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Review

A review of simple to scientific models for anaerobic digestion

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ABSTRACT

To fully model the anaerobic digestion process, biological and physico-chemical background, the kinetics of bacterial growth, substrate degradation and product formation have to be taken into account. The presented approaches differ depending on the requirements and the developer of the model. Important parameters affecting the process such as temperature, which can cause great inaccuracy, are rarely included in the models. Simple calculators are also available that estimate the applicability of the process to a specific farm and provide information to a farmer or a decision maker. Six simple calculators are presented in this study: AD decision support software, Anaerobic Digestion Economic Assessment Tool, $BEAT_2$, BioGC, FarmWare and GasTheo. The simpler calculators mainly use the relation that exists between volatile solids and biogas production. A tested case of 100 dairy cows and 50 sows was applied to the simple calculators to compare the results.

1. Introduction

Anaerobic digestion is a natural process that takes place in areas where free oxygen is not available and has been utilised by humans for the treatment of waste from the mid-1800s. Anaerobic digestion has become more popular in the recent years, mainly due to its ability to generate energy from waste.

The technology is also considered as one of the most important mitigation options for the greenhouse gases emissions (GHG) from farming. Alternative technologies to anaerobic digestion emit uncontrolled GHG to the atmosphere: (a) the lagoons emit methane and carbon dioxide if anaerobic conditions are developed in large depths or carbon dioxide from the upper layers of the lagoon, (b) aerobic treatment causes the emission of considerable amounts of carbon dioxide due to the large amounts of energy required for aeration and/or mixing. On the other hand, anaerobic digestion is a closed, airtight system, and one of the end products of the process is a gas mixture of methane and carbon dioxide known as biogas.

The typical ratio of methane to carbon dioxide in biogas when optimum conditions occur is 60:40. In cases that biogas is of sufficient quality and quantity, it is combusted to generate electricity or heat or both. This prohibits methane to be released to the atmosphere, and instead, carbon dioxide is emitted from the combustion process. Therefore, smaller amounts of greenhouse gases are emitted to the atmosphere by anaerobic digestion. This, in addition to the privilege of producing energy, makes anaerobic digestion preferable by farmers.

The main sources of greenhouse gases in a farm are enteric fermentation and manure management. The gases emitted from animal farming are predominately methane (CH_4) and nitrous oxide (N_2O). These gases have a larger impact on the greenhouse phenomenon compared to carbon dioxide since the molecules can trap more heat energy within them; i.e. they have higher global warming potential (GWP) than carbon dioxide [51]. The internationally accepted GWP for methane is 21 and for nitrous oxide 310 [51].

Governments have also recognised the importance of anaerobic digestion, and there are many countries that provide financial incentives for farmers to proceed with the installation of anaerobic systems. This is because (a) energy from anaerobic digestion is considered biomass energy and therefore a form of renewable energy and (b) anaerobic digestion reduces greenhouse gases emissions from manure management and is therefore an important mitigation measure.

Mathematical modelling of the anaerobic digestion process was motivated by the need for efficient operation of anaerobic systems in the early 70's [31]. The scientific models on anaerobic digestion have been developing for almost 40 years. Some use the kinetics of

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Abbreviations

D	flow per reactor volume
dS/dt	change of substrate concentration over change in time
$(dS/dt)_c$	rate of product synthesis
$(dS/dt)_e$	rate of maintenance and growth energy generation
$(dS/dt)_r$	reaction rate
$(dS/dt)_x$	rate of new cell material synthesis
dX/dt	change of cell concentration over time
E_a	activation energy
GHG	Greenhouse gases
G_s	gas production
GWP	global warming potential
I	inhibitor concentration
k	rate constant
k_d	death rate
k_{max}	maximum rate constant
K_i	inhibition constant; the substrate concentration, where bacteria growth is reduced to 50% of the maximum specific growth rate due to substrate inhibition
K_s	Monod-constant; the substrate concentration at 50% of the maximum specific growth rate ($\mu_{max}/2$)
L	Powell constant for diffusion and permeability
MEV	methane energy value
P	product concentration
P^*	critical inhibitor concentration; where growth stops
R	molar gas constant
S	substrate concentration
S_0	initial substrate concentration
S_i	inhibitor concentration
S^*	critical inhibitor concentration; where growth stops
X	concentration
Y_x	yield coefficient
Y_{p1}	yield coefficient of products, which result from primary energy metabolism
Y_{p2}	yield coefficient of products formed at side reactions or following interactions of direct metabolic products
Y_s	yield coefficient calculated stoichiometrically
μ	specific growth rate
μ_{max}	maximum specific growth rate

