Available online at www.sciencedirect.com

ScienceDirect

Procedia Technology 24 (2016) 654 – 660

Procedia Technology

International Conference on Emerging Trends in Engineering, Science and Technology (ICETEST - 2015)

Mathematical Modeling and Simulation of Anaerobic Digestion of Solid Waste

Manjusha C[a], Sajeena Beevi.B[b*]

[a]*MTech student, Chemical Engineering Department, Government Engineering College Thrissur,* 680009 *Thrissur, India*
[b]*Assistant professor, Chemical Engineering Department, Government Engineering College Thrissur* 680009 *Thrissur, India*

Abstract

Waste management and energy crisis are the greatest issues that the world is facing today. This problem can be overcome by anaerobic digestion of solid waste, where the waste is converted to biogas: a mixture of mainly carbon dioxide and methane gas. Because of the growing need of anaerobic digestion of solid waste, increased efforts in reducing biogas plant design cost and optimizing process operation is crucial. One way of doing this can be through mathematical modeling of the anaerobic process. The purpose of this paper is to use the Anaerobic Digestion Model no.1 (ADM1), which gives complete information about the physico-chemical reactions in the anaerobic process, to investigate how different parameters in the model affect biogas production. A model was implemented in MATLAB and can be used to find out how the factors such as pH and Volatile Fatty Acid (VFA) affect the daily biogas production.

Peer-review under responsibility of the organizing committee of ICETEST – 2015

Keywords: Anaerobic digestion; Biogas; ADM1 matrix;

1. Introduction

Energy crisis and waste management are the major issues that the world is facing today. In order to overcome this problem, an efficient way of technology is needed. Organic fraction of solid waste is required to manage in such a way as to minimize the negative environmental impact, fewer hazards to human health and maintain ecological balance. Anaerobic digestion of solid waste is an effective technology that treats different types of organic waste.

* Corresponding author. Tel.: +91 9446317516; fax: + 0-487-2334590.
*E-mail address:*sajeenanazer@gmail.com

Peer-review under responsibility of the organizing committee of ICETEST – 2015
doi:10.1016/j.protcy.2016.05.174

The main advantages of anaerobic digestion of solid waste are in terms of energy, cost, and ecological balance, which make this technology much better than other conversion process [1]. Different types of systems are available for the treatment of solid waste through anaerobic digestion, such as batch process, continuous process, single stage and multi stage process. The anaerobic digestion is one of the innovative technologies in the field of waste treatment. There are several varieties of researches undergoing in the field of waste treatment. The main aim of these researches is to analyze the parameters that will affect the production of biogas. There are a number of factors that affect the production of biogas, such as pH, Volatile Fatty Acid, temperature, quantity of substrate being used, and alkalinity. The level of these factors must be in correct proportion in order to keep the production of biogas in a particular level. Anaerobic digestion of solid waste is limited in developing countries due to the lack of proper treatment systems. Designing of reactor and selection of operational criteria depend on substrate characteristics and cost.

The anaerobic digestion of solid waste has a lot of applications over other conversion techniques. However, each mode of operation always has its own advantages and disadvantages. The purpose of this study is to develop a mathematical modeling of anaerobic digestion of solid waste and optimize the environmental condition such as pH, Volatile Fatty Acid, temperature for increasing the biogas production in a shorter retention time. Dynamic modeling and simulation is increasingly being employed as an aid in the design and operation of waste treatment especially in Europe. But most developing countries like India are still following conventional design technique based on the static models or empirical formulae derived either from past pilot scale studies or from performance of already existing waste treatment plant elsewhere. A dynamic model can be a useful tool for the prediction of process performance in transient conditions and for a better understanding of the process and its optimal working conditions. The main objective is to develop a mathematical model for the batch study of anaerobic digestion of Organic Fraction of Municipal Solid Waste (OFMSW). To achieve this objective we are adapting the default ADM1 for modeling and simulation of anaerobic digestion of organic fraction of municipal solid waste and calibrating the model using lab scale data from the batch study.

