

# Numerical Study of Anaerobic Digestion Processes and Biogas Generation from Fruit and Vegetable Waste

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**Abstract** Batch experiments with fruit and vegetable waste and sludge from biogas plant as the feedstock were conducted in this study. Mathematical models are introduced here to explain the anaerobic processes, and some unknown parameters were determined by solving inverse problems numerically. Numerical results were compared with the experimental outcomes. We conclude that the results only show for situation where there is no inhibition by intermediate compounds such as volatile fatty acids.

**Keywords** Anaerobic Digestion, Kinetics, Inverse Problem, Mathematical Model, Numerical Simulation

## 1 Introduction

Solid wastes generated largely in traditional markets, include fruit and vegetable wastes that are mostly disposed in municipal landfill or dumping sites. Due to their nature and composition, they degrade rather quickly and cause a foul smell. In some fruit and vegetable waste (FVW) and food waste (FW) samples, the volatile solids (VS) content is 80% - 90%, and the water content is 75% - 95%. The high organic and water contents are the main cause of heavy odor and plenty of leachate during the collection, transportation and landfill of municipal solid waste (MSW). Considering the high moisture and organic content, those wastes are treated more effectively in biological treatment such as anaerobic digestion than other techniques such as incineration or composting [1].

Anaerobic digestion is a biochemical process in which microorganisms breakdown the biodegradable material into biogas (methane and carbon dioxide) under the absence of oxygen [2]. Those biochemical processes are very complex and difficult to operate into the optimum conditions because numerous parameters must be taken into consideration and be controlled [3]. Additionally, some parameters are difficult to estimate due to technical or economic constraints, i.e., the substrate consumption measurement is expensive, needs

three hours and to be done off-line [4]. In this respect, mathematical modeling and computer simulation are a good tool for these purposes.

Various mathematical models have been constructed for anaerobic digestion processes. Since the initial dynamic mathematical digester models in the late 1960s by Andrews JF (1968) and Graef SP (1974) [6], additional and more complex models have been developed to account for significant microbial interactions and inhibitions [5]. These models include additional processes with more detailed kinetics with inhibition and various kind of substrates. However, the task of achieving valid kinetic constants is difficult, due to its complex dynamic process that involves several groups of bacteria. The objective of the study reported here is to introduce simulations of anaerobic digestion of fruit and vegetable waste, and to determine some unknown parameters from the proposed mathematical models [14]. The simplifying model proposed by P. Sosnowski et al., [9] was applied to this study, in order to obtain a mathematical model simulating the exact conditions.

## 2 Materials and Methods

### 2.1 Substrate and Inoculum

The FVW as the substrate was collected from the local market, while inoculum was provided from biogas plant located in Tsuyama, Okayama, Japan. The sample consisted of bananas, potatoes, paprika, apples, broccoli, lettuce, cabbage, and cucumbers. The samples were prepared into small pieces using blender. The ratio between FVW and inoculum was 50:50, with initial condition of inoculum and substrate concentration was 0.107 g TS/L and 13 g COD/L, respectively.

### 2.2 Batch Digester Setup

Batch experiment was carried out using 2 L digester made of glass. The detail of digester setup is showed in Fig.1. The working volume was 1.8 L, inoculated with 0.9 L for each FVW and inoculum, respectively. The temperature was

maintained at 37°C with waterbath, and operated for 30 days. It was done in one-run experiment, and the experiment was terminated after reaching the end of gas production.

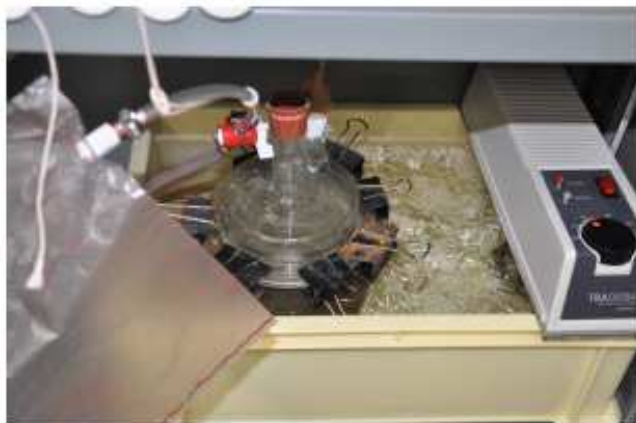


Figure 1. Batch Experiment with 2 L digester.

