Wat. Sci. Tech. Vol. 25, No. 7, pp. 61–71, 1992.
Printed in Great Britain.

0273–1223/92 $15·00

TOWARDS A USEFUL DYNAMIC MODEL OF THE ANAEROBIC WASTEWATER TREATMENT PROCESS: A PRACTICAL ILLUSTRATION OF PROCESS IDENTIFICATION

R. M. Jones*, J. F. MacGregor**, K. L. Murphy** and E. R. Hall*

**Environment Canada, Wastewater Technology Centre, P.O. Box 5050, Burlington, Ontario L7R 4A6, Canada*
***Department of Chemical Engineering, McMaster University, Hamilton, Ontario L8S 4L7, Canada*

ABSTRACT

Results are reported from a dynamic modelling study conducted on a pilot scale anaerobic fluidized bed. The objective of the study was to generate data to identify, evaluate and eventually calibrate a dynamic model for on-line estimation and forecasting in a process control system. Experiments consisted of pulse inputs of glucose, propionic acid, and acetic acid during the treatment of a distillery wastewater. The dynamic response of the methane and carbon dioxide production rates, hydrogen content of the biogas, effluent volatile acid concentrations and effluent COD concentrations are shown. A model structure was postulated based on the results observed in the dynamic experiments. An extended Kalman filter state estimation algorithm was employed to provide estimates of unmeasured process states and parameters. The use of the state estimation technique improved the performance of the model, helped locate model inadequacies, and provided information to direct further model development.

KEYWORDS

Anaerobic wastewater treatment, fluidized bed reactors, dynamic response, kinetics, modelling, state estimation, extended Kalman filter.

INTRODUCTION

The formulation of a dynamic model, often referred to as process identification, is an iterative procedure which must begin with the setting of an objective for the development of the model. The intended application of the model will influence both the model structure and the extent of calibration and verification required. An initial model structure can be formulated from a conceptual picture of the interactions in the process, or from qualitative observations on the behaviour of the process. A suitable set of process data can lead to greater confidence that the most significant mechanisms controlling the behaviour of the process will be described in the model. The initially hypothesized model structure can be tested and calibrated with the data set, with observed model inadequacies providing direction for further model development. A more detailed outline of process identification procedures, with case histories relating to wastewater treatment processes, has been summarized by Beck (1989).

A considerable amount of effort has been expended in the past two decades developing dynamic models for the anaerobic wastewater treatment process. The early research of Andrews (1969) and Andrews and Graef (1971), in which biological kinetic equations, fundamental mass balances and physical-chemical relationships for the anaerobic process were proposed, formed the basis for many later models of the anaerobic treatment

process. Some examples include the work of Hill and Barth (1977), and Rozzi (1984). As understanding improved, another level of complexity was added to published anaerobic process models. Eventually, through fundamental microbiological research (Bryant *et al.*, 1967; Boone and Bryant, 1980; McInerney et.al., 1981), the conceptual four-bacterial model of the anaerobic process emerged. A number of mathematical models were subsequently published (Mosey, 1983; Rozzi *et al.*, 1985; Ide, 1988) to formulate the interactions between the various groups of bacteria and, in particular, to incorporate the effects of hydrogen identified in the microbiological studies.

Few anaerobic dynamic modelling studies have gone beyond the model structure hypothesis stage of process identification. However, the evaluation of the model structure using actual operating process data is one of the most important steps in process identification. Not only are the initial model hypotheses tested, but information on the practicality of calibrating and applying the model for the intended purpose is obtained.

This paper provides a demonstration of process identification procedures as applied to the anaerobic wastewater treatment process, through the presentation of results from an extensive dynamic study on a pilot scale high rate anaerobic treatment reactor. The major objective of the study was to identify a dynamic model which would be suitable for on-line estimation and forecasting. One of the objectives of this paper is to highlight the inadequacies of the present state-of-the-art in process modelling and provide direction for future research. The study was conducted at Environment Canada's Wastewater Technology Centre (WTC) in Burlington, Canada.

DYNAMIC DATA COLLECTION

Pilot Plant Facilities and Operation

Non-steady state data for model identification were collected during dynamic experiments on an anaerobic fluidized bed reactor with an empty bed liquid volume of 77 L. The reactor medium was a silica sand with a Dp_{10} of approximately 120 μm. A constant expanded bed height was maintained by pumping the sand at the top of the bed through a centrifugal pump to shear excess biomass from the medium.

Sensors installed on the pilot plant allowed for the on-line measurement of biogas flow, biogas methane content, biogas carbon dioxide content, biogas hydrogen content, reactor temperature, reactor pH, and recycle flowrate. The sensors were interfaced to a microcomputer-based data acquisition and control system. Measurements made on-line were stored at 10 minute intervals. Feedback controllers maintained the levels of pH, temperature and recycle rate. Experimental forcing functions were automated through the open-loop control of two feed pumps.

Wastewater used in the study was a molasses and brandy stillage from a local distiller. The raw wastewater had an average chemical oxygen demand (COD) concentration of 46 200 mg/L. The anaerobic reactor was seeded with biomass from previously operated anaerobic hybrid and fluidized bed pilot scale reactors. Prior to final dynamic experimentation, the reactor was operated for 740 days. Steady state and dynamic loading rates were adjusted throughout this operating period through adjustments in the dilution and feedrate of the stillage wastewater, and through addition of synthetic spike solutions consisting of combinations of glucose, acetic acid, propionic acid, and butyric acid. Nutrient levels in the spike solutions were maintained by supplementing with NH_4OH and K_2HPO_4. A tracer test was conducted on the fluidized bed reactor with tritium-enriched water to determine the reactor mixing characteristics and effective volume. Further information on the pilot plant design and operation has been summarized by Jones (1992).

Experimental Design

Dynamic experimentation consisted of a series of 7 day runs in which loading pulses were implemented by adding spike solutions of either glucose, acetic acid, or propionic acid. Each spike solution consisted of 270

g COD/L of the appropriate substrate, 9 g of K_2HPO_4, and 60 mL of 29.4% aqueous NH_3. The spike solution was prepared in 20 L batches and during a pulse was added to the reactor feed at a nominal rate of 7.2 mL/min (5 L/d). The actual addition rates were monitored by measuring the volumes of spike solution used. The total feed flowrate was maintained at approximately 120 L/d throughout the experimental period.

Sampling, Analysis and Instrumentation Maintenance

Pilot plant instrumentation calibration was checked routinely and re-calibration or repairs were made as necessary. An automatic sampler was used to collect grab samples of effluent at 2 hour intervals for off-line analysis of COD and volatile acids during dynamic experiments. Samples were collected every 8 hours in the periods between pulse experiments. Sample preparation and analyses were performed according to standard WTC methods (1976).

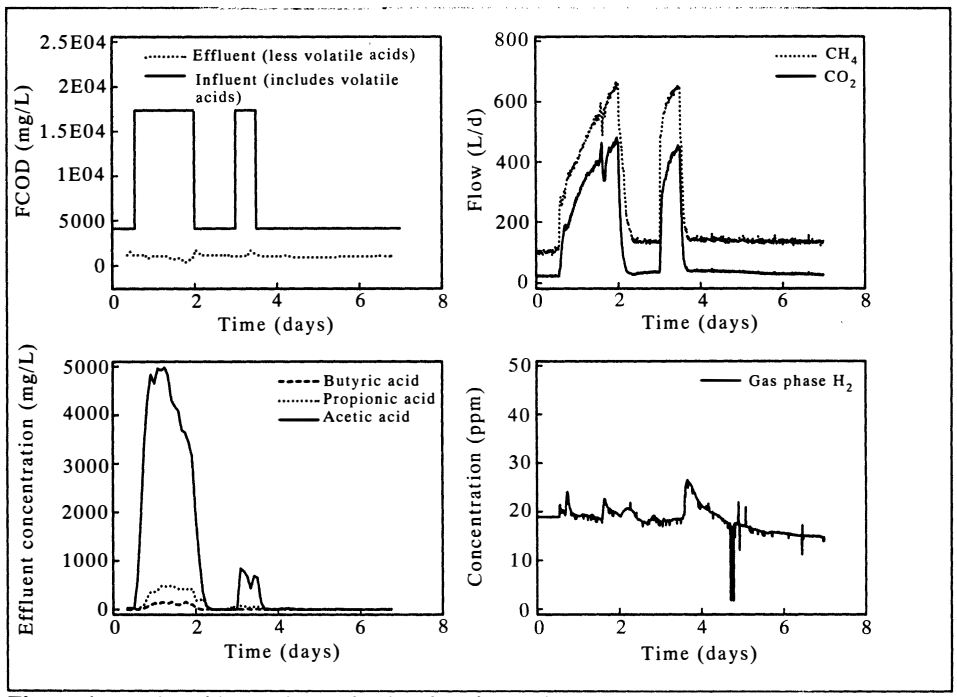

Figure 1: Acetic acid experiment forcing function and process response

DYNAMIC EXPERIMENTAL RESULTS

The experimental forcing functions and process responses during the acetic acid, propionic acid and glucose runs are shown in Figures 1, 2, and 3, respectively. The glucose run was implemented as three consecutive 7 day runs, using the same pulse sequence as the acid runs. The glucose addition rate was maintained at a midpoint (2.5 L/d) between the first and the second week. The influent concentration forcing functions plotted represent the combined concentration of the diluted distillery wastewater and the pulse addition of the synthetic spike solution. Effluent filtered COD (FCOD) concentrations were calculated by subtracting the COD equivalents of the measured effluent volatile acid concentrations from the measured effluent FCOD. The results of the tracer test indicated that the liquid-phase mixing characteristics of the fluidized bed were closely approximated by an ideal, complete-mixed reactor with an effective volume of 60 L.