2. Mathematical modelling and simulation of batch reactor

2.1. Anaerobic Digestion Model No1 (ADM1)

Because of the growing need in anaerobic digestion of solid waste, increased efforts in reducing biogas plant design cost and optimizing process operation is crucial. One way of doing this can be through mathematical modeling of the anaerobic process. This is a fact that has been recognized by researchers for a long time. Between the years 1972 and 2006 there have been about 750 publications concerning mathematical modeling of anaerobic digestion. But evaluating the merits of every scientific model on anaerobic digestion available would be a daunting task. Therefore, in recognizing both the great potential benefits of a functional model and the need of a more widely accepted mathematical description of the anaerobic process, the international water association (IWA) formed a task group aiming at the creation of a mathematical model of anaerobic digestion. Quoting Batstone et al (2002), the full aims of the so called "Anaerobic Digestion Model no.1" (ADM1) [2] are: increased model application for full scale plant design, operation and optimization, further development work on process optimization and control, aimed at direct implementation in full scale plants, common basis for further development and validation studies to make outcomes more comparable and competitive, and assisting technology transfer from research to the industry.

The ADM1 model describes the five main biochemical steps (involving biological enzymes) in an anaerobic digester. It starts with disintegration, followed by hydrolysis, acidogenesis, acetogenesis and methanogenesis. Seen in fig.1.The process can be described by the following steps:

In the disintegration step, complex biomass molecules are broken down to lipids (i.e. fats), carbohydrates and proteins. In hydrolysis, molecules of carbohydrates, lipids and proteins are broken down to long chain fatty acids (LCFAs) amino acids and sugars. In acidogenesis, these LCFAs, amino acids and sugars are broken down to volatile fatty acids (VFAs), namely propionate, valerate, butyrate and some acetate. These VFAs are then transformed into acetate in the acetogenesis. This acetate is finally transformed into methane gas and carbon dioxide, in the methanogenesis.

All in all, there are 26 different compounds taken into account by the ADM1 model. An important group of components in the ADM1 model is biomass (i.e. anaerobic bacteria groups). In the ADM1 model, there are seven types of biomass [5] that degrade eight different components (long chain fatty acids, amino acids, sugars, valerate and butyrate, propionate, acetate and hydrogen). These biomass groups have different sensibilities to process disturbances. These disturbances are referred to as inhibition. Inhibition occurs when the uptake of a compound and growth of biomass is decreased. This can lead to a less efficient process, with lower methane yields or even a

complete process failure. The ADM1 model comes in its default setting with inhibition factors describing major inhibition processes[4], namely ammonia inhibition, hydrogen inhibition, pH inhibition, competitive inhibition (competition between valerate and butyrate utilizers for valerate and butyrate) and secondary inhibition (competition for nitrogen between biomass groups). The pH dependence of ammonia is also included since a rise in pH displaces the ammonia-ammonium balance towards ammonia. Ammonia inhibition is strongly linked to the composition of the waste. Excess nitrogen, for example from high protein contents, can be converted into ammonia and that would inhibit the process. This ammonia can be created provided that the biomass (anaerobic bacteria) cannot use nitrogen in their cellular metabolism because of lack of carbon.

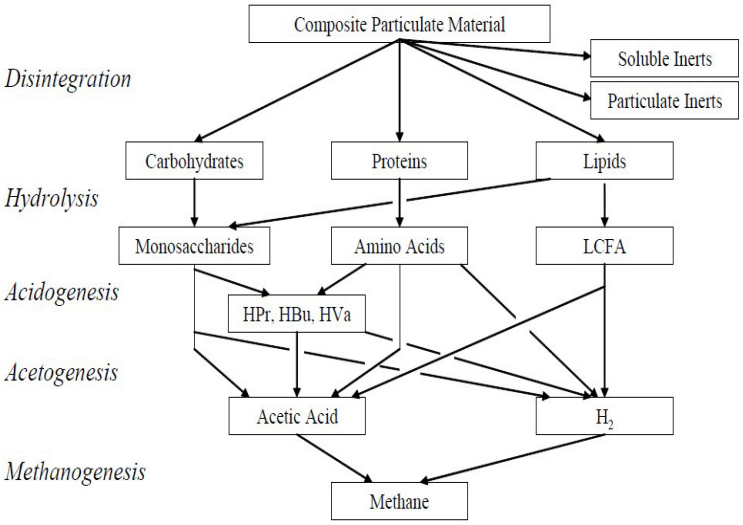

Fig.1.The disintegration and biochemical steps in the ADM1 model

After the release of the ADM1 model, many authors have showed that it possesses good predictive capabilities for different configurations of anaerobic digestion processe. Also, when published, the intent of the ADM1 was to model steady state processes; it has however been shown that a dynamic loading regime, in terms of varying masses of waste, is not a great difficulty for the model. It is common practice for authors to implement changes in the default ADM1 model to achieve a closer fit to data. The ADM1 model comes with a large set of constants, and recommended values for these constants are found in the ADM1 publication. It is a common practice among researchers to change the values of one or more of these constants to achieve a closer fit to data. Adding inhibition terms are another common practice among authors. Additional inhibition factors than those used in the default ADM1 publication can be taken into account in addition to the ADM1 model. A particular problem with the default pH inhibition function mentioned in Batstone et al (2002) is that it is discontinues and may cause numerical instabilities. Similar pH functions have therefore been devised for the ADM1 model which “mimics” the original function without these instabilities