### 2.3 Analytical Methods

The following parameters were determined: elemental analysis (C,H,N), COD, TS, biogas volume, and concentration of  $CH_4$  and  $CO_2$  which were done every six days (day 3, day 9, day 15, day 21, and day 27). VFA (volatile fatty acid) was not measured during experiment, only determined by simulation. Biogas volume was measured by using displacement method. The elemental analysis, COD, TS, and concentration of  $CH_4$  and  $CO_2$  were carried out in accordance to Standard Methods.

For elemental analysis (C,H,N), The PerkinElmer 2400ii CHN Elemental Analyzer was used. Concentration of  $CH_4$  and  $CO_2$  were determined using gas chromatograph Shimadzu GC-8A1F equipped with a 6m x 2 stainless steel column (FID). The temperature of column was set to be 60°C. The gas sample was injected to the inlet for 500  $\mu$ L. Argon was used as the carrier gas.

## 3 Results

The whole feedstock collected has been analyzed before it put inside the digester. The high moisture content in the fruit and vegetable waste (89%) facilitates the anaerobic digestion process into optimum. CN ratio of the feedstock was 33.7:1. In fact, the ratio of CN in the feedstock should be in the range of 20:1-30:1, because bacteria use up carbon 25-30 times faster than they use nitrogen [7][12]. The experiment results of CN ratio showed that it is slightly higher than the optimal range. The optimal CN ratio in feedstock is important to anaerobic process. If it is too high, the nutrient deficiency for growth and reproduction of anaerobic bacteria may occur which will lead to biogas depletion [1][7].

### 3.1 Biogas Production

Anaerobic digestion processes of fruit and vegetable wastes were done for 30 days. The measurements of biogas volume, concentration and composition were done on day 3, 9, 15, 21, and 27. In the experiment biogas increased quickly at the beginning and reached maximum in the day three, while it decreased until reached zero in the end of gas production (Fig. 2). Figure 3 illustrates that methane and carbon dioxide generation was stable after day 21. Methane-producing bacteria have 14-day regeneration, so they need longer time to produce methane [3]. Fruit and vegetable wastes are rapidly degraded in the first stage and produce volatile fatty acids. It tends to inhibit methane-producing bacteria when the feedstock is not adequately buffered [10].

From Fig.2, Fig.3, and Fig.4 showed that concentration of methane during five days was low compared to the volume. This conditions show that during start-up phase, anaerobic condition was not fully reached. This phase should be proceed slowly until it stable in about one month. It is also important to fully maintain and monitor the condition of digester during this phase, such as temperature and pH, especially when the inoculum is not in a good condition [15].

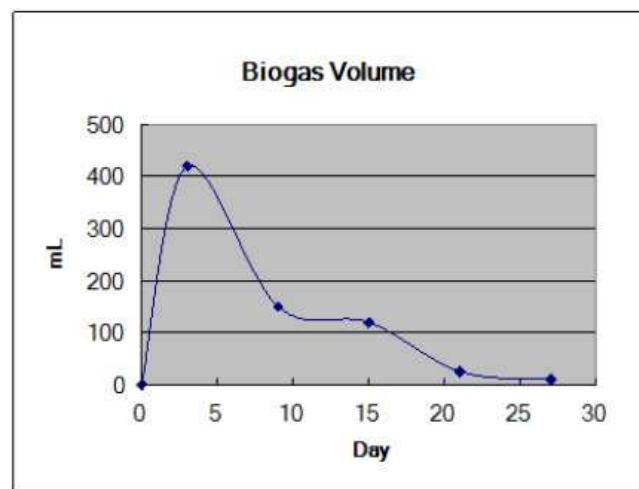


Figure 2. Biogas Volume.

