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Optimal operating conditions for maximum biogas production in anaerobic bioreactors

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HIGHLIGHTS

- We introduce a general transient mathematical model for anaerobic biodigesters.
- The model was experimentally validated.
- A simulation and optimization study was conducted with the model.
- The existence of optimal hydraulic retention time was investigated.
- The model could be a tool for simulation, design, control and optimization of biodigesters.

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ABSTRACT

The objective of this paper is to demonstrate the existence of optimal residence time and substrate inlet mass flow rate for maximum methane production through numerical simulations performed with a general transient mathematical model of an anaerobic biodigester introduced in this study. It is herein suggested a simplified model with only the most important reaction steps which are carried out by a single type of microorganisms following Monod kinetics. The mathematical model was developed for a well mixed reactor (CSTR – Continuous Stirred-Tank Reactor), considering three main reaction steps: acidogenesis, with a μ_{max} of 8.64 day^{-1} and a K_S of 250 mg/L, acetogenesis, with a μ_{max} of 2.64 day^{-1} and a K_S of 32 mg/L, and methanogenesis, with a μ_{max} of 1.392 day^{-1} and a K_S of 100 mg/L. The yield coefficients were 0.1-g-dry-cells/g-pollymeric compound for acidogenesis, 0.1-g-dry-cells/g-propionic acid and 0.1-g-dry-cells/g-butyric acid for acetogenesis and 0.1 g-dry-cells/g-acetic acid for methanogenesis. The model describes both the transient and the steady-state regime for several different biodigester design and operating conditions. After model experimental validation, a parametric analysis was performed. It was found that biogas production is strongly dependent on the input polymeric substrate and fermentable monomer concentrations, but fairly independent of the input propionic, acetic and butyric acid concentrations. An optimisation study was then conducted and optimal residence time and substrate inlet mass flow rate were found for maximum methane production. The optima found were very sharp, showing a sudden drop of methane mass flow rate variation from the observed maximum to zero, within a 20% range around the optimal operating parameters, which stresses the importance of their identification, no matter how complex the actual bioreactor design may be. The model is therefore expected to be a useful tool for simulation, design, control and optimisation of anaerobic biodigesters.

1. Introduction

One of the goals of anaerobic digestion is the production of methane, which can be converted into electricity by its combustion. The production of biogas, which is rich in methane, by such a process involves a consort of microorganisms that degrade organic substrates present in biological wastes. Not only is biogas a clean-

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Nomenclature

CSTR	continuous stirred-tank reactor
F	total molar flow rate of gas out of the gas phase, mol day^{-1}
G_3	H_2 partial pressure, atm
G_4	CO_2 partial pressure, atm
G_7	methane partial pressure, atm
H_3	Henry's constant for H_2, g L^{-1} atm^{-1}
H_4	Henry's constant for CO_2, g L^{-1} atm^{-1}
H_7	Henry's constant for methane, g L^{-1} atm^{-1}
HRT	hydraulic retention time, V/Q, day
K_h	constant for first order polymer hydrolysis, day^{-1}
K_{S1}	saturation constant for acidogens, g L^{-1}
K_{S2}	saturation constant for syntrophs A, g L^{-1}
K_{S3}	saturation constant for hydrogenotrophic methanogens regarding H_2, g L^{-1}
K_{S4}	saturation constant for hydrogenotrophic methanogens regarding CO_2, g L^{-1}
K_{S5}	saturation constant for acetoclastic methanogens, g L^{-1}
K_{S6}	saturation constant for syntrophs B, g L^{-1}
Kla_3	gas-liquid mass transfer coefficient for H_2, day^{-1}
Kla_4	gas-liquid mass transfer coefficient for CO_2, day$^{-1/}$
Kla_7	gas-liquid mass transfer coefficient for methane, day^{-1}
M_{H_2}	molar mass of H_2, g mol^{-1}
M_{CO_2}	molar mass of CO_2, g mol^{-1}
M_{CH_4}	molar mass of methane, g mol^{-1}
p_T	total pressure (gas phase), atm
Q	substrates input volumetric flow rate, m^3 day^{-1}
Q_g	biogas output volumetric flow rate, 22.4 × F, L day^{-1}
r	reaction rate, day^{-1}
R	universal gas constant, atm L mol^{-1} K^{-1}
S_j	concentration of substance j, g L^{-1}
S_j^*	liquid phase saturation concentration of substance j, g L^{-1}
$S_{j,ent}$	input concentration, g L^{-1}
t	time, days
T	temperature, K
V	liquid phase volume, L
V_g	gas phase volume, L
x_i	molar fraction of component i, G_i/p_T
X_1	acetogen concentration, g L^{-1}
X_2	syntroph A concentration, g L^{-1}
X_3	hydrogenotrophic methanogen concentration, g L^{-1}
X_4	acetoclastic methanogen concentration, g L^{-1}
X_5	syntroph B concentration, g L^{-1}
$Y_{Si/Sp}$	yield of S_i from S_p, g g^{-1}
$Y_{Si/xp}$	yield of S_i from X_p, g g^{-1}