The ADM1 only utilizes the so called first order kinetics, since all differential equations in the ADM1 model are first order equations. The ADM1 model can be implemented as either a system of differential equations (DE-implementation) with 33 state variables in total, i.e. variables described by separate differential equations, or using differential equations and algebraic equations (DAE-implementation) with 28 state variables in total [4]. In both implementations some compounds are counted twice since they exist both in gas and liquid phase, or are divided into acid base pairs.

The idea behind the DAE implementation is that it removes stiffness from the implemented system. A system is stiff when the range of time constants is large. In essence, this means that some state variables change very rapidly, such as acid base pairs, while some change much more slowly, such as biomass. Stiff systems demand special

solvers to solve computationally. These solvers can be quite slow when transient (variation with time) loads are simulated.

2.2. Batch reactor model

The ADM1 model was implemented using differential equations to describe the 33 state variables. It was coded and implemented in MATLAB and solved with the variable step size, using Euler method solver ODE15s for differential equation systems. The main assumptions to be considered during the modeling are - the reactor is well stirred, there are no effects due to fluid motion in the digester, temperatures in the reactor are considered to be the same in all parts of the digester, and hydrolysis constants were at least a factor ten lower than in the default ADM1 model.

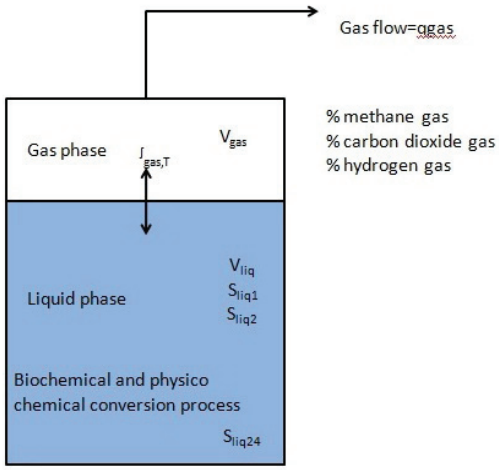

Fig.2. Process model

Equations in liquid phase

For batch reactor there is no inlet and outlet. So its liquid volume is kept constant. According to the mass balance, the state of each component in liquid phase can be expressed as follows [6]

$$\frac{dS_{liq,i}}{dt} = \sum_{j=1-28} \rho_j V_{ij} \tag{1}$$

where *Vij* is a stochimoetric constant in the ADM1 matrix. The process rate for process number j is given as ρj, it is found in the right column of the matrix and is determined by multiplying the process rates ρj for all process *j* with the specific *Vij* in the matrix for the specific *i*.

Equations in gas phase

According to the mass balance, the state of each component in gas phase can be expressed as follows

$$\frac{dS_{gas,i}}{dt} = -\frac{S_{gas,i} * q_{gas,i}}{V_{gas}} + \rho_{T,i}\frac{Vliq}{V_{gas}} \tag{2}$$

where *q* is the gas flow rate for gas *i* (*i*=hydrogen, carbon dioxide, methane gas). The transfer rate of gas is i $\rho T,i$, where *i* is temperature specific, with concern to the Henry's law coefficient $K_{H,i}$. Transfer rates are calculated according to:

$$\rho_{T,H2} = K_{La}(S_{liq,H2} - 16K_{H,H2} * P_{gas,H2}) \tag{3}$$

$$\rho_{T,CH4} = K_{La}(S_{liq,CH4} - 16K_{H,CH4} * P_{gas,CH4}) \quad (4)$$

$$\rho_{T,CO2} = K_{La}(S_{liq,CO2} - 16K_{H,CO2} * P_{gas,CO2}) \quad (5)$$

Here, $Pgas,i$ is the partial pressure of gas i, which can be calculated with the ideal gas law equation of state. $K_{H,i}$ is the Henry's law coefficient for gas i, for temperature T. Assuming that gas flow is restricted through an orifice, the gas flow, q_{gas} becomes:

$$q_{gas} = K_p(P_{gas} - P_{atm}) * \frac{P_{gas}}{P_{atm}} \quad (6)$$

3. Results and discussion

3.1. Performance of batch reactors

The plot of daily biogas production versus days is shown in figure 3(a). Initially biogas production is high due to the present of air inside the reactor and waste [3].

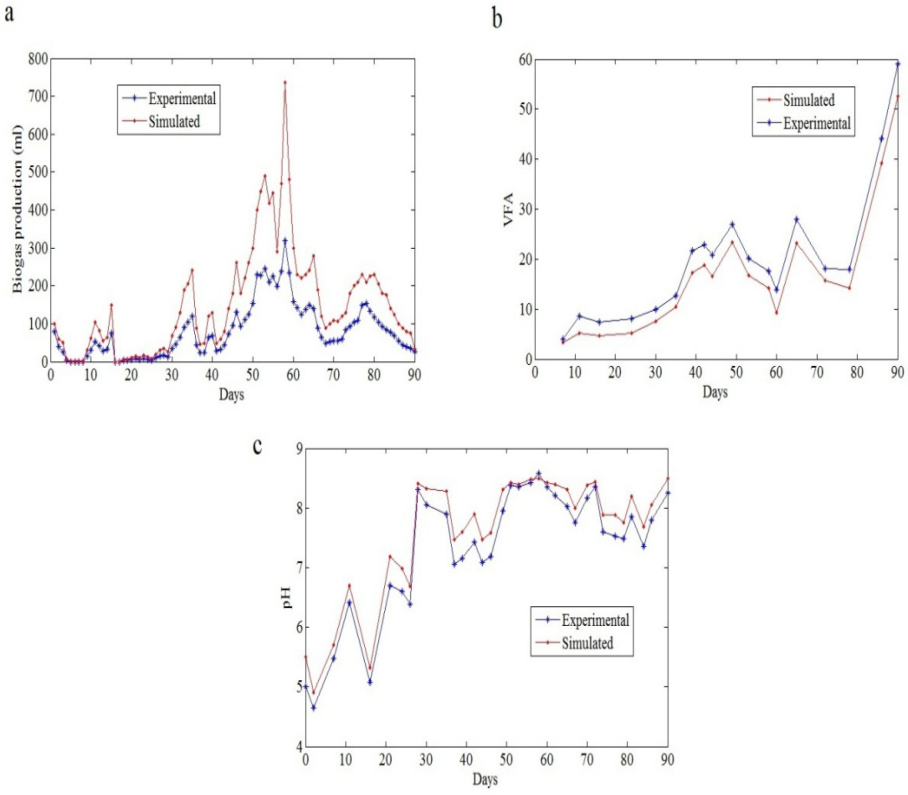

Fig.3. (a) Biogas Vs Days; (b) VFA Vs Days; (c) pH Vs Days

The maximum daily biogas production is obtained was 320ml on 58th day. The biogas production was decreased at

the end of 90 days due to the lack of substrate. Under optimized condition daily biogas production obtained was 7. 37L.This shows that optimization of the process parameter will give higher biogas production. On increasing the concentration of substrate, biogas production is high due to the accumulation of substrate. Biogas production is low on decreasing the concentration due to the lack of substrate.

The plot of VFA versus days is shown in figure3 (b). Initially VFA accumulation is very low. At the end of the digestion it increases to high value due to acidification of vegetable waste. It may reduce the pH and cause the decrease in the free ammonia and inhibition of methanogenesis. From the plot it is clear that maximum Volatile Fatty Acid was obtained at 90^{th} day of experiment. Due to the rapid acidification of vegetable wastes high VFA may form, and that leads to the instability of the reactor. At the initial condition VFA is very low.

The plot of pH versus days is shown in figure 3(c). pH was almost steady from days 50 to 60. After that the pH value gets changed due to accumulation of fatty acid and ammonia nitrogen. In anaerobic digestion process pH should be maintained at 6.8 to 7.4, which is the optimum range for methanogensis process. pH was found to be decreasing during the initial days of digestion due to the formation of volatile fatty acid. In the middle of the total days pH was maintained at 7. After that the pH value changed due to the accumulation of volatile fatty acid and ammonia nitrogen

4. Conclusion

Anaerobic digestion of solid waste is a complex process involving various microorganisms and substrate. Model contains unknown parameters which have to be estimated from experimental data. Based on the performance of anaerobic digestion of solid waste maximum biogas production was obtained at total concentration of 90g/l. It is observed that on decreasing the concentration biogas production was reduced due to the lack of substrate. On increasing the concentration, the production was high due to the accumulation of large amount of substrate. Simulation of anaerobic digestion of solid waste was done by using mat lab. In this work, a modified version of ADM1 model was proposed to model and simulate anaerobic digestion of batch study. Numerical simulations have then been used to evaluate the performance of anaerobic digestion of solid waste.

