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RESEARCH ARTICLE OPEN ACCESS

Modelling and Simulation of Anaerobic Digestion of Wastewater Sludge using Mathematica

Abdul Rafey*
**(Department of Chemical Engineering, Aligarh Muslim University, Aligarh-202002*

ABSTRACT
The increasing demand of energy has led to a chaos among the existing energy sources and the tremendous amount of solid waste generation on a daily basis is making the country a dumping ground. Hence, it becomes an urgent need to address the problem of waste management and energy crisis. Municipal solid waste (MSW) thus serves as an efficient and reliable option for the conversion of waste to energy. The anaerobic digestion of solid waste to produce biogas is gaining importance. The growing need of the process involves increased efforts in reducing biogas plant design cost and optimizing process operation. This could be possibly done through mathematical modelling of the process. This paper particularly highlights the deviation of theoretical method with that obtained during experimentation through simulation results. Simulation is done in Mathematica and the concentration profiles of the substrate, anaerobic microorganisms and methane generation are plotted against various dilution rates and specific growth rate. The results reveal that at lower value of specific growth rate and dilution rate the experimental results fit best with the simulation result. This study can contribute in solving the complex unsteady state modelling equations of anaerobic digestion using Mathematica and pre-simulation of the experimentation results.
***Keywords* -** Anaerobic digestion, biogas, modelling, municipal solid waste, simulation

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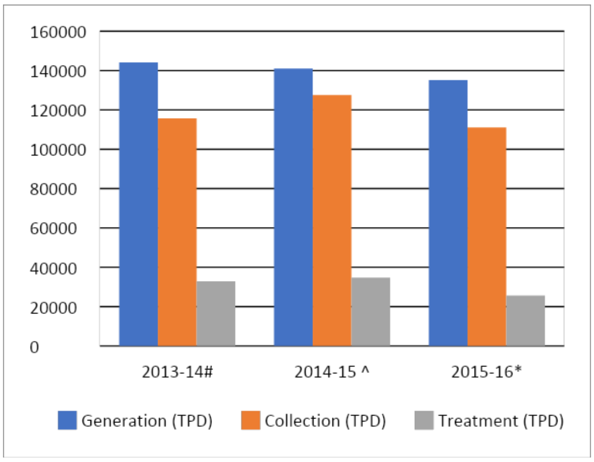
I. INTRODUCTION

With the demand of world's fossil fuel being increased at a constant pace and the substantial hike in prices, interest has rightly shifted towards the development of renewable energy sources. Renewable sources of energy offer the most potential energy conservation and development option for future. Of all the available renewable energy technologies, biogas is one of the most potential energy source with lowest financial inputs per kWh of output. There is presently an enormous amount of biomass on the globe which refers to all forms of organic matter including crop residues, agro-agricultural by-products, urban waste, animal dung, etc. [1].

Presently, more focus is on bio-chemical route of bio-energy production which is commonly known as biomethanation or anaerobic digestion. This is due to the fact that tremendous amount of solid waste is being disposed at a very large scale. This waste contains potentially useful amount of material which could cater the needs of the large masses. 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 [2]. Anaerobic digestion, therefore serves as an effective technology for the treatment of organic wastes.

Many wastes that are disposed off in landfills represent a loss of materials that could be reused, recycled, or converted to energy to displace the use of virgin (NEW) materials. The solid waste generated from the cities/towns in India has present potential to generate power of approximately 500 MW, which can be enhanced to 1,075 MW by 2031 and further to 2,780 MW by 2050 [3]. The trend of MSW management in India is shown in fig. 1.



Source: # (CPCB,2015), ^ (CPCB,2016), * (CPCB,2017)

Fig. 1: Trends in MSW Management

Nearly 62 million tonnes of MSW generated annually in urban areas of which more than 80% is indiscriminately disposed off at dump yards in an unhygienic manner. This waste has a potential of generating approximately 439 MW of power, 1.3 million cubic meter of biogas per day or 72 MW of electricity generation from biogas and 5.4 million metric tonnes of compost. Hence, 62 million tonnes annual generation of MSW will need about 3,40,000 cubic meters of landfill space everyday (1240 hectare per year) if continued to be dumped in such a manner. The status of MSW treatment in India is shown in fig. 2 [4].

