

Dynamic model simulations as a tool for evaluating the stability of an anaerobic process

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Abstract

The association of a wall growth factor with a dynamic model based on Andrews' work (1969), without pH restrictions, is used herein to study the inhibition of methanogenesis by high concentrations of volatile acids. The model considers the methanogenic bacteria as being representative of the biological phase of the anaerobic digestion, and assumes a continuous feed of acetic acid to the continuously stirred anaerobic reactor. The model can be used for simulations on transient conditions, namely the effect of initial conditions on the start-up of a digester, as well as for studying the significant improvements in stability when wall growth occurs in the reactor. The effect of changing the feed characteristics to a digester was studied in two situations: with and without wall growth. The presence of wall growth allows a better behaviour of an anaerobic process in any case, namely when a step increase in the feeding substrate concentration or in flow rate is performed.

Introduction

Anaerobic digestion is a rather complex microbiological process, which involves several biological steps performed by specific groups of bacteria. Three main steps are usually identified:

- the hydrolysis of the complex organic matter,
- the acidogenic phase, with the production of volatile acids, and
- the methanogenic phase, where methanogenic bacteria convert the volatile acids into the final products, carbon dioxide and methane.

Among the volatile acids, acetic acid is the most significant precursor of methanogenesis. Since methanogenic bacteria are the most sensitive, with the lowest growth rates, methanogenesis is frequently considered to be the rate-limiting step in modelling attempts (Andrews, 1969; Buhr and Andrews, 1977; Renard et al., 1988; Alatiqi et al., 1990; Siegrist et al., 1993; Poggi-Varaldo et al., 1997).

The use of a dynamic model allows the study of anaerobic reactor performance under transient conditions, such as start-up operations, and quantitatively measures process stability under different operational conditions. Such a model can be a valuable tool in the development of new control strategies in order to avoid process failure and to optimise reactor performance.

Keeping in mind the frequent failure situations occurring in inhibited anaerobic reactors, the importance of such dynamic models is clearly indicated. Andrews (1969) presented a dynamic model for the study of the anaerobic digestion process, considering only the reactions concerning the biological methanogenic phase of the process.

This paper presents a study of anaerobic digestion, using a dynamic model similar to the Andrews' version, without the pH restrictions assumed in that work, and a wall-growth factor is introduced in order to explain the residual stability of reactors performing in otherwise inhibitory conditions.

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☎ 09351 2343702000; fax 09351 234429290

Received 22 September 1998; accepted in revised form 26 September 2000

The model equations

The model was developed for a continuously stirred tank reactor, without recycling, and includes two mass balance equations: one for the substrate and another for the micro-organisms, with an inhibition function introduced by Andrews (1969) in order to describe the micro-organism kinetics. The use of an inhibition function is essential to develop a model that will predict failure situations in sustained continuous anaerobic processes due to inhibition of biological growth:

$$\mu = \frac{\mu_{\max}}{1 + \frac{K_s}{[HS]} + \frac{[HS]}{K_i}} \quad (1)$$

where:

- μ = micro-organisms specific growth rate (d⁻¹)
- μ_{\max} = maximum specific growth rate (d⁻²)
- $[HS]$ = un-ionised substrate concentration (g·l⁻¹)
- K_s = saturation constant (g·l⁻¹)
- K_i = substrate inhibition constant (g·l⁻¹)

This inhibition function assumes that the un-ionised volatile acids act as the inhibition agent and the limiting substrate for micro-organism growth rate. This equation can be written as a function of total acetic acid concentration, from the acetic acid equilibrium constant:

$$K_a = \frac{[S^-] \times [H^+]}{[HS]} \quad (2)$$

where:

- K_a = acetic acid equilibrium constant
- $[S^-]$ = ionised substrate concentration (g·l⁻¹)
- $[HS]$ = un-ionised substrate concentration (g·l⁻¹)
- $[H^+]$ = hydrogen ion concentration (g·l⁻¹)

since the total acetic acid concentration is given by both the ionised and the un-ionised concentrations:

$$[S]_T = [HS] + [S^-] \quad (3)$$

where:

$[S]_T$ = total substrate concentration ($\text{g}\cdot\text{l}^{-1}$).

