

## Mathematical modeling for the prediction of biogas generation characteristics of a municipal solid waste anaerobic digester.

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### Abstract

*The dependence on fossil fuels as primary energy source has led to global climate change, environmental degradation, and human health problems. The process of anaerobic digestion has the potential of converting biodegradable organics into biogas which can serve as alternative source of energy to fossil fuel. In this study, the potential of biogas production was investigated using a batch fed anaerobic digester of 10L capacity operating at an optimum temperature of 40°C and at a pH of 6.8 using vegetable/food residues as the feed. The effects of slurry concentrations of carbohydrate, protein and fat in the slurry on the biogas production rate were examined. The slurry concentration was varied from 72.0-700 kgm<sup>-3</sup>. The effect of carbohydrate, protein and fat concentrations were studied by varying their ratios in the range of 6.9:4.3:1-12.1:4.3:1, 5.6:7.0:1-5.6:13.0:1 and 7.2:10:1.6-7.2:10:5 respectively. Rate of biogas generation was found to rise from 0 to 1.1 x 10<sup>13</sup> mol/dm<sup>3</sup>.week in the first 4 weeks. A deterministic mathematical model using differential system equations was developed for predicting the behaviour of the digester.*

### Nomenclature

|            |  |
|------------|--|
| Ks         | saturation constant (kg m <sup>-3</sup> )  |
| C          | concentration (kg m <sup>-3</sup> )  |
| Ki         | inhibition constants(kg m <sup>-3</sup> )  |
| X          | biomass concentration (kg m <sup>-3</sup> )  |
| μmax       | maximum specific growth rate (d <sup>-1</sup> )  |
| Y          | yield coefficients as kilogram material consumed or Produced/kilogram of biomass synthesized |
| HAc        | acetic acid  |
| HPr        | propionic acid   |
| Hbu        | butyric acid   |
| Hval       | valeric acid   |
| LCFA       | long chain fatty acid  |
| Sl         | slurry   |
| Carb       | carbohydrate   |
| Pr         | Protein  |
| Subscripts |  |
| I.         | related to acidogenic degradation of carbohydrate  |
| I.         | related to acidogenic degradation of amino acid  |
| II.        | related to acidogenic degradation of fat   |
| II.        | related to acetogenic degradation of propionic acid  |
| III.       | related to acetogenic degradation of butyric acid  |
| IV.        | related to acetogenic degradation of valeric acid  |
| V.         | related to acetogenic degradation of LCFA  |
| VI.        | related to acetoclastic degradation of acetic acid   |

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1. related to carbohydrate in acidogenic/acetogenic/acetoclastic steps
2. related to protein in acidogenic/acetogenic/acetoclastic steps
3. related to fat in acidogenic/acetogenic/acetoclastic steps
4. related to HAc in acidogenic/acetogenic/acetoclastic steps
5. related to HPr in acidogenic/acetogenic/acetoclastic steps
6. related to HBu in acidogenic/acetogenic/acetoclastic steps
7. related to HVal in acidogenic/acetogenic/acetoclastic steps
8. related to LCFA in acidogenic/acetogenic/acetoclastic steps
9. related to CO<sub>2</sub> in acidogenic/acetogenic/acetoclastic steps
10. related to NH<sub>3</sub> in acidogenic/acetogenic/acetoclastic steps
11. related to H<sub>2</sub>S in acidogenic/acetogenic/acetoclastic steps
12. related to CH<sub>4</sub> in acidogenic/acetogenic/acetoclastic steps
13. related to H<sub>2</sub>O in acidogenic/acetogenic/acetoclastic steps

**Keywords:** Biogas, Digester, Mathematical Model, Fermentation

## 1.0 Introduction

Biogas is produced by the process of anaerobic digestion of organic material by anaerobes. It can be produced either from biodegradable waste materials or by the use of energy crops fed into anaerobic digesters to supplement gas yields. Biogas plants produce methane gas sustainably along with carbon dioxide from biomass which may come from organic household or industrial waste or from specially grown energy plants [1]. The advantage of the biogas process is the option to use the polysaccharide constituents of plant material to produce energy, such as electrical power and heat, in relatively easy-to-manage and small industrial units. Alternatively, the gas can be compressed after purification and enrichment and then fed to the gas grid or used as a fuel in combustion engines or cars. Its greatest advantage is the environmentally friendly aspect of the technology which includes the potential for complete recycling of minerals, nutrients (phosphate etc) and fibre material (for humidification) which come from the fields and return to the soil, playing a functional role by sustaining the soils vitality for future plantation. The technology is currently mature, but there is plenty of room for optimization, which will result in large high-tech production plants with integrated utilization of by-products [2].

