Application, uncertainty and sensitivity analysis of the anaerobic digestion model by Siegrist et al. (2002) on household waste digestion

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Abstract
In this paper the anaerobic digestion model published by Siegrist et al. (2002) is applied on household waste digestion. Data from two pilot scale experiments with measured characterizations were used, one with mesophilic and one with thermophilic temperature. Validation simulations with focus on the gas production rate, ammonium and VFA were first performed, using default values for model parameters. The steady state gas production could be predicted with acceptable accuracy, while the simulated ammonium and VFA concentrations were overestimated by the model. An uncertainty analysis was conducted to analyze the quality of the predictions with respect to measurements of input data. The measurement errors influenced the gas production the most, but that the VFA and ammonia predictions could not be improved with more accurate measurements. To find suitable parameters for calibration of model parameters, a Monte Carlo based sensitivity analysis was conducted, supplemented with scatter plots. The sensitivity analysis showed that the hydrolysis constant was the most important parameter to determine for both ammonium and gas production. This was problematic for the calibration, as the particulate organic matter is lumped and calibrating the ammonium from the hydrolysis constant therefore led to unrealistically low gas production. To model the protein degradation accurately, without changing the overall hydrolysis constant or the model structure, the protein content in the substrate was calibrated instead. The Siegrist model was hence not suitable for simulation of characterized household waste, unless a hydrolysis model with slower protein hydrolysis was introduced or the stoichiometry for the hydrolysis was calibrated. The VFA concentrations in the reactor were dependent on model parameters related to the aceticlastic methanogenesis and the propionate degradation. Calibration of half saturation constants for these processes was successful, but the values were increased considerably. A possible explanation for the considerable change in these parameter values could be that the mass transfer of substrate was more limiting than for the default Siegrist model.

Keywords anaerobic digestion, model, household waste, uncertainty analysis, sensitivity analysis, calibration, Monte Carlo, hydrolysis constant

Introduction
Anaerobic digestion is a complex system of biochemical and physical processes. Due to the complexity of the process, it has traditionally been treated as a black box system, and optimization has been based on experience or trial and error methods. As experiments of anaerobic digestion processes are expensive and time consuming, modeling can provide a useful tool for process understanding and optimization. Models have potentials for revealing non-linear behaviors of the system and to quantify the performance of alternative operational setups.

The aim of this report is to evaluate the applicability of a model for anaerobic digestion published by Siegrist, et al (2002), here referred to as the Siegrist model. The model was primarily developed for simulating the digestion of mixed sludge, but in this report the applicability for the model on household waste is studied. Compared to the more commonly used model by the International Water Association (IWA), called Anaerobic Digestion Model no 1 (ADM1), the Siegrist model is less complex, with a lumped hydrolysis constant and fewer Volatile Fatty Acids (VFA) included. The two models were constructed with different approaches, the Siegrist model parameters are based on experiments, whereas the ADM1 uses review consensus (Batstone, 2006). ADM1 has been validated in the literature with varying success (Parker, 2005; Batstone, et al., 2003; Tartakovsky, et al., 2008). The Siegrist model is less utilized, but interesting because of the simpler structure with fewer input variables.

The aim of the report is also to evaluate the required quality of input parameters, and to find the most important parameters to measure when modeling household waste digestion. Furthermore, the model parameters most suitable for calibration are evaluated and results with calibrated parameters are shown.

Materials & Methods
The model was implemented in Matlab as a system of differential equations with 23 liquid phase state variables and 3 state variables describing gaseous compounds. The stiff ODE-solver ode15s was used for the numerical integration. The hydrolysis rate was described with first order kinetics with respect to the degradable particulate organic matter $X_s$ (process 1 in Figure 1). Monod kinetics, in combination with inhibition expressions with respect to ammonia, pH, acetate and dissolved hydrogen, were used to simulate the microbial processes (process 2-7 in Figure 1). The model also included stripping of the gases methane, carbon dioxide and hydrogen from the liquid with a pressure control loop (Siegrist, et al., 2002).
Data from one mesophilic (35°C) and one thermophilic (55°C) pilot scale experiment was used for validation and model analysis (Davidsson, et al. 2007). The household waste used in the mesophilic experiment was collected in the city district of Västra Hamnen in Malmö, Sweden, and the thermophilic digester was fed with household waste from Aalborg, Denmark. Characterization data for fat, protein, fiber, sugar, starch, VFA and ammonium content as fractions of TS was found in Højlund Christensen, et al. (2003). The measurement errors of the characterization data were found in an evaluation of the analysis methods by la Cour Jansen, et al. (2004). Relative standard deviation for the ammonium measurements were provided by the analysis instrument manufacturer (3.5 %, Dr Lange®). The relative standard deviation for VFA was assumed to be 10 %, and 2.5 % for gas production measurements.

The experiments were divided into three phases; startup, steady state and post digestion. As the inoculums were collected from digesters fed with sludge, the startup phase was needed for the microorganisms to get accustomed to the new type of feed. Post digestion data was not available for the mesophilic digestion experiment.