Thus the inhibition function can be written as follows:

$$\mu = \frac{\mu_{\max}}{1 + \frac{K_s \times (K_a + [H^+])}{[S]_T \times [H^+]} + \frac{[S]_T \times [H^+]}{K_i \times (K_a + [H^+])}} \quad (4)$$

Andrews (1969) considered a simplification to the inhibition function, which assumes a pH range for digester operation between 6 and 8, and allowed for the consideration of the total substrate concentration which is approximately the same as that of the un-ionised substrate concentration. This simplification was not considered here; which means that the pH range can assume values of lower than 6 and higher than 8. Exclusion of restrictions to the pH range is particularly important since, under transient conditions, the pH may assume values outside the range of normal operation.

Figure 1 illustrates the tridimensional representation of the inhibition function for one set of kinetic constants and a pH range of between 5 and 8, and shows the influence of total substrate concentration and pH on the micro-organism specific growth rate.

From the graphic representation of the inhibition function, it may be concluded that at low pH values the inhibition effects are more severe, due to the high un-ionised acetic acid concentrations.

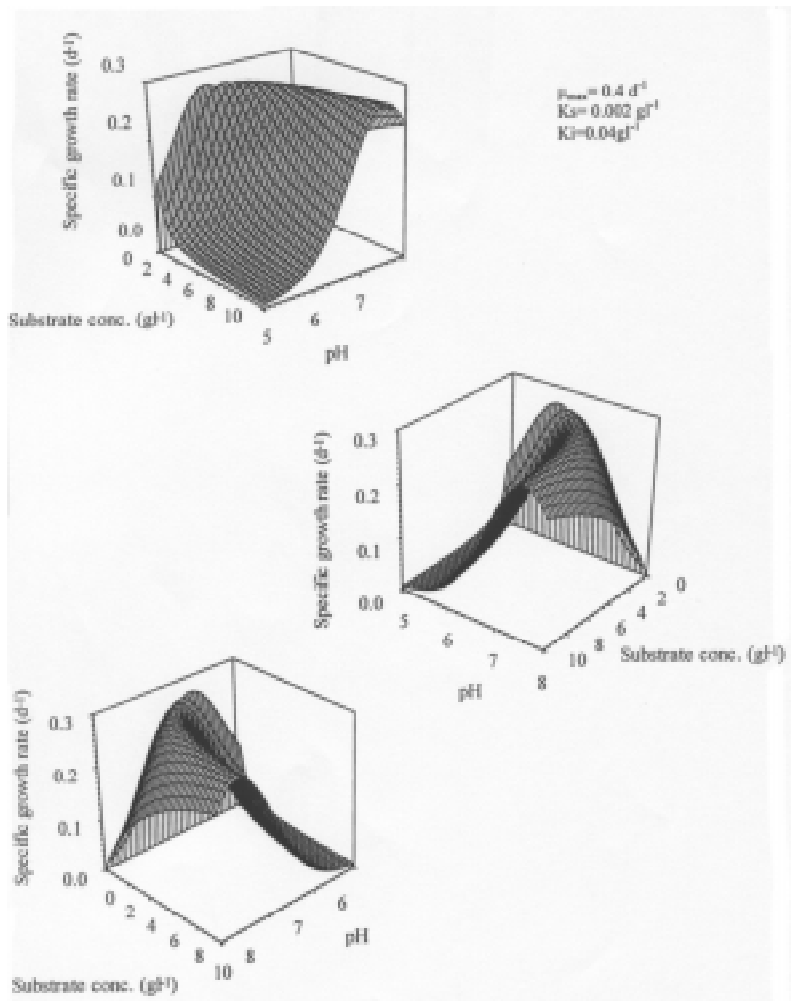


Figure 1
Tridimensional representation of the inhibition function

This suggests that low pH values enhance reactor instability and can lead to the failure of the process. At high pH values, the micro-organisms show a shorter response time, which suggests that reactor recovery is more difficult and longer recovery times will be needed.