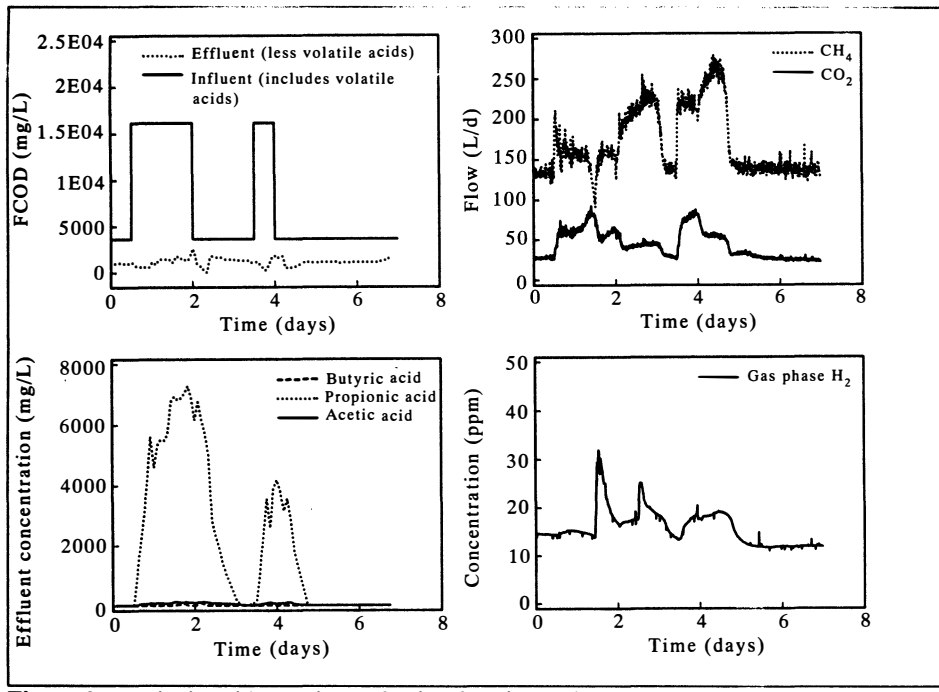

Figure 2: Propionic acid experiment forcing function and process response

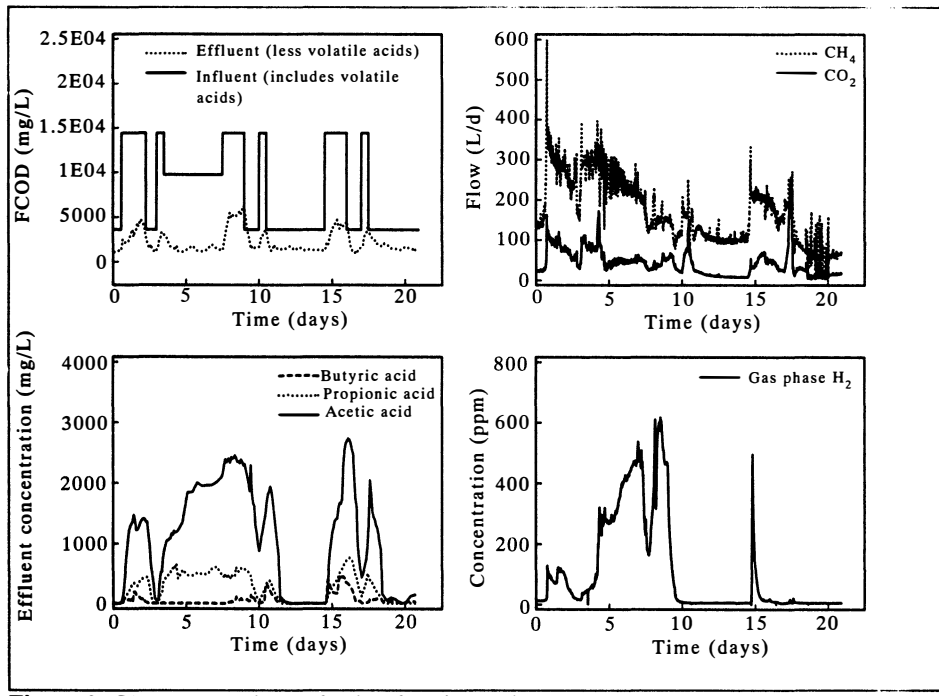

Figure 3: Glucose experiment forcing function and process response

Table 1: Anaerobic model process rate equations

$$\mu_{AF} = \mu_{max,AF}\frac{S_{G,1}}{K_{AF}+S_{G,1}}$$

$$\rho_{P,AF} = \frac{S_{A,1}}{K_{GP}+S_{A,1}}\eta$$

$$\rho_{A,AF} = \frac{1}{1+\frac{S_{A,1}}{K_{I,GA}}}$$

$$\rho_{B,AF} = 1-\rho_{A,AF}-\rho_{P,AF}$$

$$\mu_{PA} = \mu_{max,PA}\frac{S_{P,1}}{(K_{PA}+S_{P,1})(1+\frac{S_{A,1}}{K_{I,PA}})}$$

$$\mu_{BA} = \mu_{max,BA}\frac{S_{B,1}}{(K_{BA}+S_{B,1})(1+\frac{S_{A,1}}{K_{I,BA}})}$$

$$\mu_{AM} = \mu_{max,AM}\frac{S_{A,1}}{(K_{AM}+S_{A,1})(1+\frac{S_{P,1}}{K_{I,AM}})}$$

INITIAL MODEL FORMULATION

Description

A qualitative analysis of the experimental results was used to build an initial dynamic model structure. The model nomenclature is listed in Tables 2 and 3. The general form of a mass balance for a soluble component in the system is,

$$\frac{dS_{i,1}}{dt} = \frac{Q}{V}(S_{i,0}-S_{i,1}) - \frac{1}{Y_j}\mu_j X_j + \nu_{i,AF}\rho_{i,AF}\mu_{AF}X_{AF} + \nu_{i,PA}\mu_{PA}X_{PA} + \nu_{i,BA}\mu_{BA}X_{BA}$$

where, the subscript '1' refers to an effluent concentration, and the subscript '0' refers to an influent concentration. The expressions for μ_j and $\rho_{i,AF}$ are shown in Table 1. These equations are similar to those previously proposed for four-bacterial population models (Mosey, 1983; Ide, 1988). The differences are due to the observation in this study that there was little correlation between the reaction kinetics and the gas phase hydrogen concentration.

