IDENTIFICATION OF A BIO-METHANIZATION PROCESS: A CASE STUDY

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Abstract. We present the procedure that we have used to obtain a satisfactory mathematical model for a bio-methanization reactor (anaerobic digestion).
A non-linear state-space representation (five state variables) is adopted for the digester, which is inspired by the well-known work of Hill-Barth. The influent feed rate, the influent chemical composition and the gas production have been measured once every day for 160 days. From these data, the parameters of the model are, in a first step, calibrated by trial-and-error using a least-squares criterion on the gas production. In a second step, adaptative parameters are identified in order to improve the simulation capabilities of the model.

Keywords. Biotechnical processes, Identification, Parameter estimation.

INTRODUCTION

This paper presents the results of the identication of a mathematical model of a biomethanization process with special emphasis on the methodology that was used.

Biomethanization is an anaerobic fermentation process where biodegradable matter is transformed into simpler compounds with a smaller BOD. Under suitable conditions, this decomposition is linked to methane gas production and the residual sludge may be used as a liquid, non-odoreous plant fertilizer.

Hence such a process represents an interesting path for the recycle of organic wastes coming from agriculture, household, food industries, slaughterhouses, ... The identification of such a biochemical process was considered as a necessary step towards the implementation of regulation schemes for industrial-scale methanizers [1].

To the authors' knowledge, very few research have been conducted in this area, except for the well-known works of Greaf and Andrews (1974)[2] and Hill and Barth (1977)[3].

This identification was performed from an input-output sequence of daily measured data for a period of 160 days on a 60 liters methanizer of the laboratory of biotechnology of the university. This methanizer was fed with slaughterhouse wastes (cattle rumen contents).

THE MATHEMATICAL MODEL

The proposed mathematical model is a modi-

fied version of the model of Hill and Barth [3]. It consists in the following equations.

$$\frac{dS_o}{dt} = - GS_o - \beta X_1 S_o + GPS_{oi}$$

$$\frac{dX_1}{dt} = (\mu_1 - k_{d1} - G) X_1$$

$$\frac{dS_1}{dt} = - GS_1 + \beta X_1 S_o - \frac{\mu_1 X_1}{Y_1}$$

$$\frac{dX_2}{dt} = (\mu_2 - k_{d2} - G) X_2$$

$$\frac{dS_2}{dt} = - GS_2 + Y_b \mu_1 X_1 - \frac{\mu_2 X_2}{Y_2}$$

$$Q = Y_G \mu_2 X_2$$

$$\mu_1 = \frac{\hat{\mu}_1}{1 + \dfrac{K_{m1}}{S_1}}$$

$$\mu_2 = \frac{\hat{\mu}_2}{1 + \dfrac{K_{m2}}{S_2}}$$

The symbols are defined at the end of the paper. This model is suited to continuously fed, completely mixed, constant temperature (35°C) methanizers and is schematized at fig. 1.

It consists in four stages : in a first one, it is assumed that a part P of the introduced volatil solids is hydrolized at a rate βX_1, through extracellular enzymes from the group of acidogenic bacteria.

In a second stage, it is assumed that solubilized volatil organics are metabolized by the acidogenic bacteria and that this results in volatil fatty acids (VFA) in concentration S_2 in the methanizer.

In a third stage, those VFA are metabolized by methanigenic bacteria whose growth is linked with methane and carbon dioxide gas production.

EXPERIMENTAL DATA

The experiments were conducted on a 60 liters methanizer that was fed daily, except on Saturdays and Sundays. This operation took only a few minutes of the day.

The measured data consisted in :

i) the concentration in volatil solids in the feed,

ii) the daily gas production,

iii) the concentration in volatil acids in the methanizer and other more biologically oriented measurements.

Since the feed was stored in tanks whose capacity was large enough to supply a methanizer for various days, its concentration S_{oi} in volatil solids was only measured once per tank.

