Numerical Study on Anaerobic Digestion of Fruit and Vegetable Waste: Biogas Generation

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Abstract. The study provides experimental results and numerical results concerning anaerobic digestion of fruit and vegetable waste. Experiments were carried out by using batch floating drum type digester without mixing and temperature setting. The retention time was 30 days. Numerical results based on Monod type model with influence of temperature is introduced. Initial value problems were analyzed numerically, while kinetic parameters were analyzed by using trial error methods. The numerical results for the first five days seems appropriate in comparison with the experimental outcomes. However, numerical results shows that the model is inappropriate for 30 days of fermentation. This leads to the conclusion that Monod type model is not suitable for describe the mixture degradation of fruit and vegetable waste and horse dung.

Keywords: Anaerobic digestion, monod model, numerical simulation
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INTRODUCTION

Anaerobic digestion is a biochemical process in which microorganisms break down the biodegradable material under the absence of oxygen. This process can be utilized for treating both organic solid and liquid waste [1]. It has become popular because of high treatment efficiency, methane-producing ability, and requiring less nutrients and energy than aerobic process, which is major importance to the global environment [2,3,4].
Anaerobic digestion systems are complex processes that unfortunately can be unstable. This is usually caused by some conditions such as feed overload, presence of inhibitors, a drop in pH, or inadequate temperature control [3,4]. These certainly limit the optimization of anaerobic digestions application. In order to overcome these problems, and to operate and design anaerobic digestion efficiently, appropriate mathematical models need to be developed [5]. Mathematical models can serve as a useful tools to deepen the understanding of complex anaerobic digestion systems. Fruit and vegetable waste contains easy biodegradable organic content, cellulose-poor and high moisture. Most of its waste is limited by methanogensis than by the hydrolysis. A major limitation of anaerobic digestion of fruit and vegetable waste is a rapid acidification of these wastes decreasing the pH in the reactor, and a larger volatile fatty acids production which inhibit the activity of methanogenic bacteria [1]. Some of authors buffered these waste by addition of sodium hydroxide solutions, pre-treated organic matter of fruit and vegetable waste at high temperature to increase the efficiency of their anaerobic digestion [6]. The high temperature process will allow for better hydrolysis of wastes, for better sanitation and for better removal of xenobiotics during the process [5]. Various models have been constructed to provide more knowledge about anaerobic digestion processes. They involve so many external parameters and complicated mathematical equations that require numerical formulation and experimental data to evaluate various parameters. They also require significant time in computation.
The main aim of the study is to obtain a model of the anaerobic digestion process that can be applied to a small or intermediate scale of bioreactor users, such as farmers who have limited resources, technicians or engineers and want to improve the performance of their bioreactor.

FIGURE 1. Biogas digester

ANAEROBIC DIGESTION STAGE

An anaerobic digestion process for production of methane consists of three primary stages. Those stages are used to illustrate the sequence of microbial events that occur during the digestion process and the production of methane. Those stages are hydrolysis, acid forming, and methanogenesis. [8]
An anaerobic digestion process proceeds efficiently if the degradation rates of all three stages are equal. If the first stage is inhibited, then the substrates for the second and third stages will be limited and methane production decreases. If the third stage is inhibited, the acids produced in the second stage accumulate. The inhibition of the third stage occurs because of an increase in acids and, consequently, loss of alkalinity and decreases in pH. The typical upsets of anaerobic digester occur because of inhibition of methane-forming bacteria in the third stage. [8]