Due to the operation of the reactor with a constant expanded bed height, it was initially assumed that the bacterial loss rates, $B_{v,j}$, were equal to the respective growth rates, $\mu_j X_j$, in each bacterial mass balance. Therefore, a bacterial mass balance for this system is,

Table 2: Anaerobic dynamic model variables

VARIABLE	DESCRIPTION
S_G	Biodegradable (non-volatile acid) soluble organics (mg/L)
S_P	Propionic acid (mg/L)
S_B	Butyric acid (mg/L)
S_A	Acetic acid (mg/L)
S_I	Non-biodegradable compounds (mg/L)
X_{AF}	Acid-formers (mg/L)
X_{PA}	Propionic-acid-utilizing acetogens (mg/L)
X_{BA}	Butyric-acid-utilizing acetogens (mg/L)
X_{AM}	Acetoclastic methanogens (mg/L)
μ_{AF}	Acid-former specific growth rate (d^{-1})
μ_{PA}	Propionic-acid-utilizing acetogen specific growth rate (d^{-1})
μ_{BA}	Butyric-acid-utilizing acetogen specific growth rate (d^{-1})
μ_{AM}	Acetoclastic methanogen specific growth rate (d^{-1})
$\rho_{P,AF}$	Switching function for the production of propionic acid by acid-formers (d^{-1})
$\rho_{A,AF}$	Switching function for the production of acetic acid by acid-formers (d^{-1})
$\rho_{B,AF}$	Switching function for the production of butyric acid by acid-formers (d^{-1})
$B_{V,AF}$	Acid-former loss rate (mg/L·d)
$B_{V,PA}$	Propionic-acid-utilizing acetogens loss rate (mg/L·d)
$B_{V,BA}$	Butyric-acid-utilizing acetogens loss rate (mg/L·d)
$B_{V,AM}$	Acetoclastic methanogens loss rate (mg/L·d)
Q	Total feed flow rate (L/d)
$Q_{G,CH4}$	Methane flow rate (L/d)

$$\frac{dX_j}{dt} = \mu_j X_j - B_{V,j} = 0$$

The methane production was calculated by assuming that all acetic acid degraded by the acetoclastic methanogens was stoichiometrically converted to methane and carbon dioxide, and that all of the net hydrogen produced in the acidogenic and acetogenic reactions is oxidized by the hydrogen-utilizing methanogens to produce methane. The details of the model have been summarized elsewhere (Jones, 1992).