The pH during anaerobic process was not maintained in order to accomplish an anaerobic processes without any interference. A major limitation of anaerobic digestion of FVW is the rapid acidification due to the lower pH of wastes and the larger production of VFA, which reduce the methanogenic activity of the reactor. These conditions were also confirmed in some investigations, where rapid acidification of wastes can lead to VFA accumulation, pH decrease and inhibit the production of biogas [7][10][13].

### 3.2 Kinetics of Anaerobic Digestion

The proposed model was based on the stages described in paper by P. Sosnowski et al., [9]. First stage, hydrolytic bacteria hydrolyzed the organic compounds into a simple soluble compounds and then into volatile fatty acids by acid-forming

bacteria. In the second stage, acetogenic bacteria lumped together with methanogenic bacteria converted products from previous stage into methane and carbon dioxide.

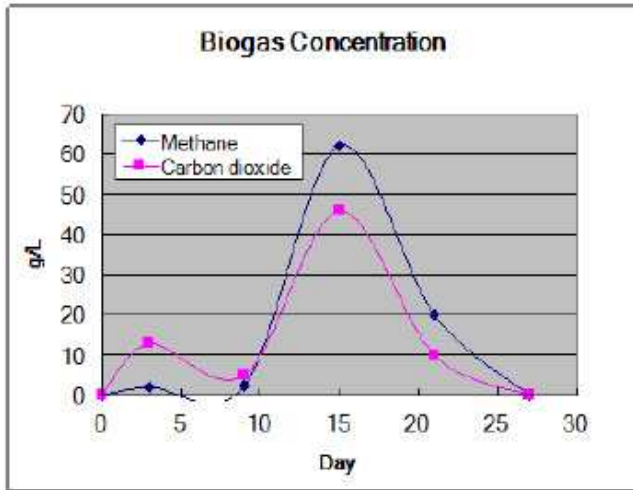


Figure 3. Biogas Concentration.

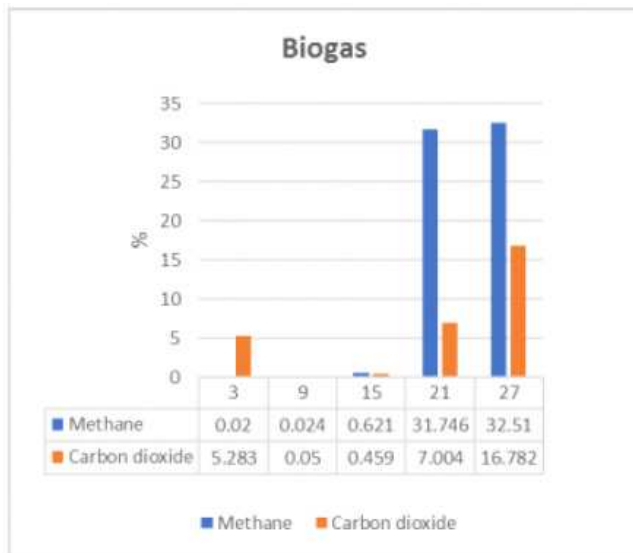


Figure 4. Biogas Composition.

The model included carbon dioxide formation both in hydrolysis and methanogenesis stages. The hydrolysis was described by the first-order kinetics. The methanogenesis was treated as Monod-like reaction. Those processes were described by the following system of differential equations:

$$\frac{dS}{dt} = -kS \quad (1)$$

$$\frac{dV}{dt} = Y_{VFA/S}kS - V_{VFA}X_0 \frac{VFA}{K_S + VFA} \quad (2)$$

$$\frac{dCH_4}{dt} = Y_{CH_4/VFA}V_{VFA}X_0 \frac{VFA}{K_S + VFA} \quad (3)$$

$$\frac{dCO_2}{dt} = Y_{CO_2/S}kS + Y_{CO_2/VFA}V_{VFA}X_0 \frac{VFA}{K_S + VFA} \quad (4)$$

