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Biogas reactor modelling with ADMI

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Preface

This report assumes the reader has at least basic understanding of the anaerobic digestion process. They should be familiar with the three fundamental steps in the anaerobic oxidation of a substrate: (1) hydrolysis, (2) acidogenesis (fermentation), and (3) methanogenesis, as well as the intermediate products associated with each.

We would like to thank all the master students who conducted lab analyses through the summer and autumn 2011 that provided the data necessary for this type of research.

Porsgrunn, Norway, March 2012

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I. Introduction

Anaerobic digestion (AD) is becoming an increasingly common method of handling agricultural waste. AD has historically been used to treat high-COD waste because it requires less energy, additives, and space than conventional aerobic processes. Research and adoption of AD to other processes has attracted more attention recently due, in large part, to the biogas (methane) it produces. At the same time, agriculture is under growing pressure to increase production and decrease emissions associated with its operation. AD can reduce odors, pathogens, and nuisance gas emissions, while preserving nutrients for a high quality fertilizer (Cantrell et al., 2008).

The traditional method of handling manure is spreading it on cropland, a very low-cost procedure. So despite the advantages of AD, its high initial capital investment is a major barrier in its development. Research at Telemark University College has shown that high rate, granular sludge reactors are a cost effective solution. However, they require improvements to minimize size and energy use, while maximizing the feed rate and methane production. Computer modeling of the AD process plays a central role in improving design and operation.

In the past few decades several dynamic models of varying complexity have been developed for anaerobic digestion. The International Water Association (IWA) task force developed Anaerobic Digestion Model No. 1 (ADM1) to be applicable to a wide range of AD processes. Batstone et al. (2002) suggest some modified parameters for digesting manure at 55 °C. Page et al. (2008) used bench-scale digesters at 35 °C and two full-scale plug-flow digesters to develop an ADM1 parameter set for dairy manure. This failed to predict biogas production, biomass, inorganic nitrogen, and volatile fatty acids (VFA) accurately. Zhang et al. (2009) also point out that the method of trial and error is very case specific and thereby limits its adoption to other reactors. Optimization algorithms were used by Zhang et al. (2009) to determine parameters for a 1700 L pilot reactor operated at 37 °C.

The goal of the work presented here is to adapt ADM1 to the AD reactor at Foss farm. After introducing the pilot plant, some theory of the model is presented, followed by a description about how it was developed and adapted to the Foss reactor. Finally, the results are discussed with some suggestions for further work.

2. Problem description

The goal of the project is to model the pilot plant at Foss farm in Skien using ADM1. Operation of the reactor began outdoors in 2008, and in 2010 it was moved inside and subjected to continuous feeding. A current process diagram of the suspended growth anaerobic digester is presented in Figure 2.1.

The ADM1 model, previously implemented in AQUASIM, is to be adapted to the anaerobic digester at Foss farm. Data from online sensor and regular lab analysis shall be used to evaluate and improve the model.