Appendix

Nomenclature

Variable	Description
VFA	Volatile Fatty Acid
$\rho T,i$	specific mass transfer rate of gas i
KLa	overall mass transfer coefficient KL times the specific transfer area
Sliq.i	concentration of gas i in liquid phase
Pgas,i	partial pressure of gas i in gas phase (bar)
KH,i	Henry's law coefficient of gas i (mole/m3/bar)
kp	pipe resistance coefficient
Sgas.i	concentration of gas i in gas phase
R	gas law constant (8.314 · 10-5 bar·m3/mole/K)
T	absolute temperature (K)

Acknowledgements

The authors thank the principal, head of the department of chemical engineering, project guide Mrs Sajeena Beevi B of Government Engineering College, Thrissur for their help and support.

References

[1] Bastogne, D .J., Keller, J., Angelidaki, I., Kalyuzhnyi, S.V., Pavlostathis, S.G., Rozzi, A., Sanders, W.T.M., Siegrist, H. & Vavilin, V.A.(2002) The IWA Anaerobic Digestion Model no.1. Water Science and Technology45 (10) 65-73.

[2] Batstone D.J. (2003) Mathematical modeling of anaerobic reactors treating domestic wastewater: Rational criteria for model use. Reviews in Environmental Science and Bio and Technology 5 (1) 57-71

[3] Jose p.p Bioenergy conversion studies of organic fraction of muncipal solid waste, 'International Journal of Scientific and Research Publications, 3(2013), pp.2-3

[4] Alina Haqgelqvist, Methane yields from anaerobic digestion of food waste Variation of load, retention time and waste composition in simulating methane yields, using the "Anaerobic digestion model no.1" (ADM1)

[5] Christian Wolf, Simulation, optimization and instrumentation of agricultural biogas plants

[6] Bhunia, P., Ghangrekar, M.M., 2008.Analysis, evaluation and optimization of kinetic parameters for performance appraisal and design of UASB reactors .Bioresource Technology 99 (7), 2132e2140.

[7] Zaher, U., Vanrolleghem, P., Rodriguez, J., Franco, A., 2004.Conceptual approach for ADM1 applications. In: Ujang, Z., Henze, M. (Eds.), Environmental Biotechnology: Advancement in Water and Wastewater Applications in the Tropics.

[8] Zaher,U.,Pandey, P.,Chen.S., 2009. A simple elemental continuity based model application to study the anaerobic microbial activity for the treatment of dairy manure. Applied Mathematical Modelling 33 (9), 3553e3564

[9] Hansen, K, Angelidaki, I, Ahring, B.K, Anaerobic digestion of swine manure: inhibition by ammonia. Water Res. 32 (1) (2008) 5–12.

[10] Metcalf & Eddy, Inc., Wastewater engineering: Treatment and reuse 4thed. McGraw-Hill, New York, 2003

[11] Volcke, E.I.P., Van Hulle, S., Deksissa, T., Zaher, U. and Vanrolleghem, P.A. (2005). Calculation of pH and concentration of equilibrium components during dynamic simulation by means of a charge balance. BIOMATH Tech. Report, Ghent University, Ghent, Belgium

[12]Gallert, C, Henning, A, winter, J, Scale-up of anaerobic digestion of the biowaste fraction from domestic wastes, Water Res. 37(2003), 1433–1441.

[13] Gernaey, K.V., Rosen, C and Jeppsson, U. (2006). WWTP dynamic disturbance modeling - an eesential module for long-term benchmarking development. Wat. Sci. Tech. 53(4-5), 225-23

[14] Copp J.B. (ed.) (2002). The COST Simulation Benchmark - Description and Simulator Manual. ISBN 92-894-1658-0, Office for Official Publications of the European Communities, Luxembourg.

[15] A. Del Borghi, A. Converti, E. Palazzi and M. Del Borghi, "Hydrolysis and thermophilic anaerobic digestion of sewage sludge and organic fraction of municipal solid waste", Bioprocess Eng., vol.20, pp. 553-560, 1999.