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Modelling and parameter estimation of a two-stage anaerobic digestion system for the treatment of tequila vinasses

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Abstract
The estimation of kinetic parameters and yield coefficients of a two-stage anaerobic digestion model based on experimental data obtained from the treatment of tequila vinasses is considered in this paper. The proposed model is derived from mass balances of two fixed-bed up-flow bioreactors where the acidogenic phase takes place in the first bioreactor, whereas the second one contains a mixture of acidogenic and methanogenic biomass. The Marquardt method via a study of parametric sensitivity was implemented for estimating parameters and initial conditions using two sets of raw experimental data. The model and the estimated parameters were statistically analyzed to validate the results. Finally, the model was tested with a different set of raw experimental data showing satisfactory prediction capabilities.

Keywords
Anaerobic digestion; two-stage; parameter estimation; modelling; Marquardt method

INTRODUCTION

Modelling of Anaerobic Digestion (AD) is a complex task because this process exhibits nonlinear behavior, the presence of influent disturbances, uncertainties on biomass concentrations, lack of online sensors, among others (Mendez-Acosta *et al*., 2010). Operational instabilities of the process are mainly due to the accumulation of Volatile Fatty Acids (VFA) (Moletta *et al*., 1985), pH variability (Rajeshwari *et al*., 2001), high organic load concentrations, low hydraulic retention times (HRT) and the presence of inhibitory compounds. Several models for one stage processes have been presented with the aim of monitoring and control AD processes (*i.e.*, Moletta *et al*., 1985; Guiot, 1990; Bernard *et al*., 2001; Batstone *et al.*, 2002).

Even though, some authors (*e.g.*, Ghosh and Klass, 1982) proposed the physical separation of AD in two stages based on pH selectivity. This configuration has been evaluated for the treatment of different kinds of wastewaters (Ke *et al*., 2005) showing, in general, that two-stage AD process increases growth rates, consumes higher organic loads, uses low start-up times, generates high-purity biogas and improves process stability (Azbar and Speece, 2001; Ke *et al*., 2005; Demirel and Yenigun, 2002; Lizarraga-Palazuelos, 2010). To our knowledge, only few two-stage anaerobic digestion models have been proposed (*e.g.*, Blumensaat and Keller, 2005) to describe this process. However, these have had limited success primarily due to their high dimension which prevent the implementation of advanced control strategies (Steyer *et al*, 2005). Recently, Palacios-Ruiz *et al*., (2008) have proposed a simple model based on mass balances that have been successfully used in the proposal of robust control schemes. In this work, such a model was modified to take into account the difference between acidogenic and metanogenic bacteria and its distribution between the two reactors (stages). The modified model was identified by using the Marquardt's method (Constatinides and Mosatoufi, 2000) through parametric sensitivity analysis (Khalil, 2006), which allows the simultaneous estimation of parameters, unknown state variables and initial conditions. Finally, the proposed model is validated using a set of independent experimental data.

MATERIALS AND METHODS

Description and Modelling of the two-stage AD system

An instrumented two-stage AD process based on two up-flow fixed-bed continuous bioreactors connected in series was used for generating VFA and COD data. Such process was applied in the treatment of tequila vinasses.

The proposed model is developed under the following assumptions: 1) the first bioreactor (stage) contains acidogenic bacteria which is in charge of hydrolysis and the transformation of organic matter into VFA; 2) the second bioreactor (stage) includes a mixture of acidogenic and methanogenic biomass which transforms VFA into methane and carbon dioxide; 3) both bioreactors operate isothermally; 4) the process pH was set to 5.4 for the acidogenic reactor, and 7.2 for the methanogenic reactor; 5) VFA are mainly composed by acetic acid. The model describes in an easy manner two-stage AD processes to promote their simple application for control purposes, and it is presented by the following differential equations:

<u>*Acidogenic Bioreactor*</u>

$$\begin{aligned}\dot{X}_{1,1} &= \mu_{1,1}(S_{1,1})X_{1,1} - \alpha_1 D_1 X_{1,1}\\ \dot{S}_{1,1} &= (S_{1,in} - S_{1,1})D_1 - k_1\mu_{1,1}(S_{1,1})X_{1,1}\\ \dot{S}_{2,1} &= (S_{2,in} - S_{2,1})D_1 + k_2\mu_{1,1}(S_{1,1})X_{1,1}\end{aligned} \tag{1}$$