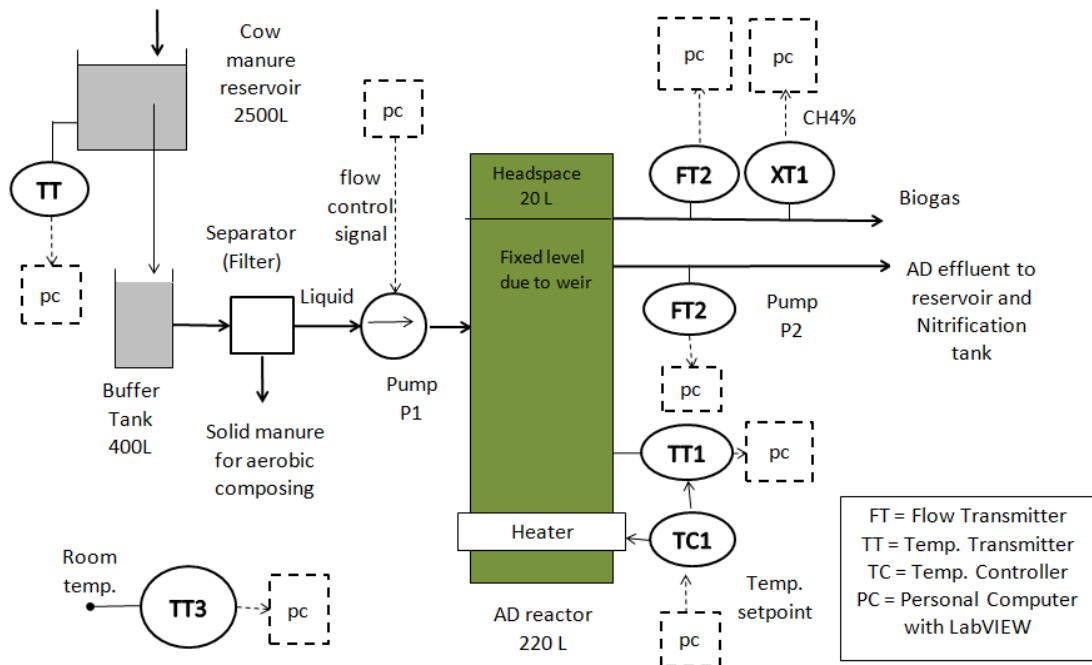


Figure 2.1: Foss farm anaerobic digester process diagram.

3. Theory

Anaerobic Digestion Model No 1, commonly referred to as ADM1, is a generic model for simulating anaerobic digestion of various substrates. Developed by the International Water Association (IWA) Anaerobic Digestion Modelling Task Group, ADM1 has 32 dynamic state variables, considers both biochemical and physicochemical processes, and contains several inhibition factors (Batstone et al., 2002). The model can be adapted to different applications by adjusting the many parameters, including reaction kinetics and substrate composition.

AQUASIM is a modeling and simulation program developed for water treatment in a variety of reactor types. Users define the parameters of the model and the processes (reactions) that occur in the compartment(s) that represents the physical design.

Implementing the ADM1 model in AQUASIM allows for comprehensive analysis and simulation of waste treatment. Users are able to adapt the model to meet the conditions of their reactor, simulate its operation, and graphically compare the results to empirical data.

4. Methods

4.1 Foss farm pilot plant

A fraction of the manure from the dairy cows on the farm is collected into batches of roughly 2500 L, which becomes the reactor feed for a few months (depending on feed rate). This manure is diluted about 25% with water as a result of the collection and cleaning process typical on these farms. The feed flow and reactor temperature can be controlled, while three temperatures (reactor, room, and reservoir), biogas flow, methane concentration, and effluent flow are measured with electronic sensors.

4.2 Data collection

Since July 11, 2011 samples have been taken from the influent and effluent three times per week (typically) for lab analysis. This includes total chemical oxygen demand (tCOD), soluble chemical oxygen demand (sCOD), total solids (TS), volatile solids (VS), total suspended solids (TSS), volatile suspended solids (VSS), inorganic nitrogen (IN), volatile fatty acids (VFA), pH, and alkalinity.

The process is controlled through the LabVIEW program on the local computer which also logs sensor data at thirty second intervals. An online connection allows remote monitoring and control of the reactor. This instrumentation has been in place since August 13, 2011

4.3 ADMI

The model adapted in this project is based on an AQUASIM file that contained the ADM1 model with parameters adjusted for an upflow anaerobic sludge blanket (UASB) reactor. The process used for developing the parameters is presented in Figure 4.1. It required many iterations of trial and error, especially to determine the substrate composition. The ADM1 model divides the influent into several specific constituents, which is rarely known in such detail. Manure composition, as defined by Lübken (2007), Rico (2007), and Zeeman and Gerbens (2002) was used to help describe the manure.

It was decided that the best solution was to have each component defined as a formula variable equal to a fraction multiplied by the related type of COD (soluble or particulate). For example, for amino acids:

$$input_S_aa_in = 0.31 * input_sCOD_inf \quad (4-1)$$

where $input_sCOD_inf$ is a list variable of the measured influent sCOD. The influent COD was observed to vary by more than 50%, so an average value did not give accurate enough simulations. Using the measured influent COD as a dynamic input to the model allowed for the impacts of other parameters to be observed and corrected more easily. The default definitions of sCOD and pCOD in the AQUASIM model included only the substrate, or degradable elements. Gosset and Belser (1982) show that the influent COD can be largely non-biodegradable in anaerobic conditions. Consequently, the definition was modified to include inerts so it would be equivalent to the experimental data that measures the entire COD.

Steady state analysis was used to determine preliminary values for parameters including component fractions. The conditions were 25 L/d feed flow, reactor temperature of 24 °C and average COD values. Matching simulated effluent COD values, