

AN EXAMPLE OF THE BENEFITS OBTAINED FROM THE LONG TERM USE OF MATHEMATICAL MODELS IN WASTEWATER BIOLOGICAL TREATMENT

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Abstract. This paper illustrates the practical benefits of the long term use of a mathematical model developed five years ago to monitor a 0.947 m³ anaerobic digestion fixed bed reactor used for the treatment of raw industrial wine processing wastewater. In particular, it is shown how simulations can be used to detect technical problems like stop of a mixing pump.

1. Introduction

Anaerobic Digestion (AD) is a complex series of biological processes that take place in the absence of oxygen and by which organic matter is decomposed and bioconverted on one hand into biogas (*i.e.*, a mixture of mainly carbon dioxide and methane, a renewable energy source) and, on the other hand, into microbial biomass and residual organic matter.

AD can be considered as one of the oldest and most efficient waste and wastewater treatment processes. It has been indeed applied over many decades for the treatment of household waste(water)s in septic tanks, of slurries in digesters, of sewage sludge in municipal treatment plants and of industrial wastewaters. It is also probably the major biological process involved in landfill wastes decomposition.

However, modeling of these processes is a tedious task that requires many efforts before obtaining satisfactory results. In addition, it is very difficult to find in the literature long-term evaluation of a model developed for AD processes.

This paper is concerned with a 0.947-m³ anaerobic digestion fixed bed reactor used for the treatment of raw industrial wine processing wastewater. The detailed description of the AD plant and its on-line instrumentation is described elsewhere [28].

A mass balance model of this process was developed from measurements obtained in 1997 and 1998 [8]. This model was built to be simple but robust and thus only included two microbial populations (*i.e.*, acidogenic and methanogenic populations) degrading organic matter (expressed as chemical oxygen demand, COD) and producing volatile fatty acids (VFAs) and CO₂ in a first step, CO₂ and CH₄ in a second step. The core of the present paper is to discuss the benefits of this five-year-old model from a practical point-of-view and to show on an example how the model can help to diagnosis a technical failure.

2. Model description

Various models have been proposed for anaerobic digestion processes. The first model included a single bacterial population [17]. The representation of the process was improved by considering three stages with solubilization of organic compounds, acidogenesis and methanogenesis [20] or even a four-population model with two acidogenesis reactions and two-methanization reactions [26]. Thereafter, these models have been improved and detailed by other authors in order to get closer to the complexity of the process (see for example [1, 6, 7, 10, 11-16, 18, 19, 21-25, 27] and related references).

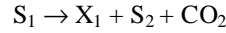
The resulting models include several bacterial populations and various substrates so that the number of parameters may become very large. The problem is that it is then difficult to use these models for monitoring and control purposes since they are hard to calibrate and to validate.

On the opposite, a simple model was chosen in the present study assuming that two main bacterial populations are present. From these considerations, a mass-balance-based model consisting of six ordinary differential

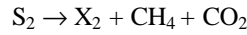
equations was derived. The state variables of this model are linked to on-line measurements of the gaseous flow rates. The model circumvents the difficulty due to the lack of reliability of the bacterial growth modeling by locating the biological variability in dedicated terms, namely the kinetic reaction rates. The use of such models for monitoring and control design has been proven to be effective [5] because it minimizes the number of assumptions during model construction [2, 8]. This mass-balance model forms also the basis for a software sensor that uses the available on line measurements of gases flow rates [9].

A drastic simplification of the digester ecosystem was thus assumed during the model development (*Cf.* Figure 1). In fact, the corresponding reaction scheme was considered as a summary of the main mass transfer throughout the digester, *i.e.*, the two steps were included in the model:

- *Acidogenesis*: the population of acidogenic bacteria (X_1) consumes the organic substrate (S_1) and produce CO_2 and volatile fatty acids (S_2) through an acidogenesis step :



- *Methanogenesis*: The second population (X_2) uses the volatile fatty acids in a methanogenesis step as substrate for growth and produces CO_2 and methane.



The total inorganic carbon is stored in the medium as bicarbonate and dissolved CO_2 form. A variable Z represents the total alkalinity within the digester.