<u>*Methanogenic Bioreactor*</u>

$$\begin{aligned}\dot{X}_{1,2} &= \mu_{1,2}(S_{1,2})X_{1,2} - \alpha_2 D_2 X_{1,2}\\ \dot{X}_{2,2} &= \mu_{2,2}(S_{2,2})X_{2,2} - \alpha_2 D_2 X_{2,2}\\ \dot{S}_{1,2} &= (S_{1,2} - S_{1,1})D_2 - k_3\mu_{1,2}(S_{1,2})X_{1,2}\\ \dot{S}_{2,1} &= (S_{2,in} - S_{2,1})D_1 - k_4\mu_{2,2}(S_{2,2})X_{2,2} + k_5\mu_{1,2}(S_{1,2})X_{1,2}\end{aligned} \tag{2}$$

with $\mu_{1,1}(S_{1,1}) = \frac{\mu_{1,1max}S_{1,1}}{k_{S1,1}+S_{1,1}}$, $\mu_{1,2}(S_{1,2}) = \frac{\mu_{1,2max}S_{1,2}}{k_{S1,2}+S_{1,2}}$, and $\mu_{1,2}(S_{2,2}) = \frac{\mu_{2,2max}S_{2,2}}{k_{S2,2}+S_{2,2}+\left(\frac{S_{2,2}}{k_{I2}}\right)^2}$, where X_{ij} represents the biomass and D_j is the dilution rate. S_{1j} and S_{2j} are the Chemical Oxygen Demand (COD) and Volatile Fatty Acid (VFA) concentrations, respectively. The subindex $j = 1$ represents the acidogenic bioreactor whereas $j = 2$ denotes the methanogenic bioreactor, and subindex $i = 1,2$ is related to acidogen and methanogen microorganisms cultures, respectively. k_{1-5} are the digester's yield coefficients. The specific growth rate $\mu_{1,j}$ correspond to Monod kinetics, meanwhile $\mu_{2,j}$ follows Haldane kinetics. Finally, α_1 and α_2 represent the fraction of biomass that is not attached to the support, and thus, leaves the bioreactor because of the dilution effect (Bernard *et al*., 2001).

RESULTS AND DISCUSSION

The Marquardt method (Constantinides and Mosatoufi, 2000) applied by parametric sensibility analysis was implemented using two sets of raw experimental data involving measurements of COD and VFA. Afterwards, an independent data set was used to validate the parameters obtained from the parameter estimation, which are shown in Table 1.

Table 1. Values of parameter estimation

Acidogenic Bioreactor			Methanogenic Bioreactor		
Parameters	Value	Units	Parameters	Value	Units
$\mu_{1,1max}$	0.27	(d^{-1})	$\mu_{1,2max}$	0.5	(d^{-1})
$k_{S1,1}$	24	$(g\ COD/L)$	$k_{S1,2}$	3.5	$(g\ COD/L)$
α_1	0.13	(-)	$\mu_{2,2max}$	0.29	(d^{-1})
k_2/k_1	3.5	$(mmol\ VFA/\ g\ COD)$	$k_{S2,2}$	16	$(mmol\ VFA/L)$
			k_{I2}	27	$(mmol\ VFA/L)^{1/2}$
			α_2	0.38	(-)
			k_5/k_3	0.9	$(mmol\ VFA/\ g\ COD)$

Regarding growth rates, tequila vinasses were degraded slower than other kind of vinasses, *e.g.*, wine vinasses, which can be explained by the lower value of $\mu_{1,1max}$ and $\mu_{1,2max}$ in comparison to those reported for wine vinasses (Bernard *et al.*, 2001). Nevertheless, notice that the estimated values are within the variation ranges previously reported for the treatment of wine vinasses. On the other hand, one of the most important values is α, which had been set to 0.5 as initial value, but it decreases in both bioreactors reflecting a good biomass adherence to the used support.

