# 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; Alatiqui 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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## 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:

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

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 ($g \cdot l^{-1}$)
[HS] = un-ionised substrate concentration ($g \cdot l^{-1}$)
$[H^+]$ = hydrogen ion concentration ($g \cdot l^{-1}$)

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

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