The inhibition function can be introduced in the micro-organism mass balance, shown in the following equation:

$$\frac{dX}{dt} = \frac{X_0}{\sigma} - \frac{X}{\sigma} + \mu \times X - K_d \times X \quad (5)$$

where:

- X = micro-organism concentration in the reactor ($\text{g}\cdot\text{l}^{-1}$)
- X_0 = micro-organism concentration in the feed ($\text{g}\cdot\text{l}^{-1}$)
- σ = hydraulic retention time (d)
- K_d = decay coefficient (d^{-1})
- t = time (d)

and it can also be introduced in the substrate mass balance, resulting in the equation:

$$\frac{dS}{dt} = \frac{S_0}{\sigma} - \frac{S}{\sigma} + \mu \times \frac{X}{Y} \quad (6)$$

where:

- S = substrate concentration in the reactor ($\text{g}\cdot\text{l}^{-1}$)
- S_0 = substrate concentration in the feed ($\text{g}\cdot\text{l}^{-1}$)
- Y = yield coefficient, mass of micro-organisms produced per mass of substrate utilised ($\text{g}\cdot\text{g}^{-1}$).

The model developed thus far assumes the following:

- methanogenesis is assumed as the limiting step;
- the substrate is acetic acid;
- there is no lag-phase for biological growth;
- there are no methanogenic micro-organisms in the influent to the reactor ($X_0 = 0$).

Since the model describes the behaviour of a continuously-fed reactor without solids recirculation, the solids retention time has the same value as the hydraulic retention time. Figure 2 resumes the equations for the biological model of the methanogenic phase of an anaerobic digester.

Simulation studies

Several simulations were performed using the biological model in order to study the anaerobic reactor performance and stability. An operational temperature of 38°C and a hydraulic retention time of 10 d were considered in all simulations. The kinetic and chemical constants used in the simulations are presented in Table 1.

Start-up of a digester

To study the effect of certain parameters on the success for reaching a steady state, several simulations on reactor start-up were performed.

Figures 3 and 4 show the effect of varying the initial concentration of micro-organisms (inoculum concentration) and pH on the start-up of an anaerobic

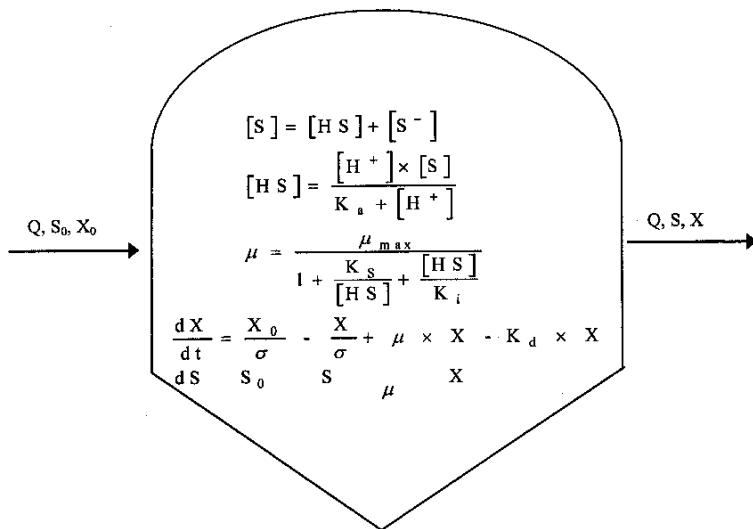


Figure 2
The biological model equations

Constants	Values	Units
μ_{max}	0.4	d ⁻¹
K_s	0.002	g·l ⁻¹
K_i	0.04	g·l ⁻¹
Y	0.05	g·g ⁻¹
K_d	0.03	d ⁻¹
pK_a	4.5	

digester. The results of the simulations were obtained for a constant substrate concentration in the feed of 10 g·l⁻¹. Simulations shown in Fig. 3 were performed for four values of initial micro-organism concentrations: X_i : 0.15 g·l⁻¹, 0.05 g·l⁻¹, 0.01 g·l⁻¹ and 0.001 g·l⁻¹. In Fig. 4 a similar study was performed for four values of pH: 5, 6, 7 and 8.

It is observed that the lower the initial micro-organism concentration the longer the time taken to attain a stationary state at any pH value. Therefore, the model agrees with the general observation in the field that the time needed for the start-up of a digester can be decreased by increasing the inoculum concentration. If the initial micro-organism concentration is not high enough, the start-up of the digester at lower pH values leads to the failure of the process and no stationary state is attained. On the other hand, high initial micro-organism concentrations provide fast substrate degradation, preventing the accumulation of inhibitory substrate concentrations in the reactor, and allowing it to reach steady state.