Substrate can be cow manure which is also useful for inoculation, manure from other farm animal such as pigs, chickens and horses, fat from slaughter waste or frying oil, organic household or garden waste, municipal solid waste and rotten foodstuff. Even organic waste from hospitals containing paper and cotton, municipal sewage sludge, waste from agriculture or food production, organic-rich industrial waste water etc. can be used as consumable substrate. Often, energy crops such as maize (whole plant including the corn), clover, grass, young poplar and willow are especially grown for biogas production and added purely or in mixture. To ensure a homogeneous substrate quality throughout the year, the green plant material is usually stored as silage, preferably by a process favouring homofermentative lactobacilli to minimize carbon loss [2]. Biogas formation from plant fibres is generally a four-stage process involving a different set of anaerobic and facultatively anaerobic microorganism in each stage:

1. Hydrolysis of polysaccharides (starch, cellulose, hemi-cellulose etc.), proteins and fats into oligosaccharides and sugars, fatty acids and glycerol.
2. Acidogenesis: the fermentation of these products into mainly acetic, propionic and butyric acid, carbon dioxide, hydrogen, alcohols and other minor compounds.
3. Acetogenesis: the production of acetic acid and carbon dioxide. Due to the long generation time of these bacteria this seems to be the limiting process step.
4. Methanogenesis with up to 70 % (v/v) CH<sub>4</sub> and 30 % CO<sub>2</sub> and the by-products NH<sub>3</sub> and H<sub>2</sub>S by slow-growing archaea, which are sensitive to acidification, ammonia accumulation, low amounts of oxygen and other factors.

The bacterial community engaged in these four stages may be similar to those in cows rumen [3] or in wastewater treatment plants [4]. However, their composition varies depending on the substrate, the type of fermenter and the process (e.g. mesophilic or thermophilic; [5-8]). Some bacteria involved have been isolated and characterized, but comprehensive studies on the biological system in pure plant biomass fermenting plants are still widely missing, especially on the hydrolytic and the thermophilic processes.

Traditional farm biogas plants are run as a single or two-stage process at around 37 °C with an uncontrolled secondary fermentation in large storage tanks. Due to different optional conditions specific for the hydrolytic and the methanogenic bacteria, two-stage processes are increasingly applied particularly in large industrial biogas plants. Most biogas fermentation tanks are run as liquid fermenters. The biogas fermentation tank may contain more than 12 % (w/v) dry mass (so-called dry fermentation) or less (liquid fermentation).

The German Renewable Energy Act (EEG) and a similar law in Austria has spurred the construction of 3500(G)+600(A) biogas plants with an average electrical power output of 500kW (and even more heat) in combined heat and power plant. Larger plants of 5 MW electrical power output are still rare, but will be constructed in increasing numbers. Their size is limited by land intensive production and the transportation costs for bulky substrate.

The large quantity of energy crops required for biogas production provoked discussions among environmentalists, especially in Germany, about the issues of monoculture and resulting soil deprivation. However, proper crop rotation and the recycling of materials, minerals and nutrients, can minimize these effects [9].

Further development of biogas technology is expected to increase production efficiency. Presently, only up to a maximum of about 70 % of the organic matter in biomass is converted to CH<sub>4</sub> and CO<sub>2</sub> in order for this to increase, the hydrolysis stage must be enhanced. The separation of the process for hydrolysis and for acetogenesis/methanogenesis allows for the application of different optimized conditions in the two stages, such as pH and temperature adjustment. The main aim of this study is to develop a mathematical model for the prediction of biogas generation characteristics of an anaerobic digester based on food/vegetable residues using suitable software.

