided gas production into two fractions, one arising from rapidly fermentable feed components and the other from slowly fermentable feed components. The aim of this study is related to how originally used models are converted into two fractions mentioned above. For this purpose, all steps of the transformations were given step by step.

Keywords Gas production, Mathematical models

Introduction

A mathematical model is a powerful tool used to get valuable knowledge about the behavior of a system by using a mathematical technique. However, the main purpose of using the mathematical models is to obtain a preliminary knowledge about the functioning of a system, reducing the product costs and improving the performance [1-2]. However, the mathematical models are collected under two classes: empirical and mechanistic models [3-4]. Empirical models contain with the parameters a, b, c, etc. Therefore, these models do not give an idea about the behavior of system, but they are used only to fit data points. Therefore, since the parameters of the empirical models do not contain any biological meaning. It is difficult to estimate their initial values. In other words, it is difficult to estimate start values for the parameters if they have no biological meaning. Since it is easy to estimate the initial values of the parameters of mechanistic model and it is possible to calculate in 95% confidence intervals. Therefore, the researchers prefer mechanistic models in their studies [3, 5]. Whereas mechanistic models describe the behavior of a system that also contain the parameters with biological meaning such as upper asymptote, representing total gas production y_∞, the value at the initial time, y_0, specific initial rapid early gas production rate μ_{0r}, specific initial the slower gas production rate μ_{0s}, the decay in specific rapid early gas production rate c_r, the decay in specific the slower gas production rate, c_s, etc. Mathematical models have been widely preferred in many disciplines such as economy, biology, chemistry and agriculture. Depending on the type of curve, the models used in these areas could be in forms which are linear, exponential, sigmoidal, logaritmic and etc. In agriculture, one of the widely used models is the model with logaritmic structure. Logaritmic models are considerably used in the studies of ruminant growth and gas production. The aim of this study is to discuss to how some of the models widely used in gas production are converted to mechanistic models which has biological meaning. In addition, more information on some new parameters of the models, namely, specific growth rate at the initial time, reached maximum value, fractional constants governing the decay and etc were also given.

Akbas [6] showed how the important parameters mentioned above in terms of growth for some growth models such as Logistic and Gompertz models may be obtained, but the equations of these parameters have not been integrated into the model. The aim of this study shows mathematically how the new parameters with biological meaning of the widely used four different logaritmic growth models which have empirical structures can be

integrated into the models. As a result, new mechanistic models that explain well the functioning of the system are obtained.

Materials and Methods

Applying Gompertz, Orskov, logistic and monomolecular models to gas production rate is assumed to be proportional to microbial activity, projected as gas production (y) with a proportionally parameter (μ) [7].

While dy/dt shows the gas production rate, the equation

$$\mu = \frac{dy/dt}{y} \qquad (1)$$

shows the specific gas production rate.

First of all, we need to change Gompertz, Orskov, logistic and monomolecular models from the classical form to the other form including the parameters with biological meaning, the gas production as t goes to infinity ($t \to \infty$), y_∞, the specific gas production at the initial time (t=0), μ_0, the decay in the specific gas production, c.

The modified models of several existing models, Gompertz, Orskov, logistic, and monomolecular were developed that basically divided gas production into two fractions, one arising from rapidly fermentable feed components and the other from slowly fermentable feed components.

A model having empirical form can define the curve very well, however it does not give any idea about the phases. To define these phases, the form of mechanistic model should be created by adding several parameters to empirical models using mathematical transformations [8]. As a result, these phases can be determined. It is possible to define these phases containing the parameters: upper asymptote, representing total gas production y_∞, the value at the initial time, y_0, specific initial rapid early gas production rate μ_{0r}, specific initial the slower gas production rate μ_{0s}, the decay in specific rapid early gas production rate c_r, the decay in specific the slower gas production rate, c_s.

There are many kinds of logaritmic models as empirical form. Four of the commonly models are given in table 1.

The following steps of the modification of these four models: Gompertz, Orskov, Logistic and Monomolecular are given;

Step 1: To obtain the specific gas production rate, the first derivatives of the function with respect to t are given in table 2, respectively.

Step 2: The specific gas production rate, μ, of the models used can be found by the formula $\left(\mu = \frac{dy/dt}{y}\right)$ in table 3.

Step 3: Specific initial gas production rate, μ_0, the parameters, b, a and gas production, y(t), of the models used in the study is given in table 4.

Step 4: The parameter, μ, is governed by a constant c describing the decay in specific gas production rate (caused by diminishing growth rate of microorganisms and increasing substrate as reflected in gas production) with specific initial gas production, μ_0, being the value of μ at t=0 in table 5.