High pH values cause low un-ionised substrate concentration and, consequently, the response time of the reactor will be much higher. Thus, the anaerobic digestion start-up must be performed in an ideal situation: The criteria of the pH range and the initial micro-organism concentration must be satisfied. Consequently, stable stationary states within short response time will be attained.

The simulations on start-up conditions for several initial micro-organism concentrations predict the failure of the process at low pH values, while at high pH values a stationary state is always attained, although the response time may be very long. The simulation with an initial micro-organism concentration of $X_i = 0.001$ g·l⁻¹, in Fig. 3, predicts the failure of the process for pH values of lower than 7. The simulation with a higher concentration of $X_i = 0.05$ g·l⁻¹ predicts the failure of the process only for pH values of lower than 6.4 and predicts smaller response times in order to attain a stationary state at pH values of higher than 6.4.

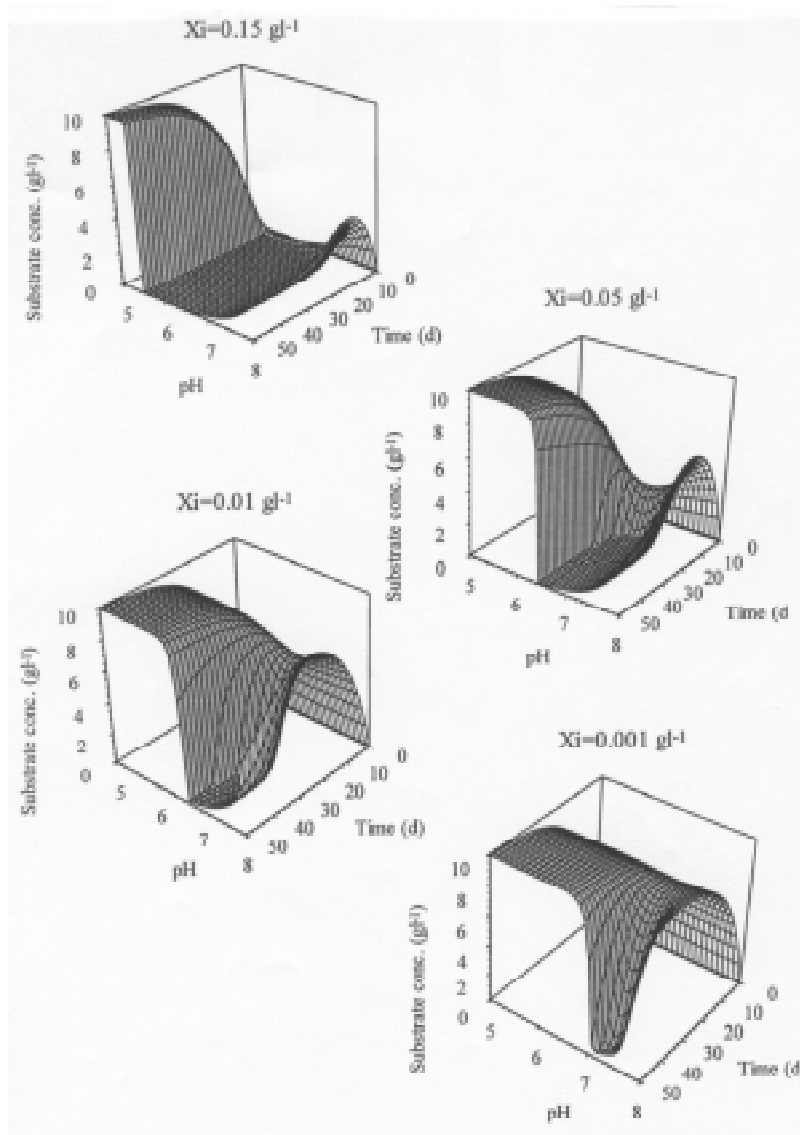


Figure 3
Simulations on start-up conditions for an anaerobic digester, for several X_i values