## 2.0 Materials and Methods

### 2.1 Experimental set up and operation

A 10 L digester with a height to diameter ratio of 3:1 was used for the experimental studies. The digester was equipped with an external jacket and a mechanical stirrer. The digester was seeded with slurry containing feed materials in various solid concentration ranges. Before the start of each run, the bioreactor was inoculated with 10%(v/v) freshly prepared seed microorganisms cultured in the nutrient agar medium from the broth of a running biogas plant of Ramakrishna Mission Ashram, Narendrapur West Bengal, India. The working volume of the digester was kept at 8 L. Biogasification of Vegetable/food residues was carried out at mesophilic condition (40 °C) by circulating warm water from a constant temperature bath through the external jacket. The entire digester was properly thermally insulated. This working temperature was selected on the basis of the observation of its poor performance above and below this temperature. Once inoculated, the bioreactor was run at a stirrer speed of 50 rpm at a temperature of 40 °C. The system pH was adjusted intermittently during experimental runs. Biogas coming out of the digester was collected continuously in a sampling bottle by the downward displacement

of water and was analyzed by a gas chromatograph. To study the effect of carbohydrate, protein and fat individually on the rate of production and the composition of biogas, their concentrations were varied in the feed slurry by using their sole sources, namely sucrose, papain, vanaspati oil, respectively, keeping the concentration of natural constituents namely vegetable waste, oil cake and whey constant. The overall slurry concentration was varied by changing the amount of vegetable/food residues.

### 2.2 Mathematical analysis

To ensure a high degree of accuracy and numerical stability, the classical Runge-Kutta method of fourth-order was adopted.

During biogas generation a complex array of degradation reactions of carbohydrate, protein and fat take place. In the present investigation biodegradation reactions as outlined by Angelidaki et al [10] in his pioneering work on anaerobic cow dung digestion was selected for developing kinetic model equations. Since the concentration of carbohydrate, protein, and fat in the slurry is very high with respect to other constituents like inorganic salts, etc., this part has been considered to be constituted of carbohydrate, protein and fat only. Moreover while selecting the reaction mechanism the concept of enzymatic hydrolysis, acidogenic, acetogenic, aceticlastic steps of carbohydrate, protein, and fat have been considered as proposed by Angelidaki et al [10]. The data from Ojolo et al [11] was applied to the model in Equation 6 and this was solved using fourth-order Runge-Kutta method using a basis of 1 mole of biogas with the aid of FORTRAN.

The differential mass balance equations for different reacting components undergoing acidogenic, acetogenic and aceticlastic steps and the corresponding bacterial masses are as follows.

$$\frac{dc_n}{dt} = \sum_n \sum_j \frac{\mu_j X_j}{Y_{jn}} \quad (1)$$

$$\frac{dx_j}{dt} = \mu_j X_j \quad (2)$$

$$Y_{jn} = \left( \frac{(dx_j / dt)}{\pm (dc_n / dt)_j} \right) \quad (3)$$

j(I-VIII) are different acidogenic, acetogenic and aceticlastic reactions occurring during biogas generation.

In all cases 'n' indicates the substrate/product consumed or generated in the array of reactions. The values of n designated to different components are as follows.

Carbohydrate: n = 1; protein: n = 2; fat: n = 3; HAC: n = 4; HPr: n = 5; HBU: n = 6; HVal: n = 7; LCFA: n = 8; CO<sub>2</sub>: n = 9; NH<sub>3</sub>: n = 10; H<sub>2</sub>S: n = 11; CH<sub>4</sub>: n = 12; H<sub>2</sub>O: n = 13.

The initial values of different components for each experimental condition have been shown by Angelidaki et al (10).  $dc_n/dt$  used in the definition of Y, is positive when  $c_n$  is a product and negative when  $c_n$  is a substrate. Equations 1 to 3 was solved numerically using fourth-order Runge-Kutta method programmed in FORTRAN. The model constants and rate expressions necessary for the simulation work were obtained from Angelidaki et al (10).

**2.3 The General Mole Balance Equation**

To perform a mole balance on any system, the system boundaries must first be specified. The volume enclosed by these boundaries will be referred to as the system volume. A mole balance on species j in a system volume, where species j represents the particular chemical species of interest, in this case biogas will be performed .

