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Design of a multi-model observer-based estimator for anaerobic reactor monitoring

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Abstract

A multi-model observer based estimator (OBE), which consists of a set of simple sub-models describing typical process states and a knowledge-based system, was developed for monitoring and long-term prediction of the anaerobic digestion process. The knowledge-based system uses biogas and pH measurements for process diagnosis, while OBE uses fluorescence-based measurements of chemical oxygen demand (COD) and volatile fatty acids (VFAs) for estimating process outputs. The approach was tested on experimental results obtained from the operation of a lab-scale anaerobic reactor. The sub-models used either Monod or a combination of zero- and first-order rate expressions. A comparison showed that while both multi-model OBEs featured rapid convergence and good stability, the combined zero- and first-order kinetic equations provided better long-term prediction accuracy.

Keywords: Multi-model; Observer-based estimator; Monitoring; Anaerobic reactor; Multi-wavelength fluorometry

1. Introduction

The anaerobic digestion process has a potential for efficient degradation of high strength wastewater while producing low amounts of biomass and using less energy than in aerobic wastewater treatment. Despite these advantages, industrial application of the anaerobic digestion is limited by its high sensitivity to uncontrollable input perturbations. This is why on-line monitoring and control of the anaerobic digestion process is an area of active research and development.

Initial attempts to control anaerobic reactors were based on real-time biogas measurements (Pullammanappallil, Svoronos, Chynoweth, & Lyberatos, 1998; Steyer et al., 1999; Vanrolleghem & Lee, 2003). Although this control approach provided acceptable reactor performance, biogas measurements only give indirect information on the effluent quality. Recently developed spectrometric methods such as near infrared (NIR) or mid infrared (MIR) spectrometry provide direct measurements of key process state variables (Harbeck et al., 2004; Steyer et al., 2002; Tosi et al., 2003; Vaidyanathan et al., 2001). Moreover, multi-wavelength fluorometry offers a less expensive solution for on-line monitoring concentrations of carbohydrates and volatile fatty acids in industrial anaerobic reactors (Morel, Santamaria, Perrier, Guiot, & Tartakovsky, 2004).

Variable structure model (multi-model) of the anaerobic digestion process has demonstrated several advantages in comparison with comprehensive process models (Dainson et al., 1995). The variable structure model (VSM) of the anaerobic reactor was shown to follow complex process kinetics with an acceptable accuracy while using relatively simple kinetic equations with a limited number of model parameters (Tartakovsky, Morel, Steyer, & Guiot, 2002). Because of its simplicity, the VSM can be conveniently used for on-line estimation of state variables and closed-loop process control (Tartakovsky et al., 2005).

In this work, a variable structure model was used as the basis for the design of a multi-model observer-based estimator for on-line monitoring of an anaerobic reactor. Then a knowledge-based system was developed to diagnose process states. The estimator used on-line measurements of chemical oxygen demand (COD)

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Nomenclature

a	volatile fatty acid concentration
D	dilution rate
F	volumetric input flow rate
l_i	Euclidean distance between the sphere surfaces
m	number of state variables
n	number of sub-models
Q	gaseous output flow rate
Q_m	methane flow rate
r_i	biotransformation rate
r_max	maximal biotransformation rate
s	substrate concentration
V	reactor volume
w, γ	OBE design parameters
y	vector of multi-model outputs

Greek letters

β	weight vector
Δ_i	Euclidean distance between the sphere centres
θ	vector of kinetic parameters
$\hat{\theta}$	vector of estimated kinetic parameters
ξ	vector of state variables
$\hat{\xi}$	vector of estimated state variables
Φ	coordinate of the experimental point
$\Phi_{i,r}$	radius of the sphere i
$\Phi_{i,0}$	center of the sphere i
Ω, Γ	matrices of OBE design parameters

and volatile fatty acids (VFA) obtained by a multi-wavelength fluorometric system (Morel et al., 2004).

2. Theory

2.1. Variable structure model

The variable structure model of the anaerobic digestion process consists of a set of sub-models each of which describes a typical process state. The choice of the active (leading) sub-model is handled by a knowledge-based system (Tartakovsky et al., 2002). The VSM used in this study describes methanogenic, organic overload, and acidogenic states of the anaerobic digestion process. This choice of typical states was based on the expert knowledge and agrees with a widely recognized classification of the process (Marsili-Libelli & Müller, 1996; Pullammanappallil et al., 1998; Steyer et al., 2002). In brief, the methanogenic state is described by a moderate organic load and a near neutral pH. At this state, most of the organic matter is transformed to methane thus leading to low concentrations of VFAs in the reactor effluent. An organic load increase or an insufficient hydraulic retention time (HRT) may lead to organic overload, which is characterized by the appearance of significant concentrations of VFAs in the effluent. The organic overload state is unstable and often leads to the acidogenic state, which occurs at high organic loads or inadequate buffering capacity. This state is characterized by incomplete removal of organic matter, poor methane production, high level of VFAs in the reactor effluent and low (less than 6.5) reactor pH. More information on the VSM definition can be found elsewhere (Tartakovsky et al., 2002, 2005).