Model Structure Evaluation and Initial Calibration

The use of an on-line or recursive technique for model calibration allows a model to track a process affected by time-varying disturbances. The extended Kalman filter (Jazwinski, 1970) is one such technique that has been applied to modelling of wastewater treatment (Beck, 1981) and other biological processes (Svrcek et.al., 1974; Bellgardt et.al., 1986). An initial investigation of the use of an extended Kalman filter for on-line estimation in anaerobic wastewater treatment processes and a detailed description of the algorithm have been summarized previously (Jones et.al., 1989).

Table 3: Anaerobic dynamic model variables

CONSTANT	DESCRIPTION	VALUE
Y_{PA}	Propionic acid acetogens yield coefficient	0.12 mg/mg
Y_{BA}	Butyric acid acetogens yield coefficient	0.50 mg/mg
Y_{AM}	Acetoclastic methanogens yield coefficient	0.055 mg/mg
Y_{AF}	Acid-former yield coefficient	0.70 mg/mg
$\mu_{max,AF}$	Maximum specific growth rate - acid-formers	25.0 d^{-1}
$\mu_{max,PA}$	Maximum specific growth rate - propionic acetogens	1.0 d^{-1}
$\mu_{max,BA}$	Maximum specific growth rate - butyric acetogens	1.0 d^{-1}
$\mu_{max,AM}$	Maximum specific growth rate - acetoclastic methanogens	0.3 d^{-1}
$\nu_{i,k}$	Stoichiometric yield of component i through reactions of bacteria group k	Derived from stoichiometry of glucose degradation (see, for example, Mosey, 1983)
V	Effective reactor volume	60 L
$K_{I,AM}$	Inhibition coefficient - acetoclastic methanogens	1000 mg/L
K_{AF}	Saturation coefficient - acid-formers	5000 mg/L
K_{PA}	Saturation coefficient - propionic acetogens	50 mg/L
K_{BA}	Saturation coefficient - butyric acetogens	7.3 mg/L
K_{AM}	Saturation coefficient - acetoclastic methanogens	30 mg/L
$K_{I,PA}$	Inhibition coefficient - propionic acetogens	500 mg/L
$K_{I,BA}$	Inhibition coefficient - butyric acetogens	1000 mg/L
$K_{I,GA}$	Inhibition coefficient - acid-former acetate production	250 mg/L
η	Maximum fraction of propionic acid from acid-formers	0.90

A conceptual illustration of the extended Kalman filter algorithm is shown in Figure 4. The following list summarizes the variables relevant to the current application.

1) The measured inputs are the feedrate (**Q**), and the feed concentrations ($\mathbf{S_{G,0}}$, $\mathbf{S_{P,0}}$, $\mathbf{S_{B,0}}$, $\mathbf{S_{A,0}}$, $\mathbf{S_{I,0}}$).

2) The deterministic states, those for which a mass balance can be written based on physical, chemical, and biological phenomena occurring in the process, are the effluent concentrations ($\mathbf{S_{G,1}}$, $\mathbf{S_{P,1}}$, $\mathbf{S_{B,1}}$, $\mathbf{S_{A,1}}$, $\mathbf{S_{I,1}}$).

3) The stochastic states are those states for which a model is written in completely probabilistic terms. The extended Kalman filter adjusts these states in response to stochastic disturbances affecting the actual process and to accommodate model imperfections. In this example, the stochastic states are bacterial concentrations ($\mathbf{X_{AF}}$, $\mathbf{X_{PA}}$, $\mathbf{X_{AM}}$). The bacterial concentration, $\mathbf{X_{BA}}$, was assumed constant.

4) The extended Kalman filter can also be used as a recursive estimator for parameters assumed to be time invariant. Depending on the identifiability of the parameters, a subset of the parameters in Table 3 can be estimated with the algorithm. In this example, the estimated parameters are $\mathbf{Y_{AF}}$, and η.

5) The measured states are the deterministic states and an additional measured output is $\mathbf{Q_{G,CH4}}$.

6) The unmeasured states in this example are the stochastic states.

Figure 5 shows the measured values and the extended Kalman filter estimates for the effluent FCOD concentration ($\mathbf{S_{G,1}} + \mathbf{S_{I,1}}$), $\mathbf{S_{A,1}}$, $\mathbf{S_{P,1}}$, and $\mathbf{Q_{G,CH4}}$, during the glucose experiment. Figure 6 shows the estimates

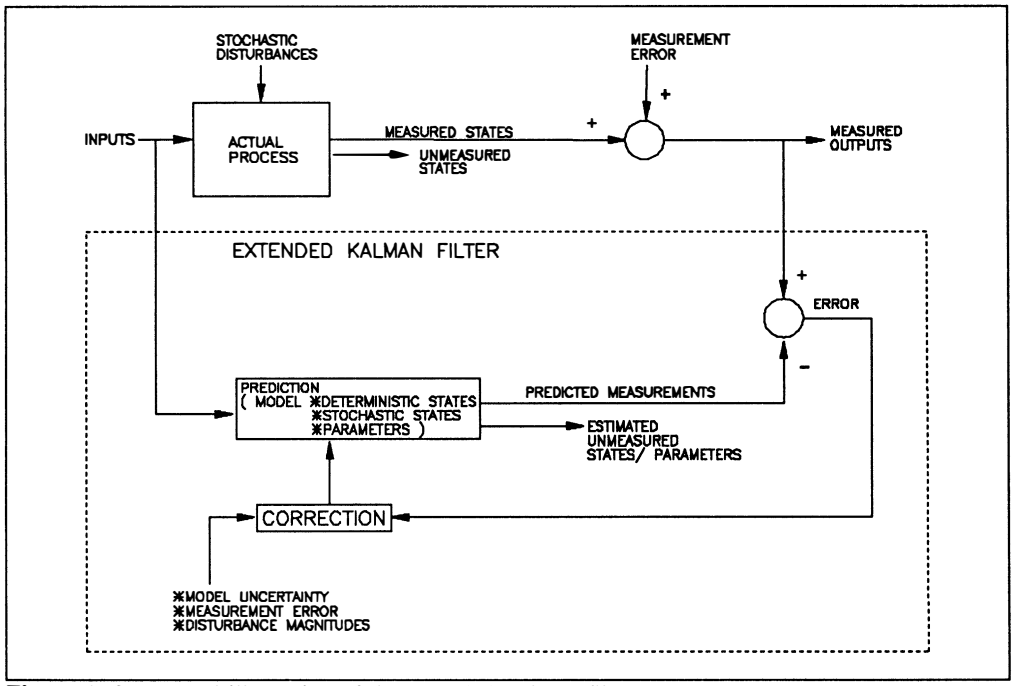

Figure 4: Conceptual illustration of the extended Kalman filter

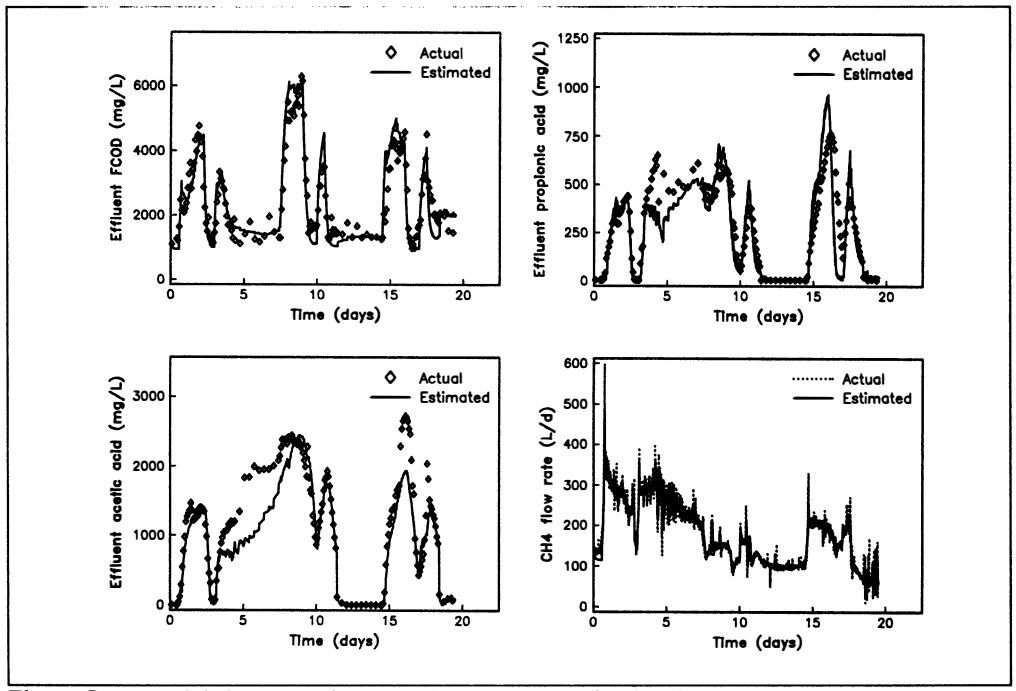

Figure 5: Deterministic state estimates and measurements for the glucose run

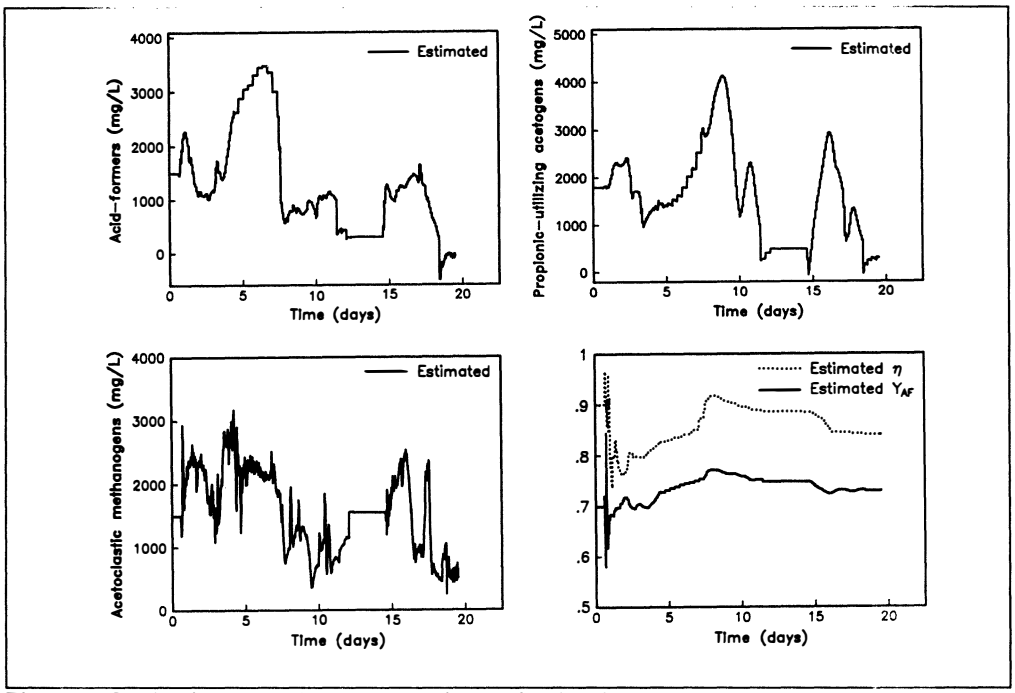

Figure 6: Stochastic state and parameter estimates for the glucose run

for the stochastic variables (X_{AF}, X_{PA}, X_{AM}), and the parameters (Y_{AF} and η). The plots show that application of the extended Kalman filter resulted in reasonable model estimates of the increasing trend in the volatile acid response and the decreasing trend in methane production observed in the experiment.

It is important to note that the performance of the model in predicting the deterministic states (Figure 5) was achieved through unrealistic adjustments of the stochastic states and time-invariant parameters (Figure 6). A qualitative analysis of the time-variable behaviour of the stochastic states can lead to insights into possible model inadequacies. For example, X_{PA} appears to be directly correlated with $S_{P,I}$, indicating that the mass balance for X_{PA} is inadequate, or that the kinetic relationship, ρ_3 is in error. Although less significant, the variations in X_{AF} and X_{AM} also display a correlation with their respective substrate concentrations.

The behaviour of the parameter estimates can also indicate possible inadequacies in the assumed model. The estimates of Y_{AF} and η appear to converge to approximately 0.73 mg/mg and 0.84, respectively. However, the estimates are not stable after an initial transient period, but vary throughout the run to accommodate inadequacies in the model structure.