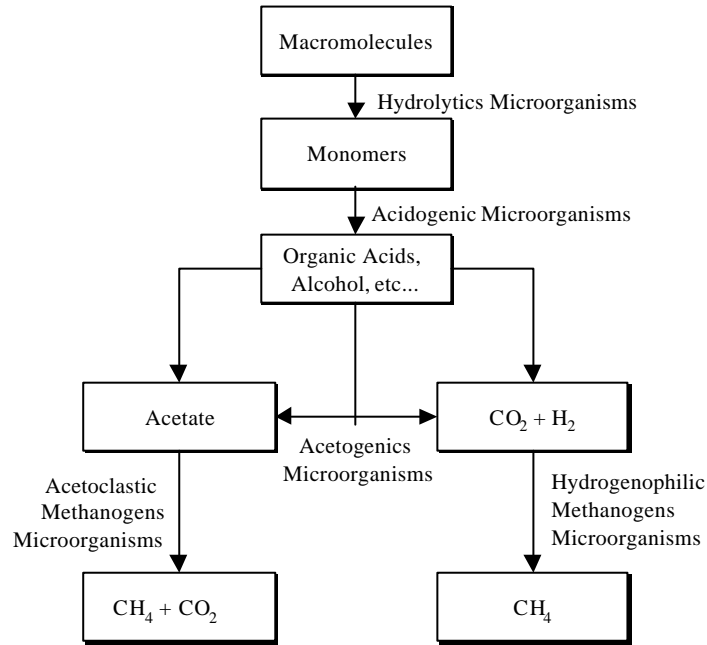


Figure 1. Main pathways in the anaerobic digestion process (from [26])

The model equations are then the following:

$$\begin{aligned}
 \frac{dX_1}{dt} &= (\mu_1(S_1) - \alpha D)X_1 \\
 \frac{dX_2}{dt} &= (\mu_2(S_1) - \alpha D)X_2 \\
 \frac{dS_1}{dt} &= D(S_{1,in} - S_1) - k_1\mu_1(S_1)X_1 \\
 \frac{dS_2}{dt} &= D(S_{2,in} - S_2) + k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2 \\
 \frac{dZ}{dt} &= D(Z_{in} - Z) \\
 \frac{dC}{dt} &= D(C_{in} - C_{tic}) + k_4\mu_1(S_1)X_1 + k_5\mu_2(S_2)X_2 - q\text{CO}_2
 \end{aligned} \tag{1}$$

The influent concentration of organic substrate, volatile fatty acids (VFA), alkalinity and inorganic carbon are denoted S_{1in} , S_{2in} , Z_{in} and C_{in} respectively. Bacterial growth rates were chosen as a Monod model for X_1 and an Haldane model for X_2 *i.e.*,

$$\mu_1(S_1) = \mu_{1max} \frac{S_1}{S_1 + K_{S1}} \quad ; \quad \mu_2(S_2) = \bar{\mu}_{2max} \frac{S_2}{S_2 + K_{S2} + S_2^2 / K_{I2}}$$

Note that it is assumed that a constant fraction (α) of the bacteria is attached on the support and therefore, this fraction is not affected by the dilution effect. The reader can refer to [8] for details on the parameter meaning and on the computation of the gaseous flow rate with respect to the state variables. In fact, the parameters were identified from experiments run in 1997 and 1998 using the steady input-output behaviour. Several equilibrium states corresponding to different (constant) inputs conditions were recorded and linear regressions were used to determine the model parameters.

The reidentification of a few of these parameters (see Table 1) was performed in order to fit the model with the data obtained in 2001. In addition, since the biomass concentrations had fluctuations of low magnitude, it was decided to consider a second model where biomass concentrations are constant. This second model simply consists in removing equations of the biomass in (1) and in taking the mean values computed from equilibrium equations as biomass values. The use of these two models (*i.e.*, with and without constant biomass) will be discussed in the sequel.