The daily gas production was measured just before the methanizer was fed. Since no measurements took place on Saturdays and Sundays, the gas production from Friday noon to Monday noon was measured on Monday and this value was divided by 3 in order to obtain a (rough) estimate of the average daily gas production during the week-end.

IDENTIFIABILITY OF THE MODEL

The model proposed above cannot be uniquely identified from sequences of measurements of G, S_{oi} and Q. That is, for such a sequence, there exists an infinity of values for the 12 parameters that will give a same $[Q - (S_{oi}, G)]$ relationship.

In order to solve this indetermination problem, it is necessary to reduce the number of parameters through the following state transformations :

$$\widetilde{X}_1 = \beta X_1 \qquad \widetilde{S}_o = \frac{S_o}{K_{m1}}$$

$$\widetilde{X}_2 = Y_G X_2 \qquad \widetilde{S}_1 = \frac{S_1}{K_{m1}}$$

$$\widetilde{S}_2 = \frac{S_2}{K_{m2}}$$

$$\widetilde{Y}_1 = \beta K_{m1} Y_1 \qquad \alpha = \frac{P}{K_{m1}}$$

$$\widetilde{Y}_2 = Y_G K_{m2} Y_2 \qquad \widetilde{Y}_b = \frac{Y_b}{\beta K_{m2}}$$
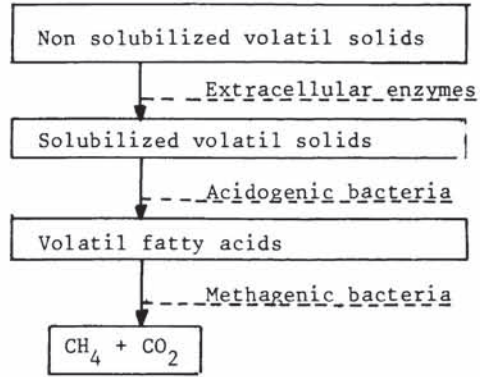
Fig.1.

Hence, the model becomes :

$$d\widetilde{S}_o/dt = - G\widetilde{S}_o - \widetilde{X}_1\widetilde{S}_o + \alpha GS_{oi}$$

$$d\widetilde{X}_1/dt = (\mu_1 - k_{d1} - G)\,\widetilde{X}_1$$

$$d\widetilde{S}_1/dt = - G\widetilde{S}_1 + \widetilde{X}_1\widetilde{S}_o - \widetilde{Y}_1^{-1}\mu_1 X_1$$

$$d\widetilde{X}_2/dt = (\mu_2 - k_{d2} - G)\,\widetilde{X}_2$$

$$d\widetilde{S}_2/dt = - G\widetilde{S}_2 + \widetilde{Y}_b\mu_1\widetilde{X}_1 - \widetilde{Y}_2^{-1}\mu_2\widetilde{X}_2$$

$$Q = \mu_2\,\widetilde{X}_2$$

$$\mu_1 = \frac{\hat{\mu}_1\widetilde{S}_1}{1+\widetilde{S}_1} \qquad \mu_2 = \frac{\hat{\mu}_2\widetilde{S}_2}{1+\widetilde{S}_2}$$

It contains only 8 parameters and is the model that we shall use in the next sections.

IDENTIFICATION : PART 1

The method :

The model was implemented on a PDP 11/34 computer and integration was performed with a Runge Kutta algorithm with 200 integration steps per day.

Its input consisted in numerical sequences of experimental data $S_{oi}(n)$ and $G(n)$ with $n = 1, \ldots, 160$ days.

The output of the model which is a sequence of computed daily gas production $\hat{Q}_i$ was compared to the sequence of experimental daily gas production Q_i and the model parameters were "manually" adjusted by a trial and error procedure so as to minimize :

$$E_N = \left[\frac{1}{N} \sum_{j=1}^{N} (Q_j - \hat{Q}_j)^2 \right]^{1/2}$$

where $N \leqslant 160$ is the length, in days, of the sequence under test.