SUMMARY AND DIRECTION FOR FUTURE MODEL DEVELOPMENT

The preceding analysis provides some indication of the inadequacies of the present state-of-the-art in dynamic mathematical models of high rate anaerobic processes. Mechanistic expressions for the reactor bacteria concentrations would improve the performance of the model in forecasting the response of a process to disturbances. However, these expressions would be difficult to verify because of the difficulties in measuring reactor and effluent concentrations of individual bacteria species. Methods are required for the on-line measurement of the activities of the bacterial groups in both the suspended and the fixed film phase

of high rate anaerobic reactor systems.

The extended Kalman filter algorithm can be used as an aid for additional model development. For example, in the analysis presented in this paper, the time-variable behaviour of the stochastic state estimates indicates that the general bacterial mass balance relating the bacterial concentrations to the respective growth rates should be tested. Completion of the bacterial mass balances would require expressions for the loss rate of each bacterial group, $\mathbf{B}_{V,i}$. One approach for quantifying the loss rates would be to run the extended Kalman filter with the bacteria concentrations as deterministic states and model the $\mathbf{B}_{V,i}$ terms as stochastic states. The model identification process would then go through a further iteration by examining the time variable behaviour of the $\mathbf{B}_{V,i}$ estimates. Alternate growth rate expressions could also be tested by examining their effect on the parameter and stochastic state estimates.