1. Stage 1-Hydrolysis
   Hydrolysis is the splitting (lysis) of a compound with water [8]. The main components of organic matter are carbohydrates, fats, and proteins [7]. In this stage, undissolved compounds of carbohydrates, proteins, and fats are broken down into monomers (water-soluble fragments) by exoenzymes (hydrolase) of facultative and obligatorily anaerobic bacteria [9]. When cellulose is hydrolyzed in an anaerobic digester, molecules of soluble glucose are liberated. Cellulose is hydrolyzed by the hydrolytic bacterium Cellulomonas. The bacterium is able to hydrolyze cellulose because it processes the enzyme cellulase, which is capable of breaking the glycosidic bonds between the monomers [8]. The hydrolysis of carbohydrates takes place within a few hours, while the hydrolysis of proteins and lipids within few days. Lignocellulose and lignin are degraded only slowly and incompletely [9].
2. Stage 2-Acid Forming stage
   In the acid-forming stage, soluble compounds produced through hydrolysis or discharged into the medium inside the digester are degraded by a large diversity of facultative anaerobes and anaerobes through many fermentative process. The degradation of these compounds results in the production of carbon dioxide, hydrogen gas, alcohols, organic acids, some organic-nitrogen compounds, and some organic-sulfur compounds. Acetate is the principal organic acid or volatile acid used as a substrate by methane-forming bacteria. Carbon dioxide and hydrogen can be converted directly to acetate or methane.[8,9]
3. Stage 2-Methanogenesis stage
   In the methanogenic stage, methane is formed from acetate, carbon dioxide, and hydrogen gas. Methane is also formed from some other organic compounds. Therefore, all other fermentative products must be converted to compounds that can be used directly or indirectly by methane-forming bacteria.[8,9]

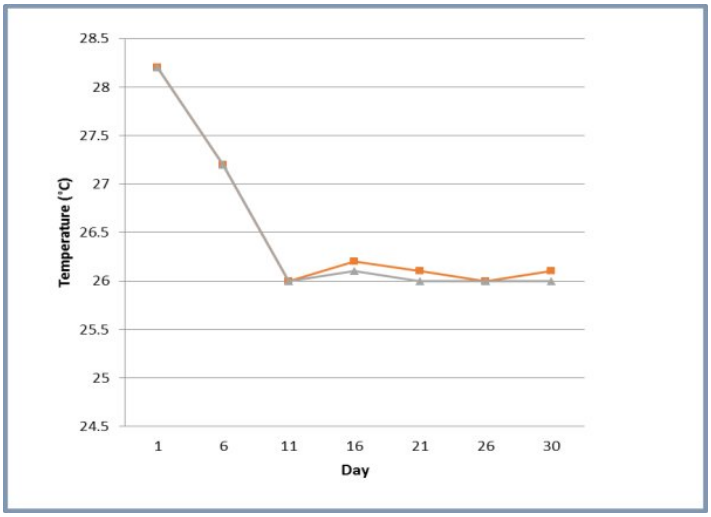

FIGURE 2. Temperature during experiment

MATERIAL METHODS

The experiment was carried out using a 50 Litres batch-floating drum type digester under ambient temperature (26-28^{o}C). Each digester was equipped with inlet and outlet for feeding and taking gas for analysis. The digester consist of 2 tanks, one tank for the substrate and the other for gas which is put inside 95 L drum filled with water. The batch-floating drum type digester was chosen because of convenience for biogas measurement. The aluminium digester was chosen as the reactor because of its nonflammability.
The substrate used in the experiment was fruit and vegetable waste from traditional markets in Padang, West Sumatra, Indonesia. Horse dungs were used as the inoculum for fermentation over 30 days. The total amount of fruit and vegetable waste and inoculum are 30 L. The amount of each fruit and vegetable waste and horse dung will be determined based on C/N content (equation 1).

$$C/N = \frac{CN_{FVW} x M_{FVW} + CN_{inc} x M_{inc}}{M_{FVW} + M_{inc}} \tag{1}$$

where CN_{FVW} is C/N content of fruit and vegetable waste, CN_{inc} is C/N content of inoculum (horse dung), M_{FVW} is mass of fruit and vegetable waste, and M_{inc} is mass of inoculum (horse dung).
The parameters measured were $C/H/N$, temperature, pH, biogas volume and biogas composition. C/N and total solids will be analysed in accordance with Standard Methods. Biogas production were measured using displacement method. Biogas composition (methane and carbon dioxide) were analyzed with adsorption methods.