A mole balance of species j at any instant in time(t), yields the following equation:

|               |   |                    |   |                 |   |                      |
|---------------|---|--------------------|---|-----------------|---|----------------------|
| Rate of flow  |   | rate of generation |   | rate of flow of |   | rate of accumulation |
| Of j into the | + | of j by chemical   | - | j out of the    | = | of j within the      |
| System        |   | reaction within    |   | system          |   |                      |
| (moles/time)  |   | the system         |   | (moles/time)    |   | (moles/time)         |
|               |   | (moles/time)       |   |                 |   |                      |

$$F_{j0} + G_j - F_j = \frac{dN_j}{dt} \tag{4}$$

Where  $N_j$  represents the number of moles of species j in the system at time t. If all the system variables (e.g temperature, catalytic activity, and concentration of the chemical species) are spatially uniform throughout the system volume, the rate of generation of species j,  $G_j$ , is just the product of the reaction volume  $V$ , and the rate of formation of species j,  $r_j$

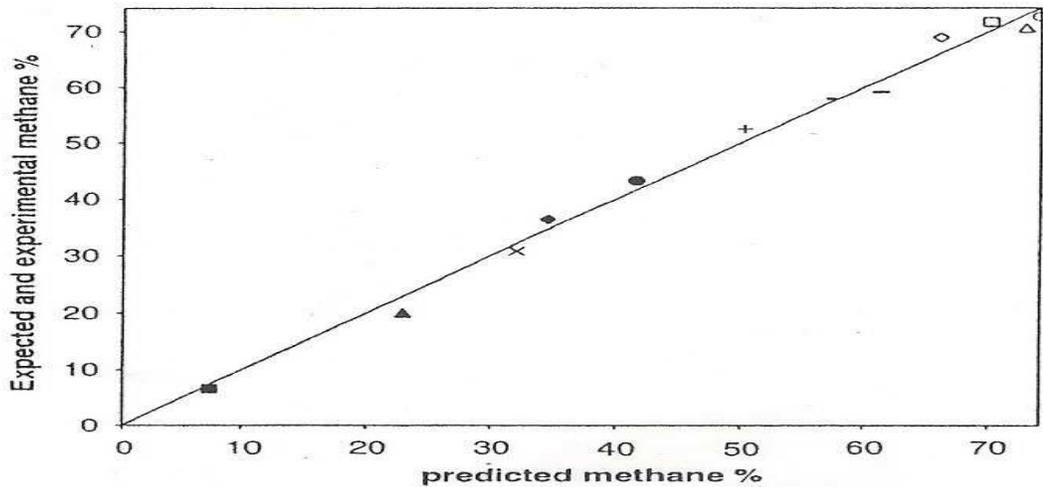
$$G_j = r_j V \tag{5}$$

**2.31 Batch Feed Digester (Batch Reactor)**

A batch reactor has neither inflow nor outflow of reactants or products while the reaction is being carried out;  $F_{j0} = F_j = 0$  [12]. The resulting general mole balance on species j is

$$\frac{dN_j}{dt} = r_j V$$

**3.0 Results and Discussion**



**Fig. 1** Assessment of scattering of experimental values of methane concentration in biogas on 15th day by comparison with the diagonal showing the plot of expected and predicted values when concentrations of slurry, carbohydrate, protein and fat are the parameters; □, Sl = 72 kg m<sup>-3</sup>, ▲, Sl = 300 kg m<sup>-3</sup>; ■, Sl = 700 kg m<sup>-3</sup>; ○, ratio of carb: Pr: fat = 6.9:4.3:1; —, ratio of carb: Pr: fat = 7.8:4.3:1; ×, ratio of carb: Pr: fat = 12.1:4.3:1; ◇, ratio of carb: Pr: fat = 5.6:7.0:1; +, ratio of carb: Pr: fat = 5.6:9.1:1; ◆, ratio of carb: Pr: fat = 5.6:13.0:1; —, ratio of carb: Pr: fat = 7.2:10:1.6; △, ratio of carb: Pr: fat = 7.2:10:2; ●, ratio of carb: Pr: fat = 7.2:10:5.