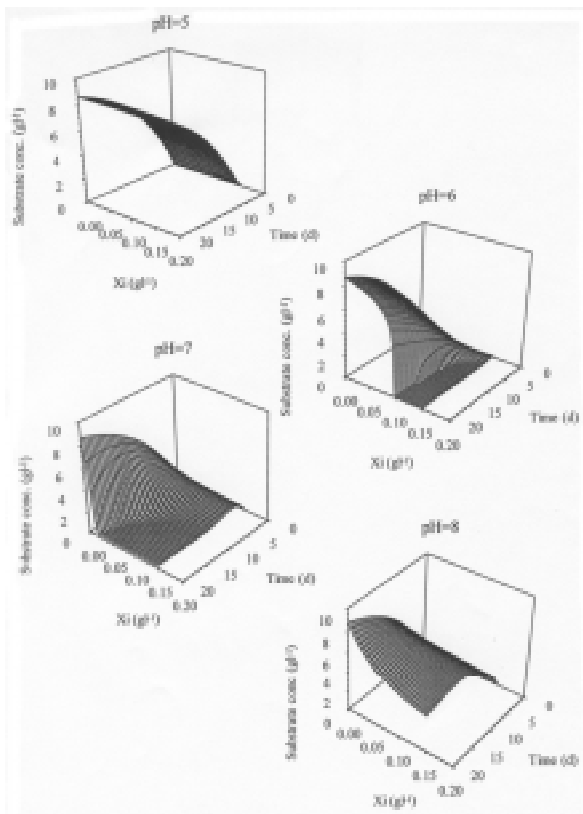


Figure 4

Simulations on start-up conditions for an anaerobic digester, for several pH values

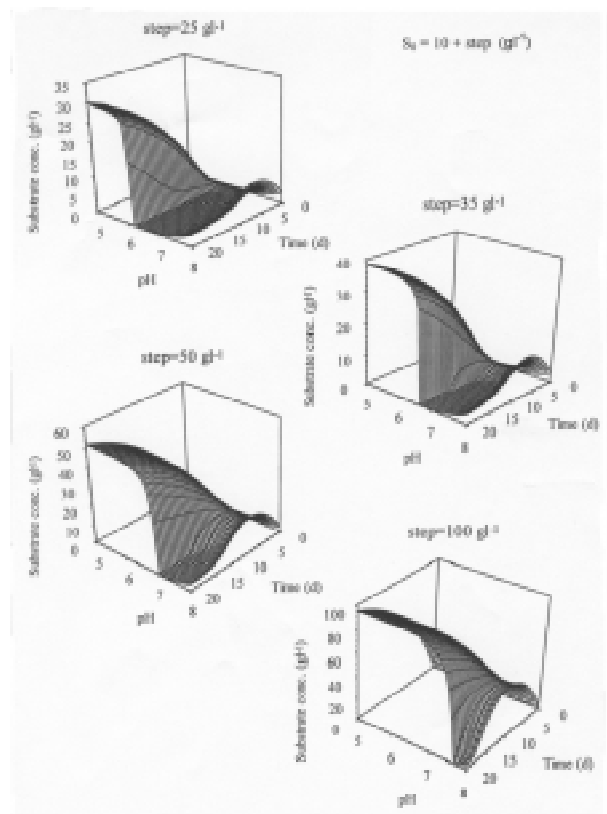


Figure 5

Simulations of an anaerobic digester response to a change in the feed characteristics - a step increase on the substrate concentration

Effects of changing the feed characteristics

Another set of simulations for the study of transient states was also performed through a change of the characteristics of the feed stream after a steady state had been reached previously. Several changes in the organic loading rate were thus simulated, utilising two different methods: The simulation of a step increase on the influent substrate concentration and the simulation of a step increase on the flow rate.

A step increase on the influent substrate concentration

Figure 5 shows the effect of a step increase on the influent substrate concentration of an anaerobic reactor, simulated for a pH range of between 5 and 8 and an initial feed substrate concentration of 10 g·l⁻¹. Simulations of the model were performed for four values of step increases: 25 g·l⁻¹, 35 g·l⁻¹, 50 g·l⁻¹ and 100 g·l⁻¹.

The small step increases in the substrate concentrations of the feed, obtained by steps of 25 g·l⁻¹ and 35 g·l⁻¹, show a good response of the process for pH values of higher than 6.1 and 6.6, respectively. The highest step increase (100 g·l⁻¹) indicates a very small stable region, slow responses and steady states with large substrate concentrations. For pH values of lower than 7.7, this step increase (100 g·l⁻¹) causes process failure, since un-ionised acid concentration escalates to a critical range. Thereafter, severe inhibition occurs. Moreover, for high pH values the response times required are considerably longer and the stationary states are obtained for high substrate concentrations, resulting in an unacceptable efficiency of the process. This is due to the low un-ionised substrate concentration levels available for the micro-organisms at those pH values.