Step 5: For getting better describing any data, especially for the samples that showed a rapid gas production during early stages of fermentation and slowly increasing asymtote: To obtain better fit, the parameter μ was modified and divided into two parts, one for rapid early gas production rates, μ_r, and one for the slower gas production rates, μ_s, and its own fractional decay constants, c_r for rapid early gas production and c_s for the slower gas production, respectively in table 6 for specific gas production rate (μ).

Step 6: Substituting the equations in table 6 into table 3 and integrating gives firstly table 7 for gas production (y) and then table 8 for the initial time gas production (y_0) and finally table 9 for the new equation of gas production (y) with y_0.

Step 7: As t goes to infinity, the gas production (y) is found with the asymptote y_∞ in table 10, it is more convenient to work with them.

Table 1: The models used

Models	Equation
1. Gompertz	y=aexp(-exp(b-ct))
2. Orskov	y=a+b(1-exp(-ct))
3. Logistic	y=a/(1+exp(b-ct))
4. Monomolecular	y= a(1-bexp(-ct))
y: gas production, exp:exponential	

Table 2: The first derivative of the models used in the study

Models	The First derivative (dy/dt)
1. Gompertz	acexp(b-ct)exp(-exp(b-ct))
2. Orskov	-bcexp(ct)
3. Logistic	acexp(b-ct)/(1+exp(b-ct))^2
4. Monomolecular	abcexp(-ct)

Table 3: The specific gas production rate of the models used in the study

Models	The specific gas production rate $\left(\mu = \frac{dy/dt}{y}\right)$
1. Gompertz	cexp(b-ct)
2. Orskov	-bcexp(ct)/(a+b(1-exp(ct)))
3. Logistic	cexp(b-ct)/(1+exp(b-ct))
4.Monomolecular	bcexp(-ct)/(1-bexp(-ct))

Table 4: Specific initial gas production rate, μ_0, the parameters b, a and gas production, y(t), of the models used in the study

Models	μ_0	b	a	y(t)
Gompertz	cexp(b)	$\ln(\mu_0 / c)$	y_∞	$y_\infty \exp(-\mu_0 \exp(-ct)/c)$
Orskov	bc/a	$a\mu_0 / c$	$cy_\infty / (c+\mu_0)$	$(cy_\infty / (c+\mu_0))(1+(\mu_0/c)(1-\exp(-ct)))$
Logistic	cexp(b)/(1+exp(b))	$\ln(\mu_0/(c-\mu_0))$	y_∞	$y_\infty / (1+\mu_0 \exp(-ct)/(c-\mu_0))$
Mono-molecular	bc/(1-b)	$\mu_0/(c+\mu_0)$	y_∞	$y_\infty(1-\mu_0 \exp(-ct)/(c+\mu_0))$

y_∞ : upper asymtote, representing total gas production

μ_0 ,the specific gas production rate the initial time (t=0); y_∞ , the gas production as t goes to infinity ($t \to \infty$); c, the decay in the specific gas production.

Table 5. Specific gas production rate μ , represented by μ_0 , specific initial gas production rate and c, the decay in specific gas production rate of the models used in the study

Models	μ
Gompertz	$\mu_0 \exp(-ct)$
Orskov	$\mu_0 c \exp(-ct)/(c+\mu_0-\mu_0 \exp(-ct))$
Logistic	$\mu_0 c \exp(-ct)/(c-\mu_0+\mu_0 \exp(-ct))$
Mono-molecular	$\mu_0 c \exp(-ct)/(c+\mu_0-\mu_0 \exp(-ct))$

Table 6: Specific gas production rate μ, represented by μ_{0r}, specific initial rapid early gas production rate, μ_{0s}, specific initial the slower gas production rate and c_r, the decay in specific rapid early gas production rate, c_s, the decay in specific the slower gas production rate, of the models used in the study ($\mu_{0r} > \mu_{0s}$ and $c_{0r} > c_{0s}$)

Models	μ
Gompertz	$\mu_{0r}\exp(-c_r t)+\mu_{0s}\exp(-c_s t)$
Orskov	$\mu_{0r}c_r\exp(-c_r t)/(c_r+\mu_{0r}-\mu_{0r}\exp(-c_r t))+\mu_{0s}c_s\exp(-c_s t)/(c_s+\mu_{0s}-\mu_{0s}\exp(-c_s t))$
Logistic	$\mu_{0r}c_r\exp(-c_r t)/(c_r-\mu_{0r}+\mu_{0r}\exp(-c_r t))+\mu_{0s}c_s\exp(-c_s t)/(c_s-\mu_{0s}+\mu_{0s}\exp(-c_s t))$
Mono-molecular	$\mu_{0r}c_r\exp(-c_r t)/(c_r+\mu_{0r}-\mu_{0r}\exp(-c_r t))+\mu_{0s}c_s\exp(-c_s t)/(c_s+\mu_{0s}-\mu_{0s}\exp(-c_s t))$