Greek symbols

μ	specific growth rate, day^{-1}

Subscript

ent	inlet
j0	polymeric phase
j1	fermentable monomer
j2	propionic acid
j3	liquid phase H_2
j4	liquid phase CO_2
j5	acetic acid
j6	butyric acid
j7	liquid phase methane
k1	acidogens
k2	syntrophs A
k3	hydrogenotrophic methanogens
k4	acetoclastic methanogens
k5	syntrophs B
max	maximum
opt	optimal

burning fuel but it also has a lower heating value close to the lower heating value of methane, i.e., 50.28 MJ kg^{-1} [1]. Such value depends strongly on the proportion of methane present in the mixture of gases, which is composed mostly by methane and carbon dioxide.

Hence the importance of biodigestion could be summarized by: while being an efficient waste treatment method, reducing the organic load of the waste stream, it also produces an environmentally friendly fuel [2]. Moreover, the remaining residues, both liquid and solid, can be used as biofertilisers [3].

Whenever anaerobic digestion is selected as the process to generate electricity by the combustion of biogas, the production rate of methane should be maximized. In that direction, Marcos et al. [4] experimentally found optimal load rates for maximal biodegradation rates and methane production obtained from the anaerobic co-digestion of solid (e.g., fat, intestines, rumen, bowels, whiskers) and liquid (e.g., blood, washing water, manure) wastes of the meat industry, particularly the ones rising from the municipal slaughterhouse of Badajoz, Spain.

Although mathematical models are efficient tools used to optimise a process, it should be noted that to obtain reliable parameters of an anaerobic digestion is very challenging. The complexity is mainly due to the large number of microorganisms and compounds (i.e. large number of parameters) [5], which are summarized in Fig. 1, therefore, determining accurate values for a specific bioreactor and substrate would be highly onerous. Therefore, for the purpose of model development and concision, the organic material can be classified into carbohydrates, proteins, fats and inert compounds. Fig. 1 sketches the hydrolysis reactions for the first three, producing sugars, amino acids and long chain fatty acids, respectively.

Several mathematical models based on each biochemical step involved in the process and address variables that affect biogas production (e.g., temperature) have been proposed. Valle-Guadarrama [6] proposed a model, based on thermodynamic principles, that predicts temperature changes in a pilot plant thermophilic anaerobic digester. Fixed and variable overall heat transfer coefficient values were used, in good agreement with experimental data, concluding that temperature variation was affected by the heterogeneity of the feeding and extraction processes, by the heterogeneity of the digestate recirculation through the heating system and by the lack of a perfect mixing inside the biodigester tank. However, the use of a searching routine based on a minimal square optimization criterion for parameters determination, model complexity and computational time are issues to be considered when control and optimization are the objectives of the model.

In general, the published models assume uniform temperature within the reactor defining a class of models that the technical literature is rich of. One of the most complete models that have been proposed is the so called Anaerobic Digestion Model No. 1 (ADM1), which is a structured model that includes multiple steps