The introduction of high step increases of 50 g·l⁻¹ and 100 g·l⁻¹, shows the failure of the process for higher pH values. The critical pH, below which the process fails due to un-ionised substrate inhibition, increases with higher step changes. High step increases lead to steady states with higher substrate concentration values.

It is, therefore, extremely important to avoid sudden changes on the feed substrate concentration, in order to allow the process to stabilise and metabolise the substrate concentration present, within a reasonable response time. Furthermore, it prevents process failure due to inhibitory un-ionised substrate concentrations.

Good process response may be obtained by a gradual increase (ramp forcing) of the feed substrate concentration instead of a step increase.

A step increase in the flow rate

Figure 6 presents the effects of step increases in the feed flow rate, for the same organic loading rate values for studied step increases of the substrate concentration.

High step increases in the feed flow rate inhibit the performance of an anaerobic digester, decreasing its stability. Different transient responses were observed for simulations of either a step increase in the substrate concentration (Fig. 5) or a step increase in the flow rate to a reactor (Fig. 6), for the same organic loading rate values. A higher degree of inhibition is observed when a step increase in the flow rate is simulated than when a step increase in the substrate concentration is performed. Accordingly, Parkin and Owen (1986) reported that a high increase in influent flow rate resulted in a decrease of SRT in a single-stage, high-rate digester, leading to wash-out.

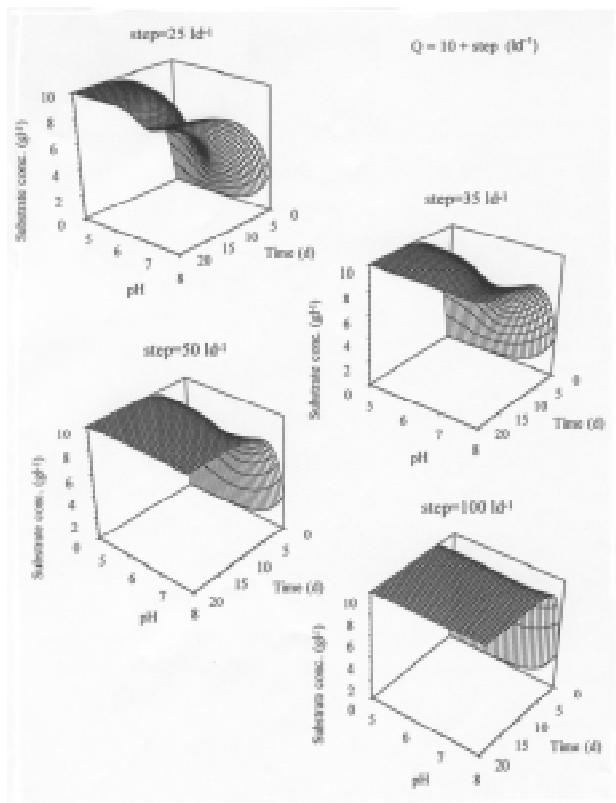


Figure 6

Simulations of an anaerobic digester response to a change in the feed characteristics - a step increase in the flow rate