Table 7: Gas production y(t) represented by μ_{0r}, specific initial rapid early gas production rate, μ_{0s}, specific initial the slower gas production rate and c_r, the decay in specific rapid early gas production rate, c_s, the decay in specific the slower gas production rate, of the models used in the study ($\mu_{0r} > \mu_{0s}$ and $c_{0r} > c_{0s}$) (k_1, k_2, k_3, k_4 are constants of the models)

Models	y(t)
Gompertz	$\exp\left(\frac{-\mu_{0r}\exp(-c_r t)}{c_r}-\frac{\mu_{0s}\exp(-c_s t)}{c_s}\right).\exp(k_1)$
Orskov	$(c_r+\mu_{0r}-\mu_{0r}\exp(-c_r t))(c_s+\mu_{0s}-\mu_{0s}\exp(-c_s t))\exp(k_2)$
Logistic	$\frac{\exp(k_3)}{(c_r-\mu_{0r}+\mu_{0r}\exp(-c_r t))(c_s-\mu_{0s}+\mu_{0s}\exp(-c_s t))}$
Mono-molecular	$(c_r+\mu_{0r}-\mu_{0r}\exp(-c_r t))(c_s+\mu_{0s}-\mu_{0s}\exp(-c_s t))\exp(k_4)$

Table 8: The initial time gas production y_0 represented by μ_{0r}, specific initial rapid early gas production rate, μ_{0s}, specific initial the slower gas production rate and c_r, the decay in specific rapid early gas production rate, c_s, the decay in specific the slower gas production rate, of the models used in the study ($\mu_{0r} > \mu_{0s}$ and $c_{0r} > c_{0s}$) (k_1, k_2, k_3, k_4 are constants of the models)

Gompertz	$\exp\left(\frac{\mu_{0r}}{c_r}-\frac{\mu_{0s}}{c_s}\right).\exp(k_1)$
Orskov	$c_r c_s\exp(k_2)$
Logistic	$\frac{\exp(k_3)}{c_r c_s}$
Mono-molecular	$c_r c_s\exp(k_4)$

Table 9: Gas production y(t) with y_0, gas production at t=0, represented by μ_{0r}, specific initial rapid early gas production rate, μ_{0s}, specific initial the slower gas production rate and c_r, the decay in specific rapid early gas production rate, c_s, the decay in specific the slower gas production rate, of the models used in the study ($\mu_{0r} > \mu_{0s}$ and $c_{0r} > c_{0s}$)

Models	y(t)
Gompertz	$y_0 \exp(\frac{\mu_{0r}}{c_r}(1-\exp(-c_r t)) + \frac{\mu_{0s}}{c_s}(1-\exp(-c_s t)))$
Orskov	$\frac{y_0(c_r+\mu_{0r}-\mu_{0r}\exp(-c_r t))(c_s+\mu_{0s}-\mu_{0s}\exp(-c_s t))}{c_r c_s}$
Logistic	$\frac{y_0 c_r c_s}{(c_r-\mu_{0r}+\mu_{0r}\exp(-c_r t))(c_s-\mu_{0s}+\mu_{0s}\exp(-c_s t))}$
Mono-molecular	$\frac{y_0(c_r+\mu_{0r}-\mu_{0r}\exp(-c_r t))(c_s+\mu_{0s}-\mu_{0s}\exp(-c_s t))}{c_r c_s}$

Table 10: Gas production y(t) with y_∞, gas production at $t \to \infty$, represented by μ_{0r}, specific initial rapid early gas production rate, μ_{0s}, specific initial the slower gas production rate and c_r, the decay in specific rapid early gas production rate, c_s, the decay in specific the slower gas production rate, of the models used in the study ($\mu_{0r} > \mu_{0s}$ and $c_{0r} > c_{0s}$)

Models	y(t)
Gompertz	$y_\infty \exp(-\frac{\mu_{0r}}{c_r}\exp(-c_r t) - \frac{\mu_{0s}}{c_s}\exp(-c_s t))$
Orskov	$\frac{y_\infty(c_r+\mu_{0r}-\mu_{0r}\exp(-c_r t))(c_s+\mu_{0s}-\mu_{0s}\exp(-c_s t))}{(c_r+\mu_{0r})(c_s+\mu_{0s})}$
Logistic	$\frac{y_\infty(c_r-\mu_{0r})(c_s-\mu_{0s})}{(c_r-\mu_{0r}+\mu_{0r}\exp(-c_r t))(c_s-\mu_{0s}+\mu_{0s}\exp(-c_s t))}$
Mono-molecular	$\frac{y_\infty(c_r+\mu_{0r}-\mu_{0r}\exp(-c_r t))(c_s+\mu_{0s}-\mu_{0s}\exp(-c_s t))}{(c_r+\mu_{0r})(c_s+\mu_{0s})}$

Results

The first derivatives and the specific gas production rate of the models used in this study were presented in tables 2 and 3, respectively. The specific initial gas production rate, μ_0, the parameters, b, a and gas production of the models were presented in table 4. The specific gas production rate, μ, represented by μ_0, specific initial rapid early gas production rate and c, the decay in specific gas production rate of the models were represented in table 5. The specific gas production rate, μ, represented by μ_{0r}, specific initial rapid early gas production rate, μ_{0s}, specific initial the slower gas production rate, and c_r, the decay in specific rapid early gas production rate, c_s, the decay in specific the slower gas production rate, of the models were represented in table 6. The gas production y(t), represented by μ_{0r}, μ_{0s}, c_r, c_s and constants of the models, k_1, k_2, k_3, k_4, respectively were given in Table 7.