MATHEMATICAL MODELING

The model proposed in this study consists of 3 stages of anaerobic digestion: Hydrolysis, Acid-Forming stage, and Methane forming stage.

Stage 1: Hydrolysis. Hydrolysis is the splitting (lysis) of a compound with water (hydro). In the anaerobic digester complex insoluble compounds such as particulate and colloidal wastes undergo hydrolysis. Particulate and colloidal wastes consist of carbohydrates, fats, and proteins [7].

Stage 2: Acid-Forming Stage. In the acid-forming stage, soluble compounds produced through hydrolysis or discharged to the digester are degraded by a large diversity of facultative anaerobes and anaerobes through many fermentative processes. The degradation of these compounds results in the production of carbon dioxide, hydrogen gas, alcohols, organic acids, some organic-nitrogen compounds, and some organic sulphur compounds [7].

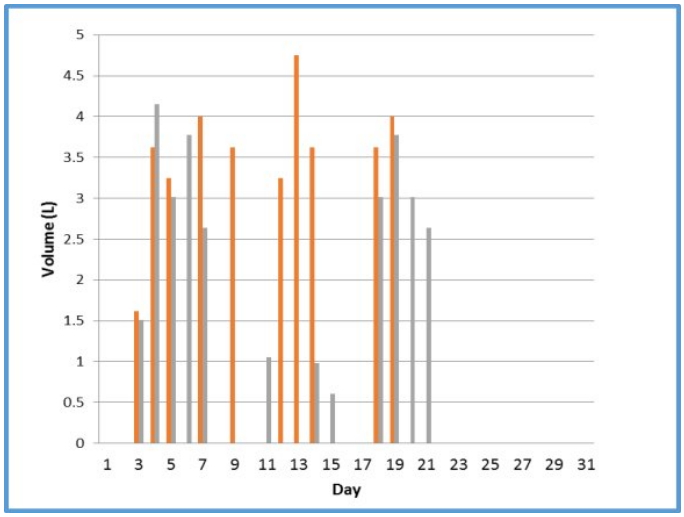

FIGURE 3. Biogas production (experimental data)

Stage 3: Methanogenesis Stage. In the methanogenic stage, methane is formed mostly from carbon dioxide and hydrogen gas[7].

The Monod equation was used to investigate the kinetics of anaerobic digestion of fruit and vegetable waste. The equation is given below.

$$\mu = \frac{\mu_{max}(T)}{1 + \frac{K_s}{S}} \tag{2}$$

where μ is maximum specific bacterial growth rate (g/l), K_s is substrate saturation constant (day^{-1}), S is soluble substrate concentration (g/l), and μ_{max}(T) is temperature dependent saturation growth rate (day^{-1}). The influence of temperature on bacterial growth is proposed in the study. The equation is expressed as [7]

$$\mu_{max}(T) = k_1 exp\frac{-E_1}{RT} - k_2 exp\frac{-E_2}{RT} \tag{3}$$

where k_1,k_2 are the rate constant (day^{-1}), E_1,E_2 are the activation energy constant (J mol^{-1}), T is temperature (^{o}K), and R is molar gas constant (J K^{-1} mol^{-1}). The first term of the right-hand side of the equation represents the common increase of the reaction rate due to temperature. The second term with typically higher activation energy corresponds to the fast decrease of the reaction rate above a certain temperature limit (rate of inactivation) [7].
The mass balance equations that describe substrate degradation, microbial growth, and product formation for batch reactor is described as [14]

$$\begin{aligned} \frac{dX}{dt} &= \mu X \\ \frac{dS}{dt} &= \frac{1}{Y}\mu X \\ \frac{dP}{dt} &= -Y\mu X \end{aligned} \tag{4}$$

where X is concentration of bacteria (g l^{-1}), S is substrate concentration (g l^{-1}), and P is concentration of product formation (g l^{-1}). By substituting eq. (2) and (3) into eq (4), the differential equations for biomass, substrate