Table 1. Values of the changing parameters of the model between 1998 and 2001

Parameter	meaning	1998	June 2001	Sept. 2001	Oct. 2001
V	Volume	947 l	550 l	350 l	see Figure 5.
K_{S1}	Half saturation constant for S1	7.1 g/l	8.9 g/l	8.9 g/l	8.9 g/l
K_{S2}	Half saturation constant for VFA	9.28 mmol/l	23.2 mmol/l	23.2 mmol/l	23.2 mmol/l
b	Bias in the pH measurement	0	0.35	0.5	0.5 and 0 after day 7 in Figure 5

3. Results

As an illustration of the benefits of the long-term use of this mathematical model, Figure 2 compares the on-line measurements obtained in September 2001 together with simulation results. As it can be seen, the model fits quite well the on-line measurements over 30 days both in the liquid and in the gas phases but some additional remarkable points should be highlighted:

- as already pointed out, compared to the thirteen parameters values determined in 1998, only two were modified (*i.e.*, the half saturation constants of the two specific growth rates, one being increased by 25 % and the other one being increased by a factor of 2.5),
- to obtain these results, the biomass was kept constant and a working volume of only 350 liters was chosen (to be compared with the 947 liters originally available),
- the simulated pH value was increased by a constant value of 0.5.

This led us to assume that:

- microorganisms affinity to the substrate had been modified with time which could be explained by large biofilm development within the reactor,
- a clogging of the reactor was suspected. The process is indeed a fixed bed reactor where clogging is likely to occur,
- a bad calibration of the pHmeter was present due to clogging of the sensor after biofilm formation around the sensor.

This was confirmed from a 20 days comparison with on-line measurements obtained two months before (*i.e.*, in June 2001 – See Figure 3). Similar results were obtained with parameter values identical to those determined from data obtained in September 2001 (*i.e.*, the process being operated for 5 years, the microorganisms adaptation to the wastewater was already over). But then, a working volume of 550 liters and a constant bias of the pH of 0.35 were needed to fit the measurements. This reinforced our belief in the suspected clogging of both the reactor and the pHmeter and pushed us to check all the components involved within the plant.

However, when analyzing in details the functioning of the reactor, it was found that the pump at the bottom of the reactor used to ensure good mixing of the liquid phase before entering the fixed part (*i.e.*, where microbial biofilm is present – See Figure 4) was not working anymore. As a consequence, the liquid phase was poorly mixed and shortcuts were surely present in the fixed phase.