The documentation of results from this anaerobic dynamic modelling study has provided a demonstration of a number of process identification procedures. Non-steady-state data were collected from an anaerobic fluidized bed reactor as the process responded to pulse inputs of glucose, propionic acid, and acetic acid. Based on the results of these experiments, a dynamic model structure was postulated from the four-bacterial conceptual model of the process. A relatively sophisticated method of model structure evaluation and calibration utilizing the extended Kalman filter was shown. However, the main purpose of the discussion was to highlight the value in following a systematic analysis of the problem while attempting to satisfy the main modelling objectives. The objective of the study reported here was to obtain a model which could be used for on-line estimation and forecasting within a process control system. In many instances, the primary objective of a modelling study is to extend engineering knowledge of the process. In any case, the evaluation of the model structure using a dynamic data set collected for that purpose is invaluable in determining the significant phenomena affecting the process response of interest.

ACKNOWLEDGEMENTS

Funding for this research was provided by Environment Canada, the Federal Panel on Energy R&D (PERD), and the ISTC Biotechnology Strategy.

REFERENCES

Andrews, J.F. (1969). Dynamic model of the anaerobic digestion process. *J. Sanit. Engng Div. Proc. ASCE*, 95 (SA1), 95-116.

Andrews, J.F., and Graef, S.P. (1971). Dynamic modeling and simulation of the anaerobic digestion process. *Anaerobic biological treatment processes*. Advances in Chemistry Series, R.F. Gould (Ed)., Vol. 105, American Chemical Society, New York, pp. 126-162.

Beck, M.B. (1989). System Identification and Control. In: *Dynamic Modeling and Expert Systems in Wastewater Engineering*. G.G. Patry and D. Chapman (Ed)., Lewis, Chelsea, MI, pp. 261-323.

Beck, M.B. (1981). Operational estimation and prediction of nitrification dynamics in the activated sludge process. *Wat. Res.*, 15, 1313-1330.

Bellgardt, K.-H., Kuhlmann, W., Meyer, H.-D., Schugerl, K., Thoma, M. (1986). Application of an extended Kalman filter for state estimation of a yeast fermentation. *IEE Proceedings*, 133, PT. D (5), 226-234.

Boone, D.R., and Bryant, M.P. (1980). Propionate-degrading bacterium, *Syntrophobacter wolinii* sp.nov.gen.nov., from methanogenic ecosystems. *Appl. Env. Microbiol.*, 40 (3), 626-632.

Bryant, M.P., Wolin, E.A., Wolin, M.J., and Wolfe, R.S. (1967). *Methanobacillus omelianskii*, a symbiotic association of two species of bacteria. *Arch. Microbiol.*, 59, 20-31.

Hill, D.T. and Barth, C.L. (1977). A dynamic model for simulation of animal waste digestion. *J. Wat. Pollut. Control Fed.*, 10, 2129-2143.

Ide, S. (1988). Dynamics, Stability, and Control of Anaerobic Packed Bed Processes. Ph.D. thesis, Rice University, Houston, Texas.

Jazwinski, A.H. (1970). *Stochastic Processes and Filtering Theory*. Academic Press, New York.

Jones, R.M., MacGregor, J.F., and Murphy, K.L. (1989). State estimation in wastewater engineering: application to an anaerobic process. *Environmental Monitoring and Assessment*, 12, 271-282.

Jones, R.M. (1992). Dynamic Modelling for Process Control of a High Rate Anaerobic Wastewater Treatment System. Ph.D. thesis, McMaster University, Hamilton, Ontario.

McInerney, M.J., Bryant, M.P., Hespell, R.B., and Costerton, J.W. (1981). *Syntrophomonas wolfei* ge.nov.sp.nov., an anaerobic, syntrophic, fatty acid-oxidizing bacterium. *Appl. Env. Microbiol.*, 41 (4), 1029-1039.

Mosey, F.E. (1983). Mathematical modelling of the anaerobic digestion process: regulatory mechanisms for the formation of short-chain volatile acids from glucose. *Wat. Sci. Tech.*, 15 (8/9), 209-232.

Rozzi, A. (1984). Modelling and control of anaerobic digestion processes. *Trans Inst M C*, 6 (3), 153-159.

Rozzi, A., Merlini, S., Passino, R. (1985). Development of a four population model of the anaerobic degradation of carbohydrates. *Env. Technol. Lett.*, 6, 610-619.

Svrcek, W.Y., Elliott, R.F., and Zajic, J.E. (1974). The extended Kalman filter applied to a continuous culture model. *Biotechnol. Bioengng.*, 16, 827-846.

Wastewater Technology Centre (1976). Analytical Methods Manual. Wastewater Technology Centre Laboratory Services Section, Environment Canada, Burlington, Ontario.