TABLE 1. Results of parameter estimation

Parameters	Interval	Optimum value	Units
$E1$	[0.4-0.8]	0.533	J/mol
$E2$	[0.2-1.0]	0.467	J/mol
Ks	[0.01-50.0]	33.337	1/day
Yp	[0.1-10.0]	5.3	g microbial/g substrate
Y	[0.01-20.0]	13.337	g microbial/g substrate
$k1$	[0.1-1.0]	1.0	1/day
$k2$	[0.1-1.0]	1.0	1/day

degradation and product formation can be described as

$$\begin{aligned} \frac{dS}{dt} &= \frac{1}{Y}\frac{\mu_{max}(T)XS}{K_s+S}, \\ \frac{dX}{dt} &= \frac{\mu_{max}(T)XS}{K_s+S}, \\ \frac{dP}{dt} &= -\frac{Y_p\mu_{max}(T)XS}{K_s+S} \end{aligned} \tag{5}$$

where Y and Y_p are yield coefficient (g microbial/g substrate), μ_{max} is the maximum specific bacterial growth rate, X is microbial concentration (g/l), Ks is saturation constant, S is substrate concentration, and P is product formation rate (g/l). P represents the concentration of CH_4 and CO_2

$$\begin{aligned} \frac{dCH_4}{dt} &= -\frac{Y_p\mu_{max}(T)XS}{K_s+S}, \\ \frac{dCO_2}{dt} &= \frac{Y_p\mu_{max}(T)XS}{K_s+S} \end{aligned} \tag{6}$$

ANALYSIS METHODS

Initial value problems for proposed model (eq.5 and 6) were solved with Adams-Bashforth-Moulton Predictor-Corrector method in conjunction with the Runge-Kutta method to generate values of numerical solutions at the first three steps, while kinetic parameters were analyzed by trial-error methods.

The fourth-order Adams-Bashforth-Moulton predictor-corrector method is a fourth order method. That means that numerical values of the solution at previous four steps are used to generate the value at the new step. It is necessary to generate numerical values of the solution at the first three steps. The Runge-Kutta method was applied for that purpose [11][12].
In particular, there are eight parameters
$k_1 : [k1_{min}, k1_{max}]$
$k_2 : [k2_{min}, k2_{max}]$
$E_1 : [E1_{min}, E1_{max}]$
$E_2 : [E2_{min}, E2_{max}]$
$K_s : [Ks_{min}, Ks_{max}]$
$Y : [Y_{min}, Y_{max}]$
$Y_p : [Yp_{min}, Yp_{max}]$
An interval was set for each of those parameters. Each of those intervals were divided into 50 subintervals of equal length. The values of the parameters which minimizes the error.

$$\sqrt{(CH_4 experiment - CH_4(numerical results))^2 + (CO_2 experiment - CO_2(numerical results))^2} \tag{7}$$

was sought among the sets of the parameter values
$k_1 = k1_{min} + i\triangle k_1$

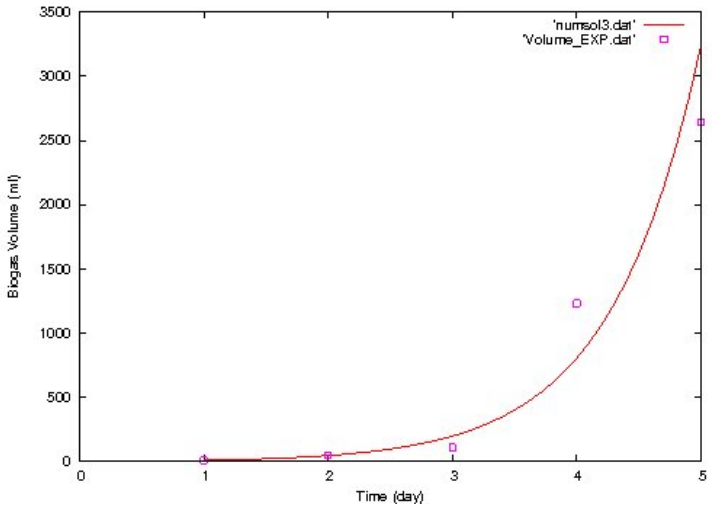

FIGURE 4. Comparison of biogas volume (line: simulation, dots: experiment)