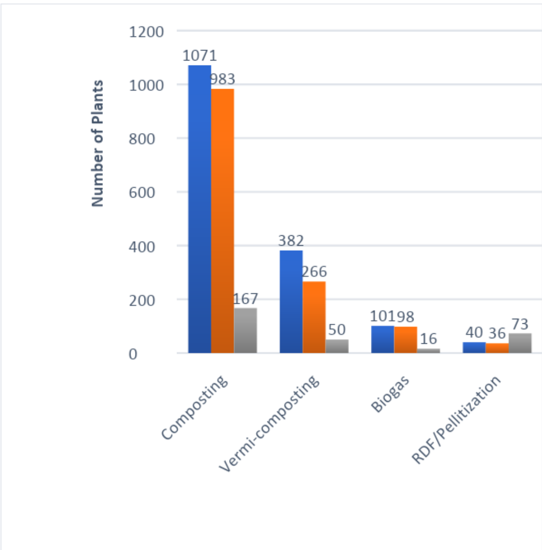


Fig. 2: Status of MSW treatment in India

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 [5]. Batch, continuous, single stage and multi-stage process are among the common systems that are implemented for the treatment of solid waste. The research is still on its pace to explore the most efficient technology for waste to energy conversion and also to address the on-site issues of waste management on landfills. A number of factors affect the kinetics of production of biogas, such as pH, volatile fatty acid, temperature, quantity of substrate being used, and alkalinity.

Modeling anaerobic digestion is very complicated because of the unsteady state behavior and the interaction of different physicochemical and biological parameters. A large number of models are available: mass balances models, black-box models or heuristic models, simulation models [5], [6], [7], [8], [9], [10], [11].

This paper presents a kinetic model of anaerobic digestion based on mass balance of substrate, microorganisms and methane production. The model is simulated using technical computing and simulation software "Mathematica" and the value of maximum specific growth rate of microorganisms is calibrated to fit the theoretical results with experimental ones regarding methane production. The experimental data is obtained from the literature [12] and reported under next section. The experimental data and the simulation results are validated to check the deviation.

II. MODELLING METHODOLOGY

Anaerobic digestion usually involves several stages each conducted by specific microorganisms and only some of them limit the process because of their slow growth. The anaerobic kinetics in this paper is described by developing a single stage model.

In order to investigate the kinetics of biogas production the process of anaerobic digestion considers the growth of microorganisms, the substrate degradation and the formation of final product, i.e. biogas. The biological reactor can be considered as a closed tank with the following hypothesis taken into account:

a) biochemical reactions occur only in the bioreactor;
b) complete mixing of sludge and microorganisms in order to maintain 36^0C in the bioreactor,
c) steady-state regime

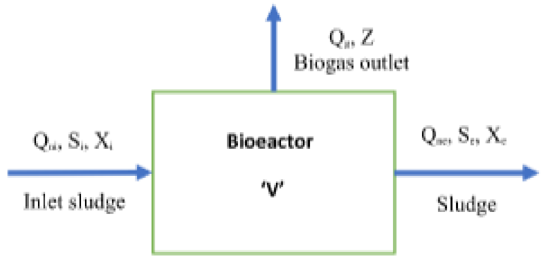


Fig. 3: Anaerobic bioreactor scheme

A bioreactor with volume 'V' is shown in fig. 3. Flow rate of inlet and outlet sludge are represented as 'Q_{ni}' and 'Q_{ne}' respectively. The concentration of the anaerobic microorganisms at the entrance and at the outlet are represented as 'X_i' and 'X_e' respectively. 'S_i' and 'S_e' represents the concentration of the substrate at the entrance and at the outlet respectively. 'Q_g' represents the flow rate of biogas being collected and 'Z' represents the corresponding methane concentration in the biogas.

The mathematical model for the microorganism's growth, the substrate decomposition and biogas formation is based on the mass conservation law. Under non-steady-state conditions, complete mixing in bioreactor is assumed and endogenous decay of the microorganisms is neglected, then the respective mass balance equations are as follows:

$$V\frac{dS}{dt} = Q_{ni}S_i - Q_{ne}S_e - r_nV \qquad (1)$$

$$V\frac{dX}{dt} = Q_{ni}X_i - Q_{ne}X_e + r_cV - r_dV \qquad (2)$$

$$V\frac{dZ}{dt} = Q_{ni}Z_i - Q_{ne}Z_e + KV \qquad (3)$$

Where, 'r_n' represents substrate degradation rate; 'r_c' represents growth rate of anaerobic microorganisms; 'r_d' represents decay rate of anaerobic microorganisms; 'K' represents the coefficient for transformation of volatile organic compounds into methane.