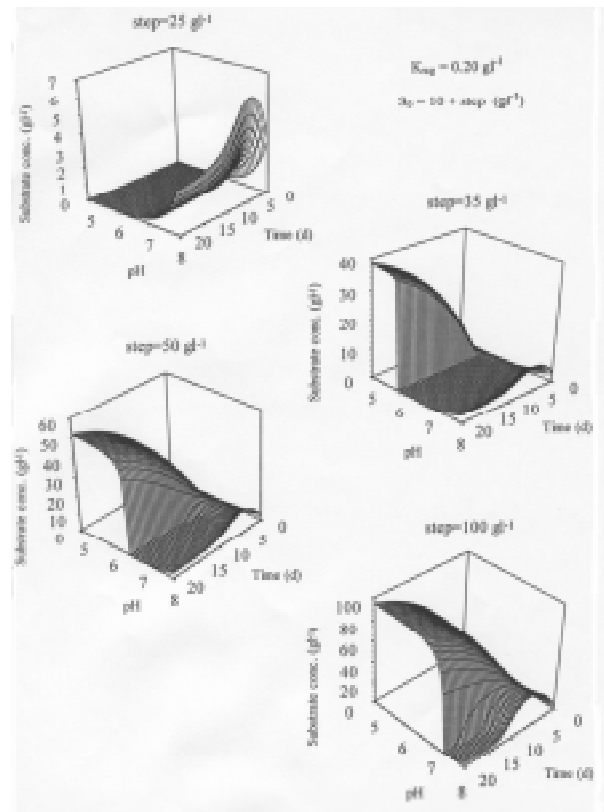


Figure 7

Simulations of the response of an anaerobic digester with wall growth to a change in the feed characteristics - a step increase in substrate concentrations

An obvious conclusion that can be drawn from this study is that the stability of an anaerobic reactor is very sensitive to the hydraulic retention time, being more severely affected by changes in the flow rate than by changes in influent substrate concentration. The maintenance of an adequate hydraulic retention time is essential for a good response of a single-stage anaerobic reactor.

The introduction of a wall-growth factor

An important problem that can appear in digester operation, and always difficult to avoid at laboratory scale, is of micro-organism growth on the digester walls. This situation often modifies the digester stability, allowing higher growth rates of the methanogenic bacteria and causing a digester to stabilise in conditions that would otherwise have led to digester instability and washout.

The kinetic equations from the dynamic model used for the simulation of digester performance can be modified to include the effects of wall growth. Topiwala and Hamer (1971) and Duarte (1981) previously considered the introduction of a factor for wall growth in modelling studies, in order to define the effect of wall growth in the steady state of an anaerobic reactor. In the present work, a wall-growth factor was also introduced in the study of transient conditions obtained in the operation of anaerobic reactors.

By introducing a wall-growth factor in the mass balance equations of the model, one can obtain the following modified model for the study of the wall-growth effects:

$$\frac{dX}{dt} = \frac{X_0}{\sigma} - \frac{X}{\sigma} + \mu \times \left(X + \frac{A}{V} \times X_w \right) - K_d \times X$$

$$\frac{dS}{dt} = \frac{S_0}{\sigma} - \frac{S}{\sigma} + \frac{\mu}{Y} \times \left(X + \frac{A}{V} \times X_w \right)$$

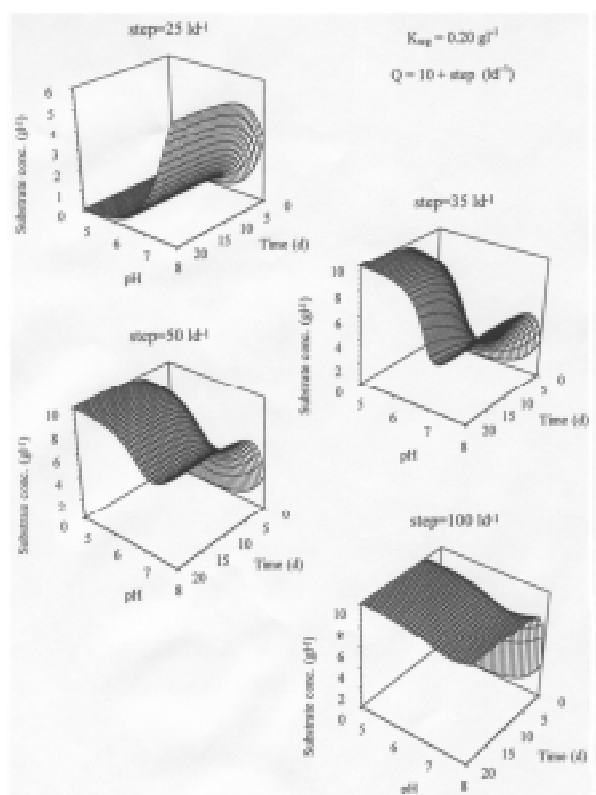


Figure 8

Simulations of the response of an anaerobic digester with wall-growth to a change in the feed characteristics - a step increase in the flow rate

where $A/V \times X_w = K_{wg}$ is the wall-growth factor, and can be defined as the mass of micro-organisms on the digester wall area divided by the digester volume. X_w is the micro-organism concentration on the wall (assumed constant), and A/V is the ratio of wetted surface area to volume of the digester. Simulations of the effect of a change in the feed characteristics (step increase) of an anaerobic reactor were again performed, this time assuming a wall-growth factor K_{wg} of $0.20 \text{ g}\cdot\text{l}^{-1}$.