$k_2 = k2_{min} + i\triangle k_2$
$E_1 = E1_{min} + i\triangle E_1$
$E_2 = E2_{min} + i\triangle E_2$
$K_s = Ks_{min} + i\triangle K_s$
$Y = Y_{min} + i\triangle Y$
$Y_p = Yp_{min} + i\triangle Y_p$
with i = 0,1,...,n
where

$$\begin{aligned}
\triangle k_1 &= \frac{k1_{max} - k1_{min}}{n}, \\
\triangle k_2 &= \frac{k2_{max} - k2_{min}}{n}, \\
\triangle E_1 &= \frac{E1_{max} - E1_{min}}{n}, \\
\triangle E_2 &= \frac{E2_{max} - E2_{min}}{n}, \\
\triangle Y &= \frac{Y_{max} - Y_{min}}{n}, \\
\triangle Y_p &= \frac{Yp_{max} - Yp_{min}}{n}, \\
\triangle K_s &= \frac{Ks_{max} - Ks_{min}}{n}
\end{aligned} \tag{8}$$

The initial value problem of equations (4) and (5) were solved numerically using the values of the parameters and the error between the experimental results and numerical results were evaluated. The interval used in parameters and the optimum value of the parameters are given in Table 1.

RESULTS AND DISCUSSION

The experiment used 50 L batch floating drum type digester without mixing under ambient temperature. In hydrolysis stage, the complex organic compounds degrade into simple compounds. The hydrolysis of carbohydrates took place within a few hours while the proteins and lipids within few days. The organic compounds that contain lignin will

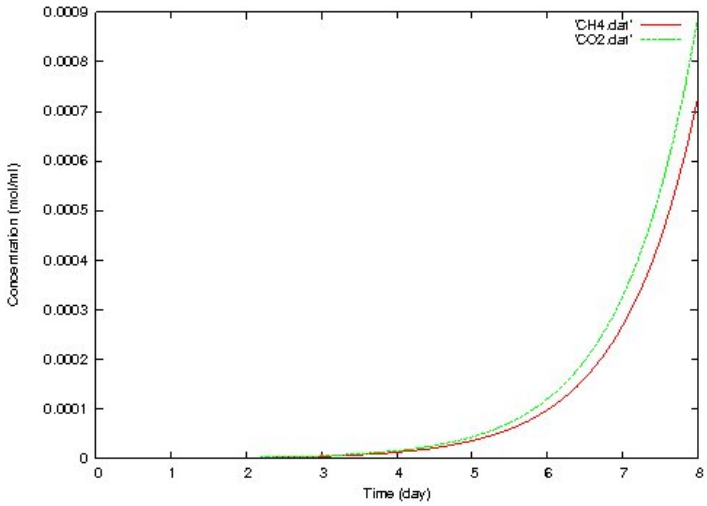

FIGURE 5. Simulation of methane and carbon dioxide concentration

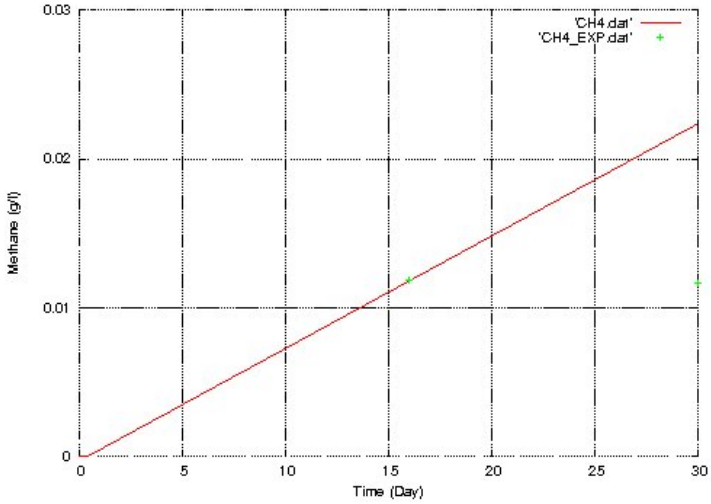

FIGURE 6. Comparison of methane concentration for 30 days (line: simulation, dots: experiment)