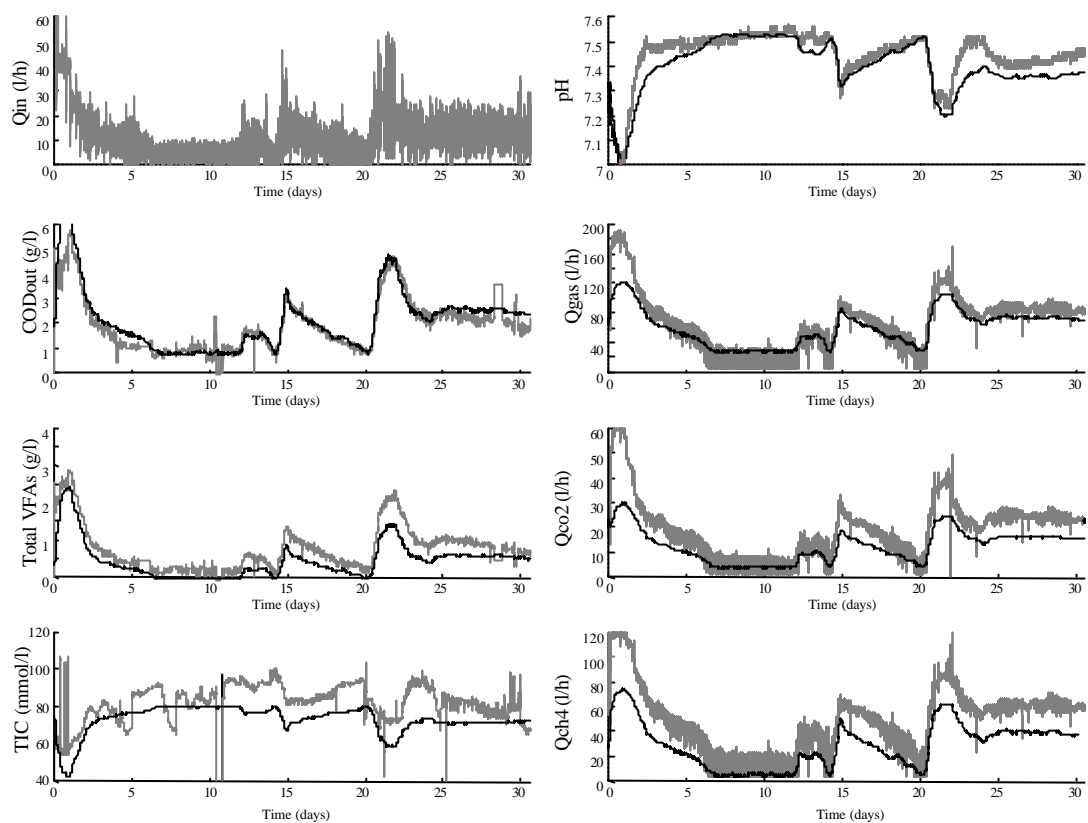


Figure 2: Comparison between on-line measurements (thin lines) obtained in September 2001 when the clogging of the reactor was suspected and simulation of the model developed in 1998 (thick lines).

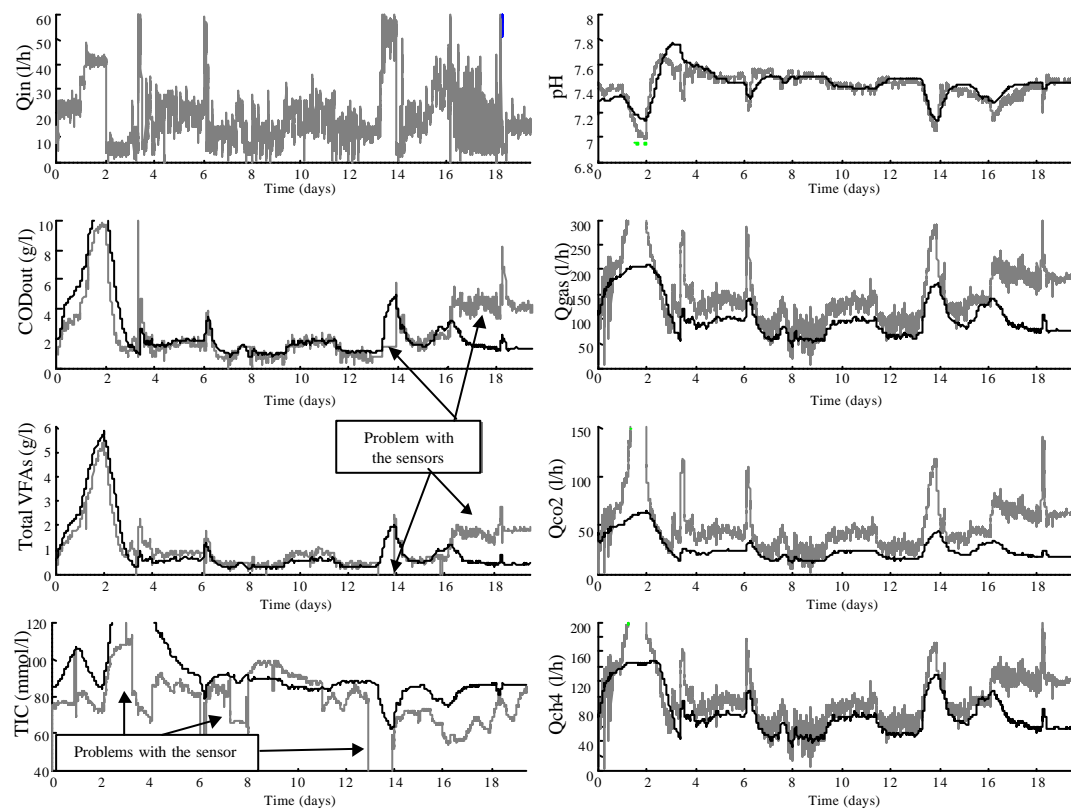


Figure 3: Comparison between on-line measurements (thin lines) obtained in June 2001 and simulation of the model (thick lines) highlighting the starting of the clogging of the reactor.