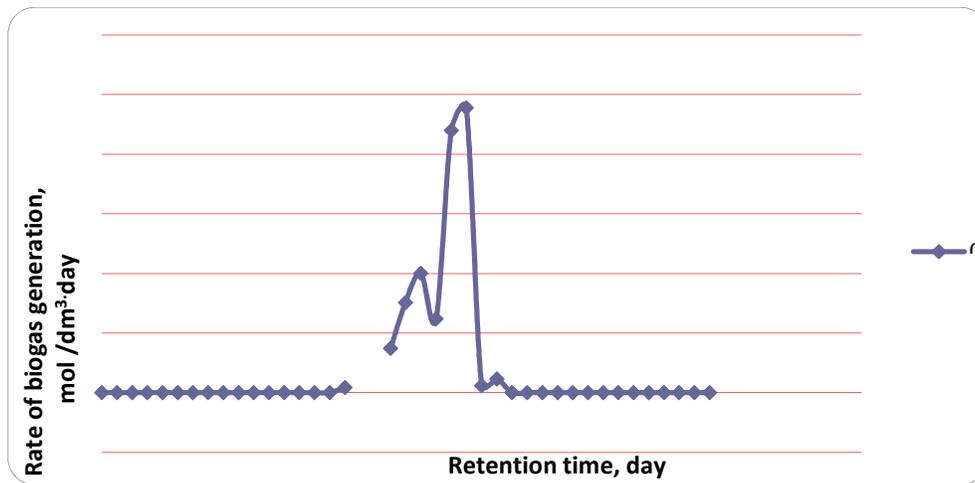


Figure 2: Profile of rate of biogas generation vs retention time

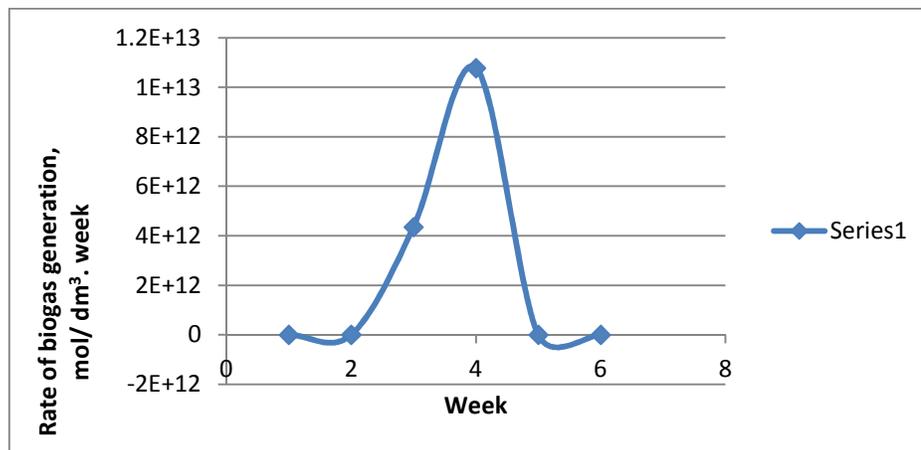


Figure 3: Profile of rate of biogas generation per week

To assess the validity of the model developed under the present investigation, in Figure1, the experimental results was compared with the simulated ones with reference to methane concentration in biogas with the variation in concentration of slurry, carbohydrate, protein and fat. In this Figure the expected values to be obtained under ideal conditions was plotted against the predicted values and the scattering of experimental values was observed.

In any bio-digester, effectiveness of the process is usually represented in terms of biogas generation rate. While assessing the effects of concentrations of slurry, carbohydrate and protein carbohydrate on biogas generation rate it is observed that the latter increases with increase in concentrations of respective parameters. This may be due to the production of larger volume of carbondioxide by the acidogenic bacteria in presence of increased quantity of respective substrates. It is also noticed that biogas generation rate is almost independent of the proportion of fat present in the system. This is possibly due to the fact that although increased quantity LCFA obtained through the lipolytic degradation of fat causes an increased methane production rate, the rate of production of other major constituent of biogas, ie. Carbon-dioxide, decreases as it is consumed simultaneously in the lipolytic degradation of fat as well as in the acetogenic degradation of LCFA. Thus due to these two antagonistic affects the overall production rate of biogas remains unaffected with respect to fat concentration.

Figures 2 and 3, shows lag-time of nine days before traces of biogas generation became observable. It was observed that the rate of biogas generation was at its peak on the 24<sup>th</sup> day of experimental period and more gas was produced in the fourth week.

## Conclusion

Mathematical modeling for the prediction of biogas generation characteristics of a municipal solid waste anaerobic digester was successfully developed and tested with experimental data. The validation of the model done with the aid of FORTRAN software. The experimental results were compared with the simulated ones with reference to methane concentration in biogas with the variation in concentration of slurry, carbohydrate, protein and fat. The comparison shows that the model can be used to predict biogas generation characteristics from municipal waste anaerobic digester to a large extent.

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