degrade slowly [9]. Fruit and vegetable waste contains easy biodegradable matter content and high moisture[9].
The biogas volume is shown in Fig. 2 [15][10][16]. It reached the maximum on day 19 and decreased until it stopped on day 30 [10]. The population of acidogenic and methanogenic bacteria were not balanced that because the regeneration of methanogenic bacteria is slower than acidogenic bacteria, which is 5-16 days [9]. This shows the products from acid stage were not used optimally to produce methane.
Temperature during the experiment was around 26-29^{o}C (Fig. 3) [10]. The change in temperature during experiment influences the biogas production and can cause the loose of biogas up to 30 percent [9]. It should be kept exactly within a range of +/- 2^{o}C [9]. It also important to maintain the temperature in optimal condition. The optimum temperature for methane bacteria is in the mesophilic range (32-42^{o}C) because most of methane bacteria belong to the mesophilics [9].
In order to fit the values of the proposed model with experimental values, equations (4) and (5) were solved numerically with Adams-Bashforth-Molton predictor-corrector methods in conjunction with the Runge-Kutta method to generate the values of the numerical solutions at the first three steps [15][16]. The coded model was to simulate biogas volume. Model fitting has been carried out by trial error methods explained in equations (9) and (10). The results are shown in Fig. 4, the models were shown to be satisfactory for simulating the biogas volume. The values of the parameters are

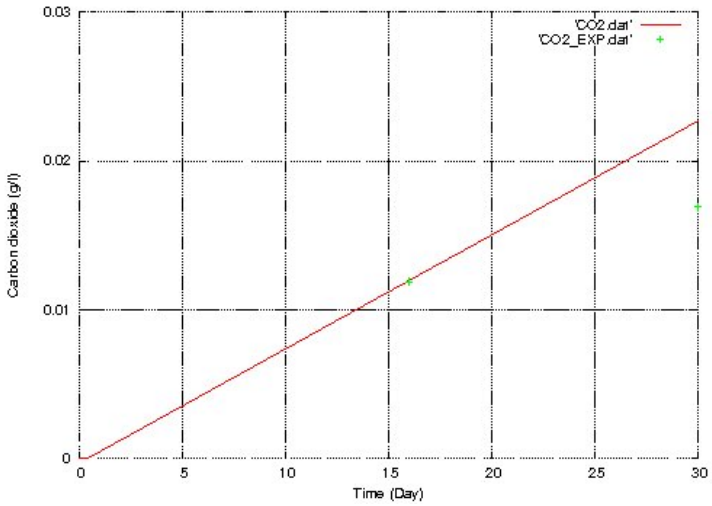

FIGURE 7. Comparison of carbon dioxide concentration for 30 days (line: simulation, dots: experiment))

shown in Table 1.
The simulation of methane and carbon dioxide concentration (methane and carbon dioxide) are shown in Figure 5. The results are likely not matches with the experimental results because in practice there is no reaction goes to full completion, and the model predicts ideal setting. This model needs an improvement in order to make the simulation more match with the experimental results.
The simulation of methane and carbon dioxide production and comparison with the experimental results are shown in Fig. 6 and Fig.7. The measurement of methane and carbon dioxide was done on day 16th and day 30th. It is shown that the numerical results does not match with the experimental results.

CONCLUSION

The simulation of biogas production is tested with the experimental results from anaerobic digestion of fruit and vegetable waste. The model consider the influence of temperature on bacterial growth. Monod model of bacterial growth rate was used to investigate the kinetics of anaerobic digestion. The equation (4) were solved numerically using Adams-Bashforth-Molton predictor-corrector methods in conjunction with the Runge-Kutta method to generate the values of the numerical solutions at the first three steps. The coded model was to simulate biogas volume. The numerical results for the first five days seems appropriate in comparison with the experimental outcomes. However, agreement between the numerical results and the experimental results is unsatisfactory for 30 days of fermentation. This shows experimental data are necessary to validate numerical results for a longer period. The disadvantage of this model is due to the lag phase which is not included in the Monod type model. The accuracy of the Monod model is very high for pure culture, but not appropriate for heterogeneous cultures or complex substrate [7]. This conclude that Monod type model is not suitable for describe the mixture degradation of fruit and vegetable waste and horse dung.