The pump was then restarted in October 2001 while step changing the feed flow for few days to induce dynamical changes of the main variables (the carbon concentration in the feeding wastewater was then kept constant). Comparison between on-line measurements and model simulation is presented in Figure 5 over 17 days (the pump was restarted at day 7). As it can be seen, again, results are quite satisfactory and the following points have to be highlighted:

- the values used for the thirteen model parameters were similar to those determined from data obtained in September 2001,
- as soon as the mixing pump is restarted, the biomass is supposed not to be fixed anymore (a washout of part of the biomass is then present and the volume is assumed to increase slowly until it reaches 830 liters four days later – see Figure 6). A tracer pulse experiment was indeed performed in June 2000 and then, the working volume was determined to be equal to 830 liters instead of 948 liters originally available in 1997. This loss of biomass and this increase of working volume explain the decrease of both the COD and total VFAs in the output of the reactor that can be noticed after day 7 in Figure 3.
- at the same time, the mixing pump was restarted, the pHmeter was changed but the numerization of the signal was kept identical, thus leading to wrong pH values recorded after day 7. Also, a technical problem of the sensor providing total VFAs and total inorganic carbon on-line measurements was discovered and then solved after day 7.

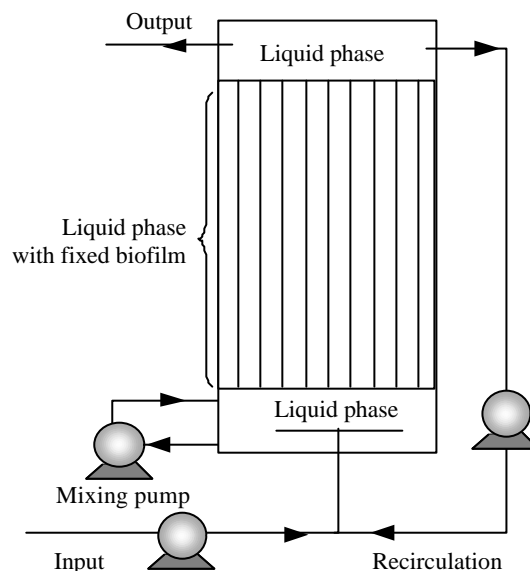


Figure 4: Schematic layout of the anaerobic digester

3. Conclusion

As a conclusion, the following points should be highlighted:

- the model was demonstrated to be very robust and efficient over a very broad range of operating conditions (*i.e.*, COD in the output of the reactor between 0 and more than 10 g/l and total VFAs between 0 and 5 g/l) and over a large period of time (*i.e.*, five years after being developed and almost two years after a complete restart of the process – the reactor being completely emptied and filled with new microbial populations in 2000 – data not shown),
- bad functioning of the overall process (*i.e.* a stop of a mixing pump at the bottom of the reactor that led to a working volume decreased by two thirds and a clogging of an important sensor, the pHmeter) could be discovered by comparison between on-line measurements and simulations of the model.