Validation simulations

Before the pilot scale experiments could be simulated, some processing of data was needed, including unit conversions and calculation of stoichiometry and the rate constant for the hydrolysis process. The elemental compositions for protein, fat etc. were found in Davidsson, et al. (2007) and converted to the unit gCOD/gTS with the Buswell formula (Buswell, et al., 1930). The default stoichiometry of mixed sludge hydrolysis in Figure 1 was hence updated to apply for the household wastes.

Data from batch experiments on the waste from Västra Hamnen was used to determine the first order hydrolysis constant for degradation of particulate degradable organic matter, $X_C$. It was assumed that the hydrolysis step was rate limiting and that there were no inhibition effects on the microbial reactions. The hydrolysis constant, $k_{H}$, was determined to 0.20 d$^{-1}$ (Figure 2).

Except for the hydrolysis constant and the composition of the waste, default values for model parameters were used for the validation simulations. The results show that the steady state gas production rate could be predicted fairly well for both household wastes, while the correlation during the start-up phase was poorer (Figure 3a and 4a). The modeled gas production rate during the startup phase was higher than measured, indicating a slower degradation before adaptation to the substrate. The fit to data for steady state ammonium concentrations were unsatisfactory for both simulations, especially for the mesophilic case (Figure 3b and 4b). The good fit to data for the startup of the thermophilic experiment was mainly due to a washout effect. The VFA concentrations were underestimated in the model predictions, especially for the thermophilic household waste digestion (Figure 3c and 4c).

Uncertainty analysis

The characterizations were based on measurements with inherent measurement errors. A Monte Carlo method with Latin Hypercube Sampling (LHS) was used to study the effects of these measurement errors on prediction uncertainty. The distributions of the measurement errors were assumed to be described by Gaussian functions, and the distributions of outputs from 5000 simulations were studied.

In Figure 5 the uncertainty of simulated outputs presented as 95% confidence intervals can be compared with measurement uncertainties of validation data (vertical intervals) for the thermophilic household waste simulation. When the confidence intervals overlap, there are no significant differences in the uncertainty. However, as the confidence intervals do not overlap, it is possible that measurement errors can explain some of the discrepancy between simulations and data for the
gas production rate, but that further calibration was needed for ammonia and VFA (Figure 5b and 5c). The confidence intervals are broader for the gas production than the ammonia and VFA, indicating that the gas production is affected more by the quality of input data than the other two outputs.

**Sensitivity analysis**

Sensitivity analysis was conducted with two main purposes; to determine the importance of measuring specific input parameters and to find model parameters suited for calibration. Sensitivity analyses of ADM1 found in the literature used sensitivity functions or other local analysis methods (Tartakovsky et al. 2008, Jeong et al. 2005, etc.). In this report, a global sensitivity analysis method was employed instead, to include the non-linear behavior of the system.

The sensitivity analysis was carried out with the same methodology as in the uncertainty analysis, e.g. Monte Carlo with LHS. This time, however, instead of varying all parameters, one parameter at a time was kept at a constant value. The relative decrease in output variance when keeping a parameter constant, compared to if all parameters varied, was used as a measure of the sensitivity for this parameter.

This variance-based method needed to be supplemented with scatters plots to enable visual evaluation of the correlation between parameters and output.

The analysis of measured input parameters was based on the same parameter distributions as in the uncertainty analysis. As no information of realistic distributions for model parameters was found, the model parameters were assumed to be uniformly distributed between ± 50 percent of the default values.
The sensitivity analysis of measured input parameters showed that the variance for prediction of gas production rate decreased the most if the TS measurements were made without errors (Table 1). Reliable measurements for TS are thus important. The most significant sources of uncertainty for the ammonium predictions were the TS, solubilized TS and protein content of the feed (Table 1). For VFA, the uncertainty from distributed input parameters was not significant, but the HCO₃⁻ of the feed was most influential (Table 1).

With the aid of scatter plots, the correlations between the measured input parameters and output could be visualized. From this analysis, the correlation between the degradable fraction of TS could be pointed out as more important for the gas production rate than the total measured TS (Figure 6 and 7). The linear correlation to the gas production is more pronounced for the degradable TS and the output values are less dispersed. This result is no surprise, however, since it is the degradable fraction of TS that is used for gas production. This result emphasizes the importance of measuring the degradability of the substrate.

VFA levels in the reactor were sensitive to parameters related to the acetotrophic methanogenesis and the anaerobic degradation of propionate (Table 2). The scatter plot analysis of the correlations revealed that the high sensitivity to these parameters was partly due to that bacteria were washed out when these constants reached extreme values. Figure 9 shows an example of a frequent washout of bacteria for low maximum growth rates for the acetoclastic methanogens.

![Figure 6 Gas production vs. total TS for the thermophilic experiment](image)

![Figure 7 Gas production vs. degradable TS for the thermophilic experiment](image)

![Figure 8 Gas production vs. $k_H$ for the thermophilic experiment](image)

![Figure 9 Gas production vs. maximum growth rate of acetoclastic methanogens](image)
In the sensitivity analysis, the most influential model parameters for each output were ranked. This result could then be used for calibration purposes, where the most influential parameters were chosen, and used to increase the fit to data. The calibration was conducted by varying parameters so that the sum of absolute errors for model predictions compared to data during the steady state phase could be minimized.