It has been assumed in the simulations, that no micro-organism growth on the digester walls was present at the time that the step increase was performed and when simulation began. This assumption allows a better comparison of the differences observed in the absence and in the presence of wall-growth, under a step increase in the feed characteristics.

Figure 7 presents the simulation of the same step increases of $25 \text{ g}\cdot\text{l}^{-1}$, $35 \text{ g}\cdot\text{l}^{-1}$, $50 \text{ g}\cdot\text{l}^{-1}$ and $100 \text{ g}\cdot\text{l}^{-1}$ on the influent substrate concentration, in the presence of wall growth, for a pH range of 5 to 8 and an initial feed substrate concentration of $10 \text{ g}\cdot\text{l}^{-1}$.

The performance of a digester observed in this case can be compared to the previous simulations of the same step additions (Fig. 5), where the assumption of micro-organism growth on the digester walls was not considered. The presence of micro-organism growth on the digester walls leads to an improvement of the response of the reactor towards inhibition, as it can be seen by comparing both step simulations (Figs. 5 and 7). Therefore, inhibition, due to a high concentration of un-ionised acetic acid, is not detected at conditions of total acetic acid concentration and pH which was expected to be responsible for micro-organism inhibition. pH values in previous step simulations led to digester failure. Consequently, a stationary state is now obtained.

Thus, the effects of wall growth, namely an increased stability of an anaerobic digester in the presence of un-ionised acetic acid concentrations at inhibitory levels, may be observed through simulations with the model and with the inclusion of a wall-growth factor.

By assuming a value of the wall-growth factor K_{wg} , less inhibitory conditions will be observed with increasing values of K_{wg} . This is dependent upon the amount of wall growth.

Simulations on the effect of a step increase in the flow rate is also presented in Fig. 8, for the same organic loading rates, and the effects of wall growth were also considered. Again, it is observed that the wall-growth effect improves the stability of an anaerobic digester under drastic changes of its operational conditions (Figs. 6 and 8).

Conclusions

The concentration of un-ionised volatile acids (assumed to be acetic acid) is a critical parameter that governs the performance of an anaerobic treatment process and its behaviour during start-up and under other transient conditions. The simulations performed in the present work emphasise the role of un-ionised acetic acid concentration as the limiting substrate and as the inhibitory agent of the microbial growth. The un-ionised acetic acid concentration depends on both total acetic acid concentration and pH. Therefore, the maintenance of ideal conditions for the process such as an adequate pH range, is essential for proper operation.

Other conditions are also important in the start-up of the process in order to attain a steady state. Simulations on the start-up of a digester with several initial micro-organism concentrations are good examples. Completely different digester behaviour was obtained for several simulations, where the same conditions were constant (the same reactor volume, the same hydraulic retention time and the same substrate concentration in the feed), but where the initial micro-organism concentrations were varied from $0.15 \text{ g}\cdot\text{l}^{-1}$ to $0.001 \text{ g}\cdot\text{l}^{-1}$. High initial micro-organism concentrations may be enough for a digester to attain a steady state, under defined operational conditions such as a given pH while the same does not happen at low initial micro-organism concentrations.

Simulations on step increases in the organic loading rate of a reactor, either by changes of the influent substrate concentration or by changes of the influent flow rate, resulted in the conclusion that the anaerobic reactor stability is more sensitive to step changes in the influent flow rate, than to similar step changes in the influent substrate concentration. The importance of the hydraulic retention time for system design or operation is reinforced by this study.

The introduction of a factor for micro-organism growth on the digester walls in the dynamic model improved the description of transient conditions in anaerobic digesters. In situations where micro-organism wall growth was observed, anaerobic digesters displayed better reaction with regard to the inhibition of un-ionised volatile acids, step increases of the feed-substrate concentration and the influent flow rate. The extent of wall-growth factor determines the extent of the improvement on the digester stability.

Acknowledgement

The authors would like to acknowledge a grant from Fundação para a Ciência e a Tecnologia (PRAXIS XXI/BTI/14342/97).

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