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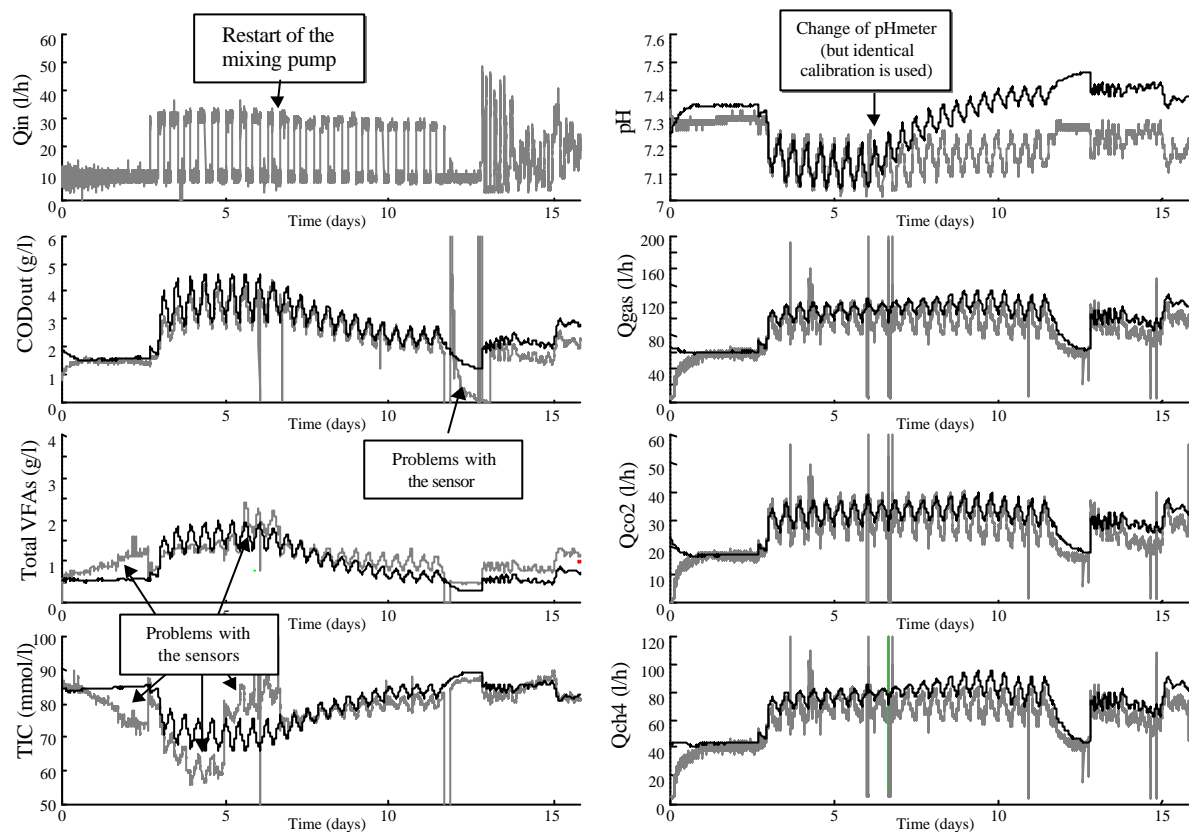


Figure 5: Comparison between on-line measurements (thin lines) obtained in October 2001 and simulation of the model (thick blue lines)

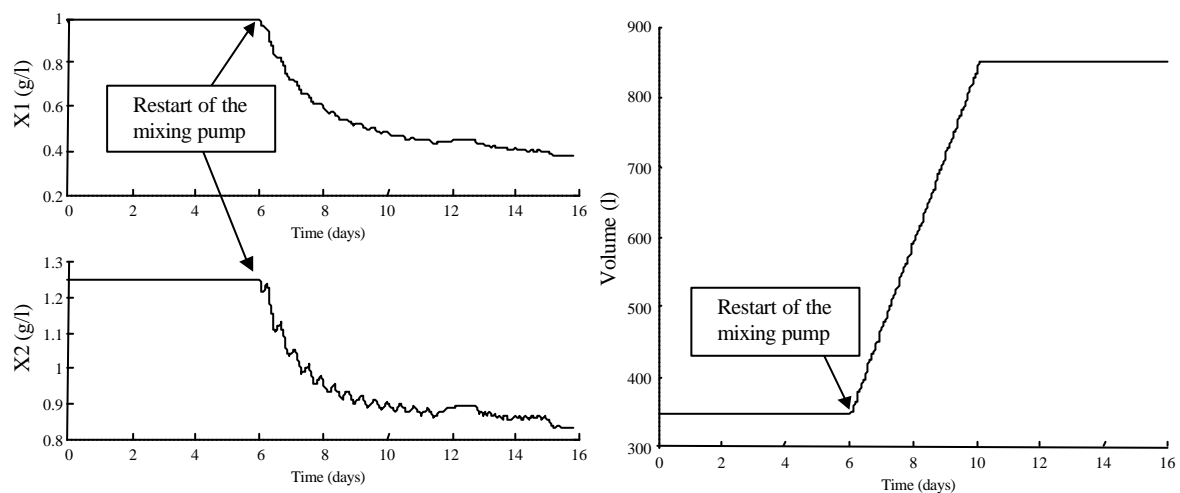


Figure 6: Dynamic evolution of the biomass concentrations and working volume just before and after restarting the mixing pump in October 2001.

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