where  $k$  is the constant of first-order kinetics ( $d^{-1}$ ),  $S$  is substrate concentration (g/L),  $VFA$  is volatile fatty acids concentration (g/L),  $Y_{VFA/S}$  is the yield factor of  $VFA$  from  $S$ ,  $V_{VFA}$  is the maximum specific utilization of  $VFA$  rate,  $K_S$  is the saturation constant (g/L),  $X_0$  is the biomass concentration (g/L),  $Y_{CH_4/VFA}$  is the yield factor of  $CH_4$  from  $VFA$ ,  $Y_{CO_2/S}$  is the yield factor of  $CO_2$  from  $S$ , and  $Y_{CO_2/VFA}$  is the yield factor of  $CO_2$  from  $VFA$ .

Initial value problems for proposed model (Eq.1-4) 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 PECE (Predictor-Evaluate Corrector-Evaluate) mode 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 [8][11]. In particular, there are five parameters.

$$\begin{aligned} k &: [k_{min}; k_{max}] \\ Y_{VFA/S} &: [Y_{vfamin}; Y_{vfamax}] \\ V_{VFA} &: [V_{vfamin}; V_{vfamax}] \\ Y_{CH_4/VFA} &: [Y_{ch4vmin}; Y_{ch4vmax}] \\ Y_{CO_2/VFA} &: [Y_{co2vmin}; Y_{co2vmax}] \end{aligned}$$

An interval was set for each of those parameters. Each of those intervals were divided into 10 subintervals of equal length. The values of the parameters which minimizes the error for all five experimental points for each methane and carbon dioxide:

$$\sqrt{(CH_4exp - CH_4num)^2 + (CO_2exp - CO_2num)^2} \quad (5)$$

It was sought among the sets of the parameter values

$$\begin{aligned} k &= k_{min} + i\Delta k \\ Y_{VFA/S} &= Y_{VFA/S} + i\Delta Y_{VFA/S} \\ V_{VFA} &= V_{VFA} + i\Delta V_{VFA} \\ Y_{CH_4/VFA} &= Y_{CH_4/VFA} + i\Delta Y_{CH_4/VFA} \\ Y_{CO_2/VFA} &= Y_{CO_2/VFA} + i\Delta Y_{CO_2/VFA} \end{aligned}$$

with  $i = 0, 1, \dots, n$

where

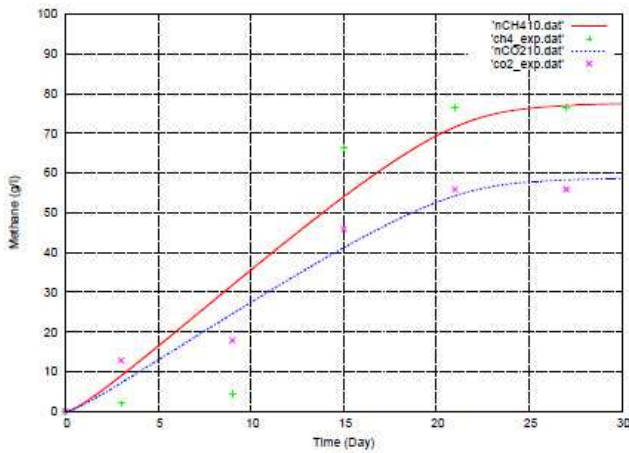
$$\begin{aligned}
\Delta k &= \frac{k_{max} - k_{min}}{n}, \\
\Delta Y_{VFA/S} &= \frac{Y_{vs_{max}} - Y_{vs_{min}}}{n}, \\
\Delta V_{VFA} &= \frac{V_{vfa_{max}} - V_{vfa_{min}}}{n}, \\
\Delta Y_{CH_4/VFA} &= \frac{Y_{ch4v_{max}} - Y_{ch4v_{min}}}{n}, \\
\Delta Y_{CO_2/VFA} &= \frac{Y_{co2v_{max}} - Y_{co2v_{min}}}{n},
\end{aligned} \quad (6)$$

for  $n = 12000$ . Results of parameter estimation are explained in Table 1.