the growth of microorganisms to predict the behaviour of the system, whereas others depend purely on the chemical reactions that take place.

The recent interest in anaerobic digestion however, has given rise to several publicly available simple software applications in addition to the scientific models. These applications have been developed to assist farmers assess (i) whether anaerobic digestion is financially viable for their farm (ii) the reduction of greenhouse gases emissions that can be accomplished from the application of anaerobic digestion at their farm and (iii) the energy that can be produced through anaerobic digestion of their waste. Most of the available applications are for people with limited scientific knowledge on anaerobic digestion and biogas production and are simple web-based calculators.

The aim of this paper is to present a review of scientific models available for anaerobic digestion and some simple software applications that can be used in cases that the available information is not sufficient to apply the detailed scientific models.

2. Scientific models simulating anaerobic digestion

Due to the complexity of the process, each model is developed for a different purpose. As a result, there is currently a variety of models that vary according to the purpose that they were designed for. Among them, are comparatively simple models developed exclusively for calculating the maximum biogas rate, which will theoretically be produced during digestion. Others calculate the biogas rate taking into consideration degradation or digestion rates of different components of the biomass.

Due to the limitation of many models to present the dynamic nature of the digestion, complex models have been developed to include the kinetics of the growth of microorganisms. The activity of microorganisms and consequently the biogas production rate can thus be investigated for a variety of substrates rates of death rate and washout of microorganisms via different mechanisms.

Several models are designed for a specific substrate or a small number of substrates, and are therefore not applicable to other types of substrate. Nevertheless, most of the available models allow for the calculation of biogas and methane production rate. To design biogas plants and to evaluate the efficiency of such plants both parameters are very important. Additionally, some models are very specialised and aim exclusively at the assessment of an effect, for example the evaluation of the influence of mixing on biogas production.

2.1. Theoretical biogas yield

The potential biogas yield of the anaerobic digestion of a particular type of waste and the gas composition can be determined by the chemical composition of a feedstock. Simple ways to calculate the biogas production are the models developed by Refs. [23,21,11,54,5]. These models are based on data for basic elements or components of organic matter and result only in estimates of the production of methane and carbon dioxide. These models are time independent, therefore the necessary retention time of the waste in the digester cannot be estimated.

According to Refs. [23]; methane and carbon dioxide yield can be calculated with an uncertainty of about 5% using relation (1), given that the chemical composition of organic matter is known. However, relation (1) does not take into consideration the degradation of organic matter for the bacteria metabolism (i.e. synthesis of cell mass and energy for growth and maintenance). According to this relationship, the methane fraction of fully degraded glucose is 50% since $C_6H_{12}O_6 \rightarrow 3CH_4 + 3CO_2$.

$$C_aH_bO_c + \left(a - \frac{b}{4} - \frac{c}{2}\right)H_2O \rightarrow \left(\frac{a}{2} + \frac{b}{8} - \frac{c}{4}\right)CH_4 + \left(\frac{a}{2} - \frac{b}{8} + \frac{c}{4}\right)CO_2 \quad (1)$$

Ref. [21] modified relation (1), to include nitrogen and sulphur in the composition of organic matter. This enabled the fraction of ammonia and hydrogen sulphur in the produced biogas to be estimated according to relation (2).