Following assumptions are made to simulate the kinetics:

- $Q_{ni}.Z_{ni} = 0$, $Q_{ne}.Z_{ne} = 0$; since no presence of biogas in inlet and outlet sludge
- $Q_{ni} = Q_{ne} = Q$; flow rate is assumed to be constant throughout and not varying with time
- Dilution rate 'D' = Q/V; where 'V' represents the volume of bioreactor

Equations (1), (2) and (3) on simplifying based on the assumptions described reduces to;

$$\frac{dS}{dt} = D(S_i - S_e) - r_n \qquad (4)$$

$$\frac{dX}{dt} = D(X_i - X_e) + r_c - r_d \qquad (5)$$

$$\frac{dZ}{dt} = K \qquad (6)$$

Growth rate of microorganisms 'r_c' is given by;

$$r_c = \mu.X$$

where, 'μ' represents the specific growth rate of microorganisms

Decay rate of anaerobic microorganisms 'r_d' is given by;

$$r_d = K_d.X$$

where, 'K_d' represents decay rate constant of microorganisms

The mass balance equation for the concentration of anaerobic microorganisms thus can be written as;

$$\frac{dX}{dt} = D(X_i - X_e) + \mu.X - K_d.X \qquad (7)$$

Based on Andrews relation for substrate inhibition [13], the specific growth rate of microorganisms is given by;

$$\mu = \mu_{\max}\frac{1}{1 + \frac{K_s}{S} + \frac{S}{K_i}} \qquad (8)$$

The substrate degradation rate 'r_n' is a combination of three different parameters namely;

- New cells formation:

$$r_{nx} = \frac{\mu.X}{Y_x}$$

where, 'Y_x' represents yield coefficient

- Energy supply for the growth and maintenance of microorganisms

$$r_{np} = K_{sx}.X.\mu + K_{mx}.X.\frac{S}{K_s + S}$$

where, 'K_{sx}' represents substrate degradation rate to supply energy for microorganisms growth and 'K_{mx}' represents substrate degradation rate to supply energy for microorganisms maintenance

- Product formation

$$r_{nc} = \frac{1}{Y_s}.\frac{dZ}{dt}$$

Thus, combining all the substrate degradation parameters, equation (4) for mass balance of substrate concentration becomes;

$$\frac{dS}{dt} = D(S_i - S_e) - \frac{\mu.X}{Y_x} - K_{sx}.X.\mu - K_{mx}.X.\frac{S}{K_s + S} - \frac{1}{Y_s}\frac{dZ}{dt} \tag{9}$$

Coefficient for transformation of volatile organic compounds into methane 'K' follows the relation;

$$K = Y_p.\mu.X \tag{10}$$

Therefore, equation (6) for methane concentration in biogas can be written as;

$$\frac{dZ}{dt} = Y_p.\mu.X \tag{11}$$

The theoretical simulation for the concentration of anaerobic microorganism, substrate concentration and methane concentration varying with time can be obtained from equations (7), (9) and (11) respectively. The equations are simulated using Mathematica software.

For modelling purpose, the volume of one reactor is considered to be three times the volume of a single reactor. Hence, the volume of the reactor for the experimental study came out to be; V = 3x4000 = 12000 m^3. The inlet sludge flow rates are given as 350 m^3/d, 298 m^3/d and 312 m^3/day. Thus the dilution rates are calculated as 0.0292 d^{-1}, 0.02843 d^{-1} and 0.026 d^{-1}. Retention time is for 30 days. The inlet substrate concentration is S_0 = 6 g/l and the microorganisms concentration is X_0 = 3 g/l.

The values of kinetic constants are taken from the literature:

μ_m = 0.2…..1.2 d^{-1}; K_s = 7.1…..360 mg/l COD; K_d = 0.02…0.04 d^{-1}; K_i = 0.5, 1.0, 10.0, 100.0; Y_x = 0.3…0.82; Y_s = 0.04…0.27; Y_p = 4.35; K_{mx} = 0.4; K_{sx} = 0.983

III. RESULTS AND DISCUSSION

The simulation data represent variation of substrate concentration, concentration of anaerobic microorganism and methane concentration with time. The mass, concentration and flow rate of methane is calculated from the equations as given below:

Methane flow rate:

$$Q_{CH_4}[kg/d] = Q_{biogas}[m^3/d].x.\rho_{CH_4}$$

where, 'x' represents the methane percentage in biogas, which is assumed to be 60% and density of methane is 0.717 kg/m^3

Mass of methane:

$$M_{CH_4}[kg] = Q_{CH_4}[kg/d].t_{retention}$$

Concentration of methane:

$$Z_{CH_4}[g/l] = M_{CH_4}[kg]/V[m^3]$$

The simulations were done for dilution rates 0.0292 d^{-1}, 0.02483 d^{-1} and 0.026 d^{-1}, according with experimental measurements. The specific growth rate of microorganisms (μm); 0.35 d^{-1}, 0.38 d^{-1} and 0.4 d^{-1}, were simulated for corresponding dilution rates.

