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Evaluating a Mathematical Model of Anaerobic Digestion of Organic Wastes Using System Identification Techniques

Robert P. Anex
Science and Public Policy Program
University of Oklahoma
100 E. Boyd St, Rm S-202
Norman, Oklahoma 73019
Voice: (405) 325-2299
Email: rpanex@ou.edu

Ger Kiely
Civil and Environmental Engineering
University College
Cork, Ireland

Abstract: Anaerobic digestion of the organic fraction of municipal solid waste (MSW), on its own or co-digested with primary sewage sludge (PSS), produces high quality biogas, suitable as renewable energy. We report on the parameter estimation and evaluation of a two-stage mathematical model of the anaerobic co-digestion of the organic fraction of MSW and PSS. Measured data are from a bench scale laboratory experiment using a continuously stirred tank reactor and operated at 36°C for 115 days. The two-stage model simulates acidogenesis and methanogenesis, including ammonia inhibition. Model parameters are estimated using an output error, Levenberg-Marquardt (LM) algorithm. Sensitivity of the estimated parameter values and the model outputs to non-estimated model parameters and measurement errors are evaluated. The estimated mathematical model successfully predicts the performance of the anaerobic reactor. Sensitivity results provide guidance for improving the model structure and experimental procedures.

INTRODUCTION

Anaerobic digestion of the organic fraction of municipal solid waste (OFMSW), on its own or co-digested with primary sewage sludge (PSS), produces high quality biogas and could contribute significantly to the renewable energy budget while reducing waste disposal through other routes such as landfilling. The Danish Energy Agency (1994) reports on 18 plants in operation in the European Union and at least 26 plants under construction world wide, with feedstock mixtures of OFMSW and other organic wastes.

Biogas production has been shown to be about 2 m^3/m^3 of reactor, for digesters containing low solids (<5% dry solids) mixtures of OFMSW and PSS at mesophilic temperatures (Kiely *et al.* 1994). Kayhanian *et al.* (1992) have reported biogas output as high as 7 m^3/m^3 of reactor for high solids mixtures (>20% dry solids) at thermophilic temperatures. One of the major problems in operating anaerobic digesters is inhibition of microbial growth by ammonia. Accurate mathematical models would be useful to help avoid such problems in analyzing the design and operation of production-scale digesters. This paper reports on the performance of a two-stage model the parameters of which have been estimated from experimental data. Further, the paper presents the results of sensitivity and model form evaluations performed using system identification techniques.

MATHEMATICAL MODEL

The mathematical formulation is based on Hill and Barth (1977), Havlik *et al.* (1986), Moletta *et al.* (1986), and Kiely *et al.* (1997). The model considers the production of methane during anaerobic digestion as being the result of a first stage of hydrolysis/acidogenesis producing acetate and a second stage of aceticlastic methanogenesis producing methane. The nine state model includes conservation of the equilibrium between CO_2 and HCO_3^- and conservation of mass for CO_2 cations and NH_4^+, and ammonia inhibition of methanogenic biomass growth. The model requires influent rates for substrate and COD loading and substrate glucose equivalent concentration. Also required are the bicarbonate, cation and ammonium concentrations. The model is solved numerically to simulate reactor operation. There are 13 model variables. Variables output for comparison with measured data are pH, ammonium (NH_4), methane (CH_4), and total volatile fatty acid (VFA). The model contains 19 parameters that are candidates for estimation.

SYSTEM IDENTIFICATION TECHNIQUES

Model parameters are estimated using an output error, Levenberg-Marquardt (LM) algorithm (Levenberg 1944, Marquardt 1963, More 1977). The LM algorithm is used to solve the nonlinear least squares problem

$$\min_{x \in R^n} \frac{1}{2} \sum_i F_i(x)^2$$

where

$$F(x) = \begin{bmatrix} y(x,t_1) - \phi(t_1) \\ y(x,t_2) - \phi(t_2) \\ \cdots \\ y(x,t_m) - \phi(t_m) \end{bmatrix}$$

and $y(x,t)$ is the model output, and $\phi(t)$ is the observed system output. The LM algorithm uses a search direction that is a blend of the Gauss-Newton direction and the steepest descent direction. In this way the LM algorithm overcomes the convergence problems of the steepest descent method and the Gauss-Newton method's reliance on an accurate estimate of the Hessian matrix (i.e., the matrix of second partials of F, also known as the Fischer Information Matrix).

The paper describes additional system identification tools that are used to analyze the identifiability and sensitivity of the model. For the purposes of this discussion identifiability is defined as a measure of the likelihood that any estimated parameter is within a specific range of the actual parameter. Sensitivity refers to the bias effects that one parameter has on the estimation of another. At convergence of the parameter estimation process identifiability and sensitivity information can be obtained through manipulation of the Hessian matrix since it is formed from the partial derivatives of the model innovations with respect to the model parameters. That is, by decomposing the

Hessian matrix the sensitivity of the model's performance to the measurements and model parameters can be generated in an elegant and useful form (Anex 1990, Anex *et al.* 1986).