Table 1
Zero- and first-order kinetics used in the OBE#1

State variable	Process state		
	Methanogenic	Organic overload	Acidogenic
(s) COD	$-r_{\mathrm{max},s}s$	$-r_{\mathrm{max},s}$	$-r_{\mathrm{max},s}s$
(a) VFA	$-r_{\mathrm{max},a}a$	$-r_{\mathrm{max},a}s$	$-r_{\mathrm{max},a}s$
(Q_m) CH_4 flow rate	$-r_{\mathrm{max},m}s$	$-r_{\mathrm{max},m}$	$r_{\mathrm{max},m}\frac{K_\mathrm{I}}{K_\mathrm{I}+a}$

Notations: $r_{\mathrm{max},s}$, $r_{\mathrm{max},a}$, $r_{\mathrm{max},m}$ are the maximum biotransformation rates for COD, VFA, and methane flow rate, respectively. K_I is the VFA inhibition constant.

With the assumption of ideal mixing, material balances of carbohydrates (described as chemical oxygen demand, COD) and total VFAs in a continuous reactor are given by the following ordinary differential equations:

$$\frac{\mathrm{d}\zeta_{i,j}}{\mathrm{d}t} = r_{i,j}(\zeta_{i,j},t) + \frac{F}{V}(\zeta_{i,j}^{\mathrm{in}} - \zeta_{i,j}) - \frac{Q}{V};$$
$$i = 1,\ldots,n, \quad j = 1,\ldots,m \tag{1}$$

where ζ is the vector of state variables (species concentration), ζ^{in} the influent species concentration vector, r the biotransformation rate vector, F the volumetric input flow rate, V the reactor volume, n the number of sub-models, Q the gaseous output flow rate ($Q=0$ for COD and VFA), n the number of sub-models, and m is the number of state variables.

If an instant methane transfer from liquid to gas phase is assumed, then the methane flow rate (Q_m) can be expressed as:

$$Q_{m,i} = r_{i,j}(\zeta_{i,j},t)V; \quad i = 1,\ldots,n, \quad j = 1,\ldots,m \tag{2}$$

The vector of VSM outputs (y) is described as:

$$y_j(t) = \sum_{i=1}^{n}\beta_i\zeta_{i,j}; \quad \sum_{i=1}^{n}\beta_i = 1; \quad \beta_i \in [0,1] \tag{3}$$

where β_i is the weighting function.

In this study, two sets of kinetic dependencies $r_{i,j}(\zeta, t)$, were used in material balances (1) and (2). First, process kinetics was described by zero- and first-order kinetic equations given in Table 1 (VSM#1). Next, a combination of first-order and Monod kinetics was used (VSM#2, Table 2). This selection of equations

Table 2
First-order and Monod kinetics used in OBE#2

State variable	Process state		
	Methanogenic	Organic overload	Acidogenic
(s) COD	$-r_{\mathrm{max},s}\frac{s}{K_\mathrm{s}+s}$	$-r_{\mathrm{max},s}\frac{s}{K_\mathrm{s}+s}$	$-r_{\mathrm{max},s}\frac{s}{K_\mathrm{s}+s}$
(a) VFA	$-r_{\mathrm{max},a}a$	$r_{\mathrm{max},a}s$	$r_{\mathrm{max},a}s$
(Q_m) CH_4 flow rate	$r_{\mathrm{max},m}\frac{s}{K_\mathrm{s}+s}$	$r_{\mathrm{max},m}\frac{s}{K_\mathrm{s}+s}$	$r_{\mathrm{max},m}\frac{s}{K_\mathrm{s}+s}\frac{K_\mathrm{I}}{K_\mathrm{I}+a}$

Notations: $r_{\mathrm{max},s}$, $r_{\mathrm{max},a}$, and $r_{\mathrm{max},m}$ are the maximum biotransformation rates of COD, VFA, and methane flow rate, respectively. K_I is the VFA inhibition constant, and K_s is the Monod half-saturation constant.