The Mathematica program for simulation for each dilution rate and corresponding specific growth rate is shown below. The same program with alteration of values for dilution rate and specific growth rate; can be used for the study.

```
Anaerobic digestion model (1).nb

In[398]:= ClearAll["Global`*"]
μmax = 0.35; Ks = 7.1; Ki = 0.5; D1 = 0.0292; Xi = 3; Kd = 0.02;
Si = 6; Ys = 0.27; Yx = 0.82; Ksx = 0.983; Kmx = 0.4; Yp = 4.35;

(*Andrews Relation*)
μ = μmax / (1 + Ks / S[t] + S[t] / Ki)

(*Anaerobic microorganism concentration*)
Eqn1 = X'[t] == D1 * (Xi - X[t]) + μ * X[t] - Kd * X[t]

(*Substrate concentration*)
Eqn2 = S'[t] == D1 * (Si - S[t]) - μ * X[t] / Yx - μ * Ksx * X[t] - Kmx * X[t] * S[t] / (Ks + S[t]) -
   1 / Ys * Yp * μ * X[t]

(*Methane concentration*)
Eqn3 = Z'[t] == Yp * μ * X[t]

soln = NDSolve[{Eqn1, Eqn2, Eqn3, X[0] == Xi, S[0] == Si, Z[0] == 0}, {X, S, Z}, {t, 0, 30}]
Plot[{X[t], S[t], Z[t]} /. soln, {t, 0, 30}, PlotRange → All,
 AxesLabel → {"time [d]", "Concentration [g/l]"}, LabelStyle → Directive[Blue, Bold]]
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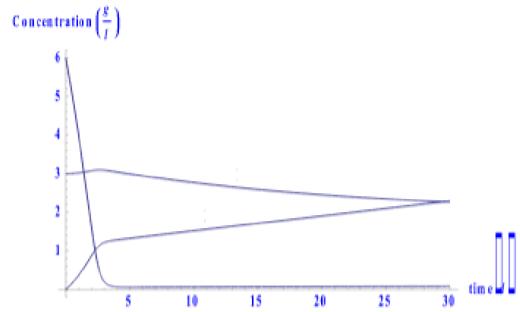
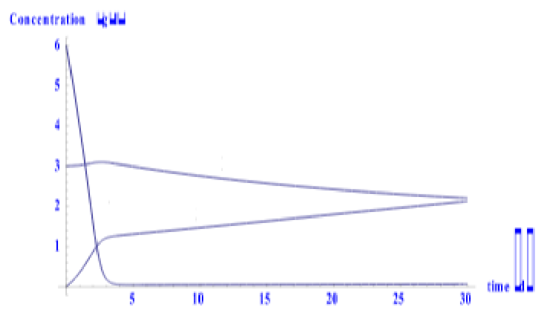
The graphical results for the concentration corresponding to each dilution rate and specific growth rate of microorganisms are shown from fig. 4 to fig. 12.





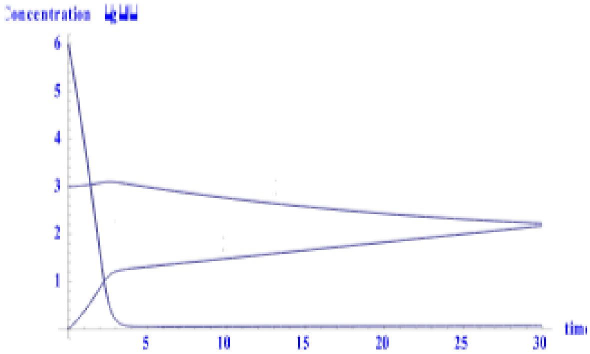


Fig. 7: Concentration vs. time variation (μ_{max} = 0.38 d^{-1}, D = 0.0292 d^{-1})

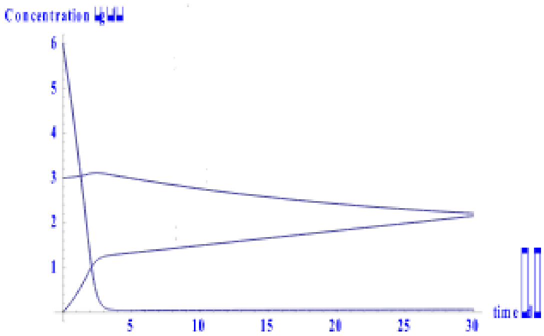


Fig. 8: Concentration vs. time variation (μ_{max} = 0.38 d^{-1}, D = 0.02843 d^{-1})

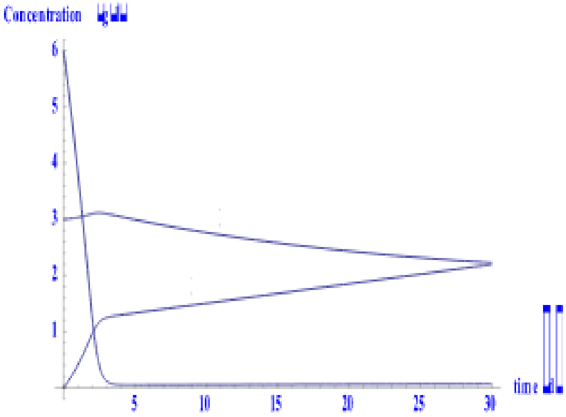


Fig. 9: Concentration vs. time variation (μ_{max} = 0.38 d^{-1}, D = 0.026 d^{-1})

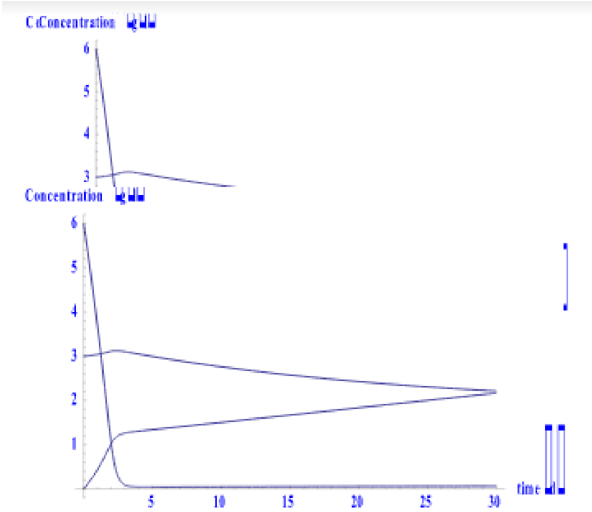


Fig. 10: Concentration vs. time variation (μ_{max} = 0.4 d^{-1}, D = 0.0292 d^{-1})

Fig. 11: Concentration vs. time variation (μ_{max} = 0.4 d^{-1}, D = 0.02483 d^{-1})