Measured data are from a bench scale laboratory experiment using a continuously stirred tank reactor and operated at 36°C for 115 days. The reactor was 2 L in volume and operated at a constant temperature in a water bath, with daily feed. The reactor was seeded with 1.5 L of inoculum from two full scale operational anaerobic digesters, allowed to acclimatize for 13 days, and was then fed pig slurry for 21 days. This "setting-up" period resulted in a reactor with pH of 7.75, an alkalinity of 5.5 g/l and an ammonia level of 1.5 g/l. These were the initial conditions at day one of the experiment. Full details of the experimental set-up and procedures were reported by Kiely *et al.* (1994).

RESULTS

The paper reports the results of identifiability and sensitivity analyses of the model's nineteen parameters. Theses analyses indicate which model parameters are most critical, and which must be known (or identified) because they have strong bias effects (error in their values will bias the estimated values of others). Model parameters previously identified as being most important are the maximum specific growth rate of acidogenic bacteria, the yield coefficient for acidogenic bacteria, and the yield coefficient of acetic acid. The identifiability and sensitivity analyses also show which measurements are most important in the estimation process and quantify how measurement error will bias model parameter estimates.

The set of model parameters selected during the identifiability and sensitivity analyses are then estimated from the observed data. A set of ten model parameters have been estimated. The estimated parameter values are compared with values suggested in the literature and outputs of the estimated model are compared with the observed reactor performance. In Figure 1 the methane production measured in the digestion experiment is compared with methane production simulated by an uncalibrated model and the estimated model.

CONCLUSIONS

The estimated model simulates pH, NH_3 and CH_4 well. The estimated model simulation performance is improved compared to the model using manually calibrated parameters. Although not verified by simulating measurements not used in the estimation process, the estimated model is the first thoroughly calibrated model of this type. Identifiability and sensitivity analyses indicate which parameters in this model structure are critical and how accurately measurement must be made to allow parameter estimation. The methods described provide valuable information to the modeler and should have broader application in environmental engineering.

Appendix I. References

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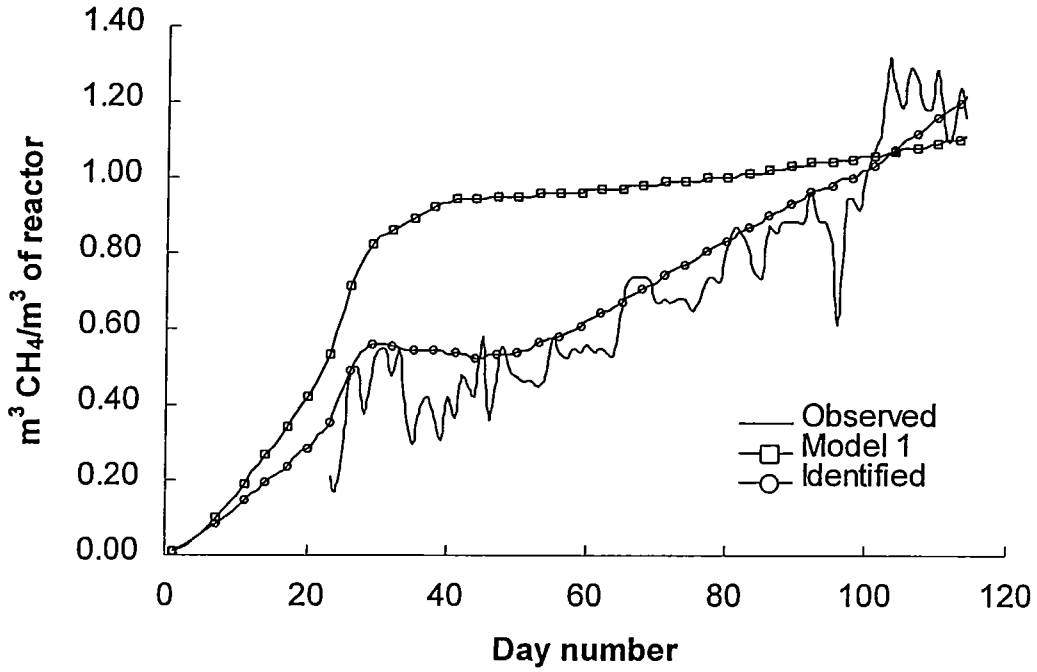

Figure 1. Comparison of observed methane production and methane production simulated by the uncalibrated and calibrated models.