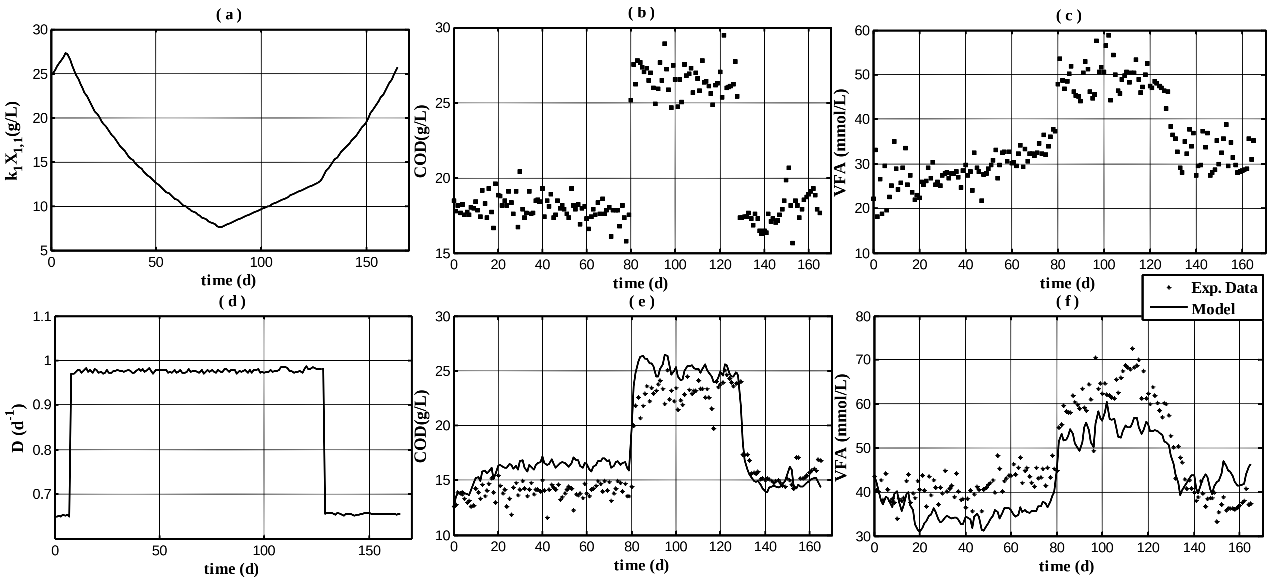

Figure 1. Acidogenic Bioreactor: (a) Biomass prediction, (b) Inflow COD concentration, (c) Inflow VFA concentration, (d) Dilution rate, (e) Comparison of COD experimental data and model predictions, (f) Comparison of VFA experimental data and model predictions.

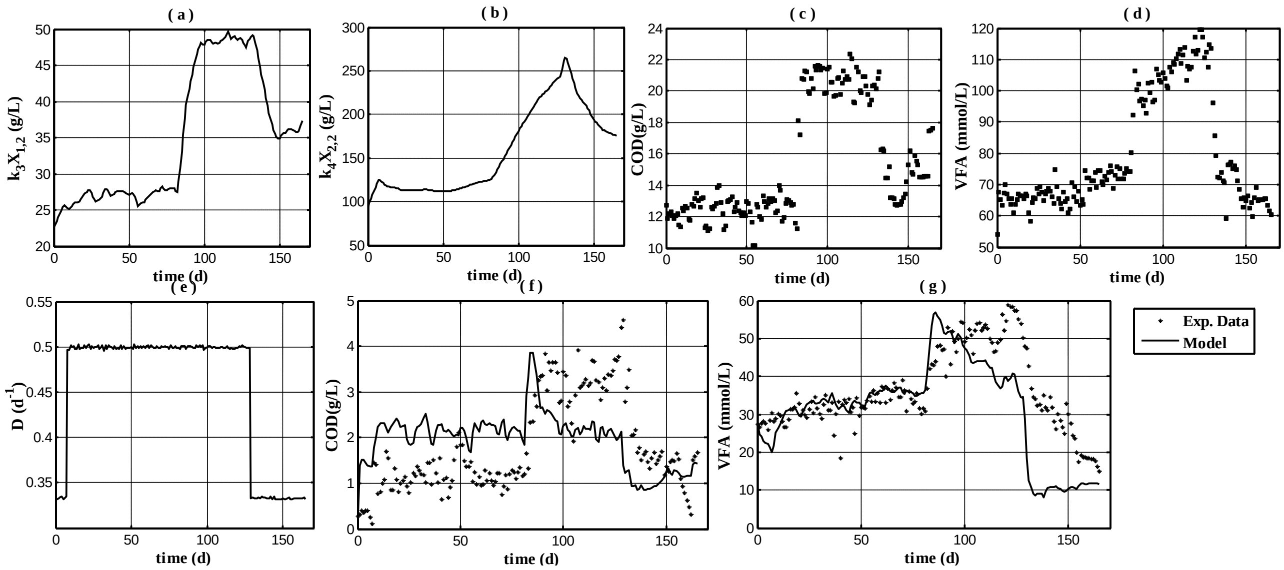

Figure 2. Metanogenic Bioreactor: (a) Acidogenic biomass prediction, (b) Inflow COD concentration, (c) Inflow VFA concentration, (d) Comparison of VFA experimental data and model predictions, (e) Dilution rate, (f) Comparison of COD experimental data and model predictions, (g) Comparison of VFA experimental data and model predictions.

Table 2. Statistical analysis results

Bioreactor	Square Residuals	Determination Coefficient R^2	F_0	F^*
Acidogenic	2.952	0.932	889.744	2.460
Mehtanogenic	14.356	0.851	853.174	2.102

In order to validate the proposed model (1-2), a statistical analysis (Table 2) was applied for both bioreactors represented by determination coefficients and the Fisher's test (Foment and Bishoff, 1990, Aceves-Lara, *et al.*, 2005). Notice that the model is not fully identifiable and the risk of parameter compensation is always possible. In fact, it was only possible to estimate $k_1X_{1,1}$, $k_3X_{1,2}$, and $k_4X_{2,2}$ instead of $X_{1,1}$, $X_{1,2}$, and $X_{2,2}$, independently. However, predictions for VFA and COD computed with the set of estimated parameters, fit acceptably experimental data even in the presence of noisy and corrupted data and follow an adequate dynamical behavior (see Figures 1-2).

CONCLUSIONS

In this paper, a two-stage anaerobic digestion model was proposed and satisfactorily identified with two different experimental data sets, and successfully validated using an independent data set. Results show that the proposed model, together with the computed parameters, reproduces in a good way the digester behavior. The model was rigorously tested and statistically proved what makes it a reliable model that can be used for control purposes, as well as for further scaling up of the two-stage AD process to pilot and industrial levels having a high impact in tequila industry.

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