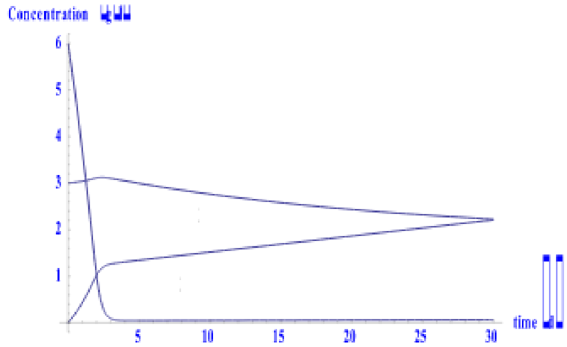


Fig. 12: Concentration vs. time variation (μ_{max} = 0.4 d^{-1}, D = 0.026 d^{-1})

The simulation results from the graph for methane concentration is shown in table 1. It is evident from the curve and the corresponding values that, with increase in specific growth rate for a constant dilution rate, the methane concentration increases. Although the specific methane yield of a substrate is a function of the substrate itself, the methane productivity is dependent on the rate at which it is produced, and importantly on the bioreactor volume that produces it [5].

Table 1: Experimental and simulation data

Experimental Data			
Inlet Sludge flow rate, Q_{ni} [m^3/d]	350	298	312
Dilution rate, D [d^{-1}]	0.0292	0.02483	0.026
Methane concentration, Z [g/l]	2.065	2.41	1.67

μ_{max} = 0.35 [d^{-1}]			
Methane concentration, Z [g/l]	2.276	2.105	2.142
μ_{max} = 0.38 [d^{-1}]			
Methane concentration, Z [g/l]	2.299	2.145	2.181
μ_{max} = 0.40 [d^{-1}]			
Methane concentration, Z [g/l]	2.311	2.145	2.181

The study clearly depicts that the experimentation results fits best with the simulation results for a lower value of the specific growth rate of microorganisms. However, as the growth rate increases along with the dilution rate, the deviation increases from the experimentation results.

IV. CONCLUSION

Anaerobic digestion process involves complex unsteady state behaviour and interaction of numerous parameters that are interlinked and form simultaneous differential equations. This paper presents simulation model for single stage anaerobic digestion kinetics. The modelling equations are solved using Mathematica and the results are validated with the experimental data to check for the best fit amongst the simulation results and the experimental ones.

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