On calibration of ADM1 model parameters to modified AMOCO model

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Abstract. Anaerobic digestion (AD) is a key technology for renewable energy production, that would largely benefit from accurate process models for effective monitoring and optimization. The Anaerobic Digestion Model No. 1 (ADM1) and the advanced monitoring and control (AMOCO) model are widely used for simulating AD processes. This study aims to calibrate ADM1 to the modified AMOCO model to validate state and parameter estimator which is designed based on the modified AMOCO model. Calibration was performed using simulation data from ADM1 and nonlinear programming optimization solver in MATLAB. The results demonstrate that, after calibration, the modified AMOCO closely matches ADM1 in predicting key digester states. These findings support the development of robust estimator validation frameworks, enabling model-based control and optimization of AD systems.

Keywords: Anaerobic digestion, ADM1, modified AMOCO, Calibration.

1 Introduction

Biogas from anaerobic digestion (AD) offers a clean energy solution with potential to reduce greenhouse gas emissions. Due to the nonlinear and time-varying nature of AD and limited affordable sensors, there is a need for accurate state and parameter estimation. This work aims to derive AMOCO-equivalent ADM1 parameters to support estimator validation.

2 Anaerobic digestion models

In this work, the data is generated by simulating the ordinary differential equation (ODE) implementation of ADM1 proposed by [1]. This ADM1 implementation includes a system of equation with 35 differential and 1 algebraic equation in which 29 variables represent the concentrations of liquid and gas outflows, while ionized volatile fatty acids, bicarbonate and free ammonia concentrations determine the remaining 6 variables. The AMOCO (advanced monitoring and control) model for anaerobic processes is a model that was primarily derived for the design of monitoring and control algorithms [2] and later modified to better match experimental and simulated data [3], [4]. The modified AMOCO model consists of seven differential equations, corresponding to the seven states, and 2 algebraic equations.

3 Methodology

The first step in generating the AMOCO equivalent state variables of the ADM1 simulations is done by using the conversion formulas presented in [3] with a slight modification to account for the hydrolysis stage [4]. Next a nonlinear programming solver, fmincon in MATLAB, is used. This solver is used so that it finds the minimum of the objective function expressed by:

$$\min f(\Theta) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{9} \sum_{j=1}^{9} \frac{|z_{amoco} - z_{adm1}|}{s_i}$$
(1)
s.t. $lb \le \Theta \le ub$

Where $\theta = [N_{bac} k_0 k_1 k_2 k_3 k_4 k_5 k_6 k_{I2} k_{s1} k_{s2} \mu_0 \mu_{1,max} \mu_{2,max}]$, *n* is the number of samples, $z = [x_1 x_2 x_0 s_1 s_2 z c r_c r_{CH4}]^T$ with z_{amoco} and z_{adm1} being the corresponding *z* vectors for simulated results by modified AMOCO and by ADM1 for the same inputs. s_i is a normalization vector used as the magnitude of the span of z_i . In this case the range of z_{adm1} is used, i.e. $s_i = \max(z_{adm1}) - \min(z_{adm1})$. Normalization is done along the *n* values of each variable in *z*. The lower and upper bounds, *lb* and *ub*, for the search space of the parameters, θ , are based on the results of the parameter identification in [4].

4 Results and Discussion

The optimal parameters are obtained to minimize the problem in (1) using the fmincon. Thus fmincon did not succeed finding the optimum parameters, and manual tuning was performed to achieve acceptable model performance. Hence, the final optimal parameters are presented in Table I below.

Parameters	N_{bac}	k _o	k1	k2	k₃	k₄	k₅	k6	k 12	k s1	ks2	μø	$\mu_{1,\max}$	$\mu_{2,max}$
Optimal values	52.21	0.78	9.02	115.56	399.34	79.23	54.83	426.94	50.76	2.45	6.13	3.38	1.90	0.18

Table I. Optimal values of the parameters

The modified AMOCO is simulated using the ode15s solver in MATLAB taking the initial states to be equal to the ones used in the ADM1 simulation using the conversion formulas in [3]. The inputs for the simulation of ADM1 are the steady-state inputs presented by [1] and adding 20 % of the steady-state composite material input every five days. Hence, the first seven elements of z_{amoco} are the solutions of the ode15s solver and the last two variables are obtained using the algebraic equations stated in the modified AMOCO model. The comparison of the two models with respect to these variables is shown in Fig. 1.



Fig. 1. Comparison of modified AMOCO variables and AMOCO equivalent ADM1 variables

Some challenges were encountered in capturing transient behaviors. This study successfully demonstrated a method for deriving AMOCO-equivalent ADM1 parameters using simulation data from a detailed ADM1 implementation. This approach enhances the development and validation of estimators for state and parameter monitoring in AD processes. The results may thus contribute to improving the reliability and efficiency of biogas production processes.

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