**Table 1.** Description of Kinetics Parameter Used in the Model

Kinetics Parameters	Value	Unit
$k$	0.000208	$\text{day}^{-1}$ (* numerical)
$K_S$	11.25	$\text{g/l}$ (** [9])
$Y_{VFA/S}$	35.3	- (* numerical)
$Y_{CH_4/VFA}$	0.46	- (* numerical)
$V_{VFA}$	0.00307	$\text{day}^{-1}$ (* numerical)
$Y_{CO_2/S}$	0.29	- (** [9])
$Y_{CO_2/VFA}$	0.34	- (*)

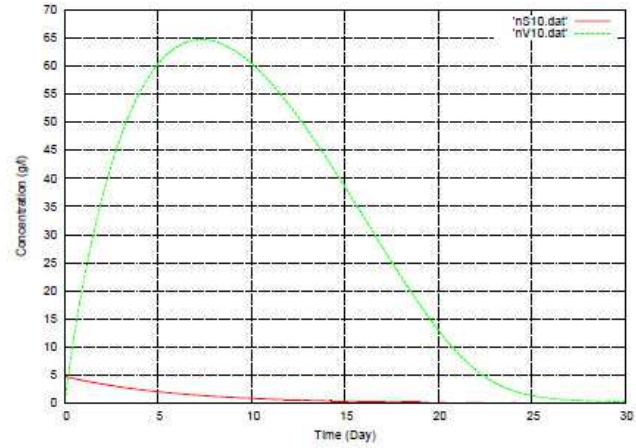
The comparison between experimental and simulation results for  $CH_4$  and  $CO_2$  concentration are shown in Fig. 5, while simulation results for concentration of substrate and volatile fatty acids are shown in Fig. 6, respectively. As stated before, FVW contains low cellulose, which can lead to a rapid acidification process. If it is not maintained properly, the pH digester will decrease and inhibit the methane bacteria [1].



**Figure 5.** Comparison between Numerical and Experimental. (line: simulation, dots: experimental.)

VFAs are produced as the end products of bacterial metabolism of protein, fat, and carbohydrate. These products are converted to methane by methanobacteria (methane-producing bacteria). The inhibition of methane bacteria can

lead to accumulation of VFA which decrease the pH further. Fig. 6 illustrates VFA degradation in ideal condition where there are no inhibitions. Anaerobic digestion processes without inhibitions mean the methanobacteria are able to convert all VFA to methane.



**Figure 6.** Degradation of Substrate (red) and Volatile Fatty Acid (green): Simulation.

Fig. 5 illustrates that the proposed model lack of fit with the experimental data. The generation of methane and carbon dioxide starts very slowly from the beginning of experiments, while the simulations show that it generates rapidly until it reaches maximum and then stops producing at the end of the process. The Monod kinetic proposed here is incapable of describing the anaerobic digestion processes under inhibitions.

## 4 Conclusions

Batch experiments were conducted in laboratory scale bioreactor with fruit and vegetable waste and sludge from biogas plants as the feedstock. It was found that the biogas production increased rapidly at the beginning of experiments until it decreased at the end of experiments, and the concentration of methane and carbon dioxide was stable after day 21. The experiment results also showed that the compositions of methane and carbon dioxide were low. Fruit and vegetable waste contains small amounts of cellulose, which caused rapid acidification and lead to the increase of volatile fatty acid and pH decrease. This may inhibit the production of methane. pH monitoring is need to be done in order to maintain the production of volatile fatty acid and prevent the digester failure.

The mathematical models introduced here can be a good tool to explain the whole anaerobic processes. However, Monod kinetics is incapable of describing the anaerobic digestion processes under inhibitions. Some investigations were introduced to explain kinetics of anaerobic digestion under inhibition [13] which can be considered in the future investigations.

Batch experiments are commonly used in anaerobic digestion process for kinetic parameter estimation. However, the main disadvantage of batch test for parameter estimation is the lack of input, since the only input is the initial condition. This can be mitigated by using different sets of initial condition [14].

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