Calibration of the hydrolysis constant to the gas production measurements resulted in an unchanged value for the mesophilic experiment, while the best fit to data for the thermophilic experiment was slightly decreased (from 0.2 to 0.15). This indicated a successful determination of $k_H$ from batch experiment for the household waste from Västra Hamnen. To enable calibration during the startup phase, the hydrolysis constant was iteratively increased until a good fit to data was achieved. The results from the calibration of the hydrolysis constant to the gas production errors are presented in Figure 10a.

The hydrolysis constant was also the most influential parameter when it came to determining the ammonia levels in the reactor. When calibrating the hydrolysis constant with the ammonia measurements, the resulting hydrolysis constants were lower, indicating slower degradation of protein than other particulate constituents. The fact that the particulate organics were lumped into one state variable, $X_S$, complicated the calibration process. As the hydrolysis constant determined both the protein degradation and the gas production rate, only one of the two processes could be calibrated at the same time. The model structure hence needed to be revised, to include a separate process of hydrolysis of particulate protein. The model structure was however not changed in this project, but is suggested for further studies. The problem was instead solved by decreasing the stoichiometric coefficient of protein in the degradation of $X_S$. The result from this calibration is presented in Figure 10b.

The sensitivity analysis showed that the maximum growth rate constants for the acetoclastic methanogenesis and the propionate degradation were most important for the VFA concentration. As discussed in the sensitivity analysis section, this result was partly due to the high rate of washout for extreme values of these parameters. This indicated that they may not be suited for calibration purposes. When calibrating with these values, the fit to data only improved slightly, and when changing the value further, the errors increased rapidly. An example when calibrating the maximum growth rate constant for the aceticlastic methanogens is presented in Figure 11a.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mean</th>
<th>Unit</th>
<th>Sensitivity (Gas)</th>
<th>Sensitivity (VFA)</th>
<th>Sensitivity (NH4-N)</th>
</tr>
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<tbody>
<tr>
<td>$\mu_{max6}$</td>
<td>0.6</td>
<td>d^{-1}</td>
<td>Rank</td>
<td>Relative</td>
<td>Rank</td>
</tr>
<tr>
<td>$\mu_{max7}$</td>
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<td>d^{-1}</td>
<td>24</td>
<td>1.00</td>
<td>6</td>
</tr>
<tr>
<td>$k_H$</td>
<td>0.2</td>
<td>d^{-1}</td>
<td>7</td>
<td>0.001</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 2 Results from sensitivity analysis of model parameters
Better calibration results were instead achieved when using half saturation constants. A better fit to data was obtained, and the process was stable for a wide range of values (Figure 12). The minimum error was acquired for a $K_S$ of 100 g COD/m$^3$ for propionate degradation and 260 g COD/m$^3$ in the thermophilic digester (compare with the default values 20 and 40 g COD/m$^3$ respectively). For mesophilic digestion, only $K_S$ for acetoclastic methanogenesis was calibrated, to 190 g COD/m$^3$.

The physical explanation for changing the half saturation constants could be that the mass transfer conditions was different than suggested in the implementation by Siegrist et al. The resulting simulation after calibration is showed in Figure 10c.

**Figure 12** Sum of absolute errors for VFA for the thermophilic simulation when varying half saturation constant for the acetoclastic methanogenesis

**Conclusions**

Applying the Siegrist model on household waste experiments gave acceptable predictions of the steady state gas production. The simulation of the startup phase, i.e. before the inoculum was adapted to the substrate, was less successful. The correlation of ammonia and VFA predictions to data was not satisfying for simulations without calibrated values.

The uncertainty analysis showed that measurement errors could explain some of the discrepancy for gas production predictions to data, but not to the same extent for ammonium and VFA. From the sensitivity analysis it could be concluded that the most important parameters to determine for predictions of gas production are the amount of degradable TS in the substrate, and the hydrolysis rate constant. The VFA concentrations of the reactor were mostly influenced by the availability of VFA as substrate in propionate degradation and acetoclastic methanogenesis. This implied that the mass transfer in the digester was more important for the VFA level than the input variables.

The calibration showed that the hydrolysis rate constant determined from batch experiments gave the best fit to data for the gas production; this method for determining the hydrolysis constant could thus be used in this case.

The ammonium concentration in the reactor was determined from the degradation of protein. As the particulate organics are lumped in the Siegrist model, the individual hydrolysis of particulate protein could not be modeled. This was problematic, since the protein degradation was much slower in the simulated experiments. It was therefore concluded that a hydrolysis model with separate hydrolysis rates as in ADM1 is preferable when modeling household waste degradation. This applies particularly when characterization measurements of the substrate are used; otherwise calibrations of the stoichiometric coefficients are needed.

**References**