REFERENCES

1. H. Bouallagui, H. Lahdheb, E. Ben Romdan, B. Rachdi, and M. Hamdi, Improvement of fruit and vegetable waste anaerobic digestion performance and stability with co-substrates addition, *Journal of Environmental Management*, 90, 1844-1849, (2009).
2. Q. Wang, M. Kuninobu, H. I. Ogawa, and Y. Kato, Degradation of volatile fatty acids in highly efficient anaerobic digestion, *Biomass and Bioenergy*, 16, 407-416, (1999).
3. B. K. Ahring, Perspective for Anaerobic Digestion, *Advances in Biochemical Engineering/Biotechnology: Biomethanation I*, 81, 2-30, (2003).

4. Rittmann, E. Bruce, and P. L. McCarty, *Environmental Biotechnology: Principles and Applications*, McGraw-Hill, 2001 (McGraw-Hill series in water resources and environmental engineering. McGraw-Hill international editions, biological sciences series), ISBN 0071181849.
5. H. N. Gavala, I. Angelidaki, and B. K. Ahring, Kinetics and modeling of anaerobic digestion process, *Advances in Biochemical Engineering/Biotechnology*, 81, 57-93, (2003).
6. H. Bouallagui, Y. Touhami, R. B. Cheikh, and M. Hamdi, Bioreactor performance in anaerobic digestion of fruit and vegetable wastes, *Process Biochemistry*, 40, 989-995, (2005).
7. M. Gerber and R. Span, An analysis of available mathematical models for anaerobic digestion of organic substances for production of biogas, *International Gas Union Research Conference 2008*, Paris, October 8-10, 2008. Association Francaise du Gaz. Curran Associates, Inc. Vol. 2, 1294-1323 (2008).
8. M. H. Gerardi, *The microbiology of anaerobic digester*, A John Wiley and Sons, Inc., Publication, 2003, ISBN 978-0-471-20693-4.
9. D. Deublein and A. Steinhauser, *Biogas from waste and renewable resources*, A John Wiley and Sons, Inc., Publication, 2008, ISBN 978-3-527-31841-4.
10. P. K. Wardhani, Uji Pembentukan Biogas dari Sampah Sayur dan Buah dengan Penambahan Kotoran Kuda tanpa Pengkondisian Lingkungan Digester, Tugas Akhir. Universitas Andalas Padang, Indonesia, 2011.
11. J. D. Lambert, *Computational methods in ordinary differential equation*, John Wiley and Sons, 1977, ISBN 0-471-511943.
12. A. Ralston, *A first course in numerical analysis*, Int. Student ed. McGraw-Hill, 1965, NCID BA10359845.
13. J. H. Mathews and K. K. Fink, *Numerical methods using matlab, 4th Edition*, Prentice-Hall Inc, 2004, ISBN: 0-13-065248-2.
14. J. Srisertpol, P. Sinarkorn, A. Kheawnak, and K. Chamniprasart, Mathematical modeling and parameters estimation of an anaerobic digestion of shrimp of culture pond sediment in a biogas process, *International Journal of Energy and Environment*, Issue 4, Volume 4, pp. 213-220 (2010).
15. P. K. Wardhani and M. Watanabe, Numerical Simulation of Fruit and Vegetable Waste, Proceeding of *International Research Conference on Engineering and Technology*, pp. 666-673. ISBN 978-986-89844-6-2 (2014).
16. P. K. Wardhani, Modeling and Simulation of Biogas Production from Anaerobic Digestion of Fruit and Vegetable Waste, Thesis, Okayama University, 2014.