The gas production at the initial time (y_0), represented by μ_{0r}, μ_{0s}, c_r, c_s and constants of the models, k_1, k_2, k_3, k_4, respectively were given in table 8.

Then, the gas production y(t) with the initial time (y_0), represented by μ_{0r}, μ_{0s}, c_r and c_s were given in Table 9.

Finally, The gas production y(t) with y_∞, gas production at $t \to \infty$, represented by μ_{0r}, μ_{0s}, c_r and c_s were given in table 10.

Discussion

The first and second partial derivatives of the models are given in Tables 2 and 3, respectively. The first partial derivatives and the specific gas production rate are necessary not only to convert the model from the empirical form into mecanistic form, but also to find the values of parameters of the model in the algorithm of some computer programs [5,9]. Many authors such as Akbas and Oğuz [10]; Narinc et al. [11] described the time and values of the inflection point in different forms of the models of Gompertz and Richard in their studies. In addition, Sezer and Tarhan [12] conducted a similar study for the model of Richard to calculate the time and values of the inflection point in their studies.

The mechanistic models of the studied four empirical models are given in table 10. Similarly, to improve the effectiveness of the models Zwitering et al. [5] and France et al. [13] gave transformations from empirical models to mechanistic models in their studies. Moreover, Beuvink and Kogut [7] gave the transformations from table 1 to table 10 for Gompertz model. Beuvink and Kogut [7] reported that fitting of the modified Gompertz model in Table 10 resulted in residual mean squares (RMS) lower than or similar to Gompertz model fit, which was influenced by the fact that the Genstat computer program used the parameters of Gompertz model as starting values for modified Gompertz model and tried to lower RMS. Beuvink and Kogut [7] also reported that the modified Gompertz model gave a good description of the gas production curves obtained by incubation of different feedstuffs with buffered ruminal fluid. In addition, the other parameters from the modified models could give valuable additional information about ruminal degradation of feedstuffs [7].

The formulas of some mechanistic models were much longer than the formulas of the empirical models (table 10). Since all calculating processes for finding the parameters are made by using the package programs, the major factor limiting the use of a model is not related to the length of the model. It is related to the number of parameters [14, 5, 15]. Modified equation of each model seems like a long equation, but number of parameters in each equation just varied in the range of 3 to 5. The parameters of each model are biologically important to understand what they mean. Indeed, it is very important to know the meanings of the parameters in each model. When the meanings of the parameters are known, the model can easily fit in the data set. The models which have fewer number of parameters are easy to fit compared with the models with more number of parameters. Zwitering et al. [5] emphasized that in case of the model which has fewer number of parameters to define the data set, this model should be preferred to the model with more number of parameters. The reasons for this are that the models which has more number of parameters are difficult to fit compared with the model with fewer number of parameters and the parameters of the models which has more number of parameters have some correlations with each. However, France et al. [13] reported that the models which have fewer number of parameters may not give enough information about system. This situation should not be ignored. Therefore, When selecting a model, the researhers should take into account how much of the system is explained by the model and how the model agrees with the system. To do this, many researchers advice some statistical tests and criteria such as Akaike Information Criteria (AIC), Bayesian Information Criteria (BIC), Mean Square Error (MSE), Determination coefficient (R^2), Accuracy Factor (AF) and F-ratio test [1, 3, 4, 14, 16,17]. The comparison of the models is not given in this study.These criteria will help the researchers to model selection.

Some researchers generally do not know whether the studied model is mechanistic or empirical. Korkmaz and Uckardes [18] mentioned the recognition of this distinction. Moreover, the transformations from some of the important sigmoidal empirical models to mechanistic models were gradually given in their study. Similarly, transformations of gas production by using rapid early and the slower gas production rates with their own fractional decay constants were gradually given in this study.

Conclusion

In this study, it is shown step by step how to obtain the new models with the parameters which have biological meaning from the commonly used four different logistic growth models which have empirical structures. More information about the growth with the parameters of the new models will be obtained. Experimental data has not been employed since this work has been prepared in a theoretical manner. In other study, the similarities and differences of the new forms of the models can be investigated by using experimental data.

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