Before to start this procedure, a sensitivity analysis of the model output with respect to the various parameters was performed with nominal parameters values proposed in [3] and a nominal steady state corresponding to imput conditions :

$$G = 0.1 \ d^{-1} \text{ and } S_{oi} = 2.5 \ gr/l$$

These nominal values of the parameters are :

$$K_{d1} = K_{d2} = 0.02 \quad \tilde{Y}_1^{-1} = 200 \quad \hat{\mu}_1 = 0.4$$

$$\tilde{Y}_2 = 1.7 \quad \tilde{Y}_b = 120 \quad \alpha = 2.25 \quad \hat{\mu}_2 = 0.4$$

The various computed sensitivities are given in table I with

$$\sigma(Q, p) = \frac{\partial p/p}{\partial Q/Q}$$

Table I.

$\sigma(Q, \hat{\mu}_1) = 0.05$	$\sigma(Q, \tilde{Y}_1) = 6$
$\sigma(Q, \hat{\mu}_2) = 0.04$	$\sigma(Q, \tilde{Y}_2) = 1$
$\sigma(Q, k_{d1}) = -0.008$	$\sigma(Q, \tilde{Y}_b) = 1$
$\sigma(Q, k_{d2}) = -0.066$	$\sigma(Q, \alpha) = 1$

It is seen that Q is quasi-insensitive to variations of $\hat{\mu}_1$, $\hat{\mu}_2$, k_{d1}, k_{d2}. Hence it was decided to keep $\hat{\mu}_i$, k_{di}, $i = 1, 2$ at their nominal values and to adjust only the parameters $\tilde{Y}_1$, $\tilde{Y}_2$, $\tilde{Y}_b$ and α during the identification procedure.

The results :

As a first step, it was tried to fit a model on the 80 first days of data from the process.

The results of the parameter estimation are given in table II. They consist in the 8 trials which were successively improving the criterion E_{80}.

Trial	1	2	3	4	5	6	7	8
Y_1	250	200	200	200	250	310	375	375
Y_2	1.7	1.7	2.0	1.7	1.9	2.0	2.2	2.4
Y_b	120	100	100	90	120	150	180	180
α	2.0	2.0	2.0	2.0	1.8	1.8	1.8	1.8
E_{80}	17.4	15.1	14.6	14.4	13.8	13.4	13.3	12.7

Computed and experimental daily gas productions are represented in Fig. 2 with parameters adjusted at their values given in column 8 of table II.
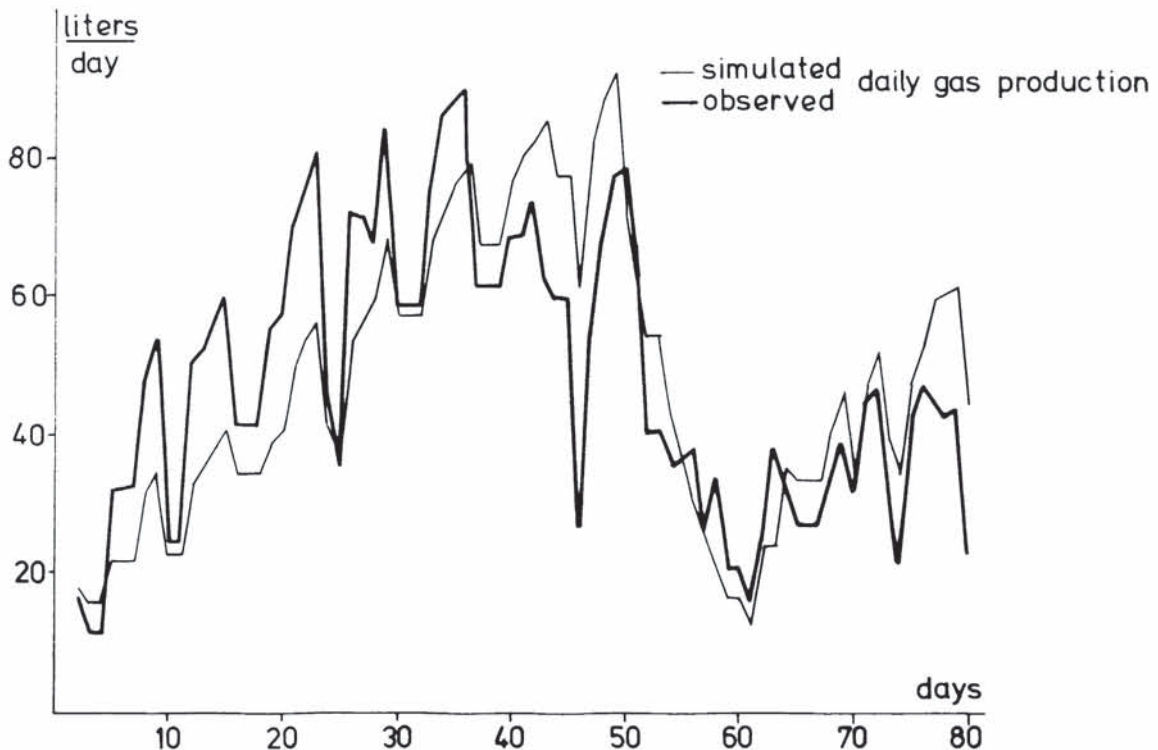
IDENTIFICATION : PART II

During the parameter adjustment procedure des-
cribed in the former section, it was observed
that the entire period of 160 days could be
divided in subperiods characterized by the
model's performance level : in some subperiods,
the model behaved quite well while for other
subperiods, the performance was consistently
poor.

Knowing that the bacterial activities are
sensitive to the concentration in VFA in the
methaniser, it was decided to model the pro-
cess with two submodels whose yield factors
$\tilde{Y}_1$, $\tilde{Y}_2$ and $\tilde{Y}_b$ are different.

The first submodel was used when the measured
volatil acids concentration was below a limit
$[VFA]_c$ while the second one was used in the
other situation.

Using the same experimental data as before,
the values of $\tilde{Y}_{1,i}$, $\tilde{Y}_{2,i}$, $\tilde{Y}_{b,i}$ and $[VFA]_c$,
i = 1,2 were adjusted in order to minimize
E_{80}.

Results are given at table III. They consist
in trials 9 and 10 and one can see by compa-
rison with trial 8 on table II that there is
a weak improvement of the model performance.

Table III. $[VFA]_c$ = 0.5 gr/lit.

Trial nr		9	10	11
$\tilde{Y}_1^{-1}$	1	175	310	175
	2	400	400	340
$\tilde{Y}_2$	1	1.8	2.4	1.8
	2	2.5	2.5	2.2
$\tilde{Y}_b$	1	100	150	100
	2	195	195	170
α		1.8	1.8	(*)
E_{80}		12.4	11.3	9.9
E_{160}		15.3	14.6	10.6

Table IV gives the sequence of uses of each
of the two submodels.

Table IV.

days	model
1-40	1
41-60	2
61-126	1
127-145	2
146-160	1

IDENTIFICATION : PART III

As a further refinement of the model, it was
decided to allow for a change in the value

of α, the digestibility parameter of the
feed.

Since the value of α is related to the
quality of the feed, it was allowed to
change whenever the tank of feed was repla-
ced. However this value was constrained to
be a constant for each feed tank.

Parameter adjustment from the same experi-
mental data as before gave the following
values for α :

| days	tanks	α
1-20	1	2.6
20-110 and 140-160	2-3-4 5-8	1.8
110-140	6-7	1.4

Results of this identification are given in
table III (trial nr 11) and graphically
presented in Fig. 3 for the whole of 160
days.

CONCLUSIONS

i) It was possible to improve the model in
taking into account biochemical phenome-
na like inhibitions and digestibility.
The challenge is probably to include in
the model those dominant biochemical
phenomena without obtaining an unmana-
gable model.

ii) The obtained model is time-varying and
further researchs are needed in order
to evaluate the possible benefits of
including a stochastic component into
this model.

iii) More experimental data from the bioche-
mical laboratoires are needed in order
to insure the validity of the proposed
models.

REFERENCES

[1] ANTUNES S. and INSTALLE M., "The Use of
Phase-Plane Analysis in the Modeling and
the Control of a Biomethanization Pro-
cess". Proceedings of 8th IFAC Triennal
World Congress, Kyoto, August 1981.

[2] ANDREWS J.F. and GRAEF S.P., "Dynamic
Modeling and Simulation of the Anaerobic
Digestion Process" - Anaerobic Biologi-
cal Treatment Processes. Dept. of
Environment Systems Eng., Clemson
University, 1974.

[3] HILL D.T. and BARTH C.L., "A Dynamic
Model for Simulation of Animal Waste
Digestion". Journal W.P.C.F., October
1977.
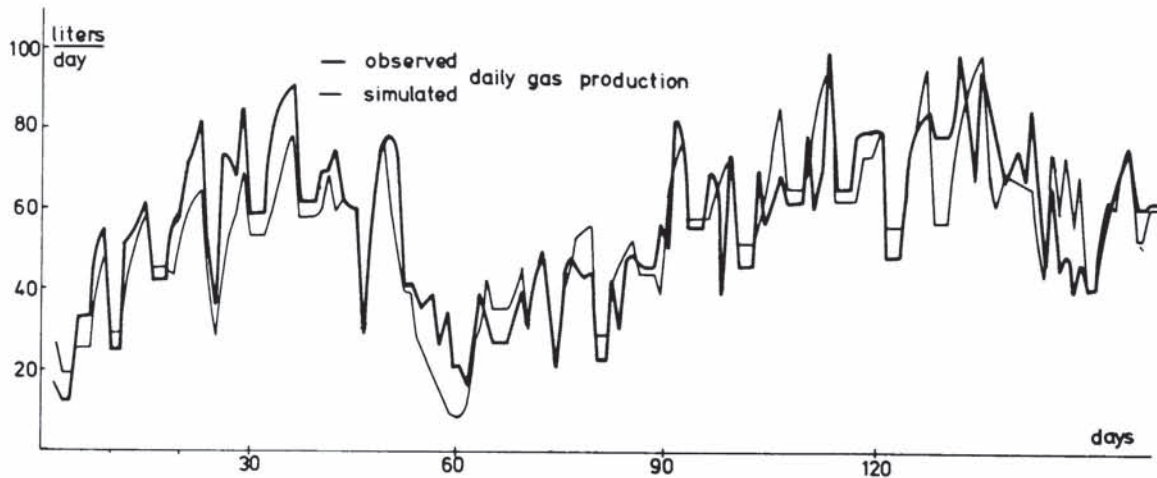
APPENDIX : SYMBOLS OF THE MODEL

G : dilution rate (day^{-1})

X_1 : concentration in acidogenic bacteria (mg/lit.)

X_2 : concentration in methanigenic bacteria (mg/lit.)

S_o : concentration in volatil solids (mg/lit.)

S_{oi} : concentration in volatil solids in the influent (g/lit.)

S_1 : concentration in solubilized volatil organics (mg/lit.)

S_2 : concentration in volatil acids (mg/lit.)

$\mu_1 (\mu_2)$: specific grow rate for acidogenic (methanigenic) bacteria (day^{-1})

$\hat{\mu}_1 (\hat{\mu}_2)$: maximum specific grow rates (day^{-1})

$k_{d1} (k_{d2})$: specific rate for acidogenic (methanigenic) bacteria (day^{-1})

$K_{m1} (K_{m2})$: saturation constant for acidogenic (methanigenic) bacteria (mg/lit.)

Y_1 : Yield coefficient (msX_1/mgS_1)

Y_2 : Yield coefficient (mgX_2/mgS_2)

Y_b : Yield coefficient (mgS_2/mgX_1)

Y_G : Yield coefficient $(lit. CH_4/mgX_2)$

Q : daily production of methane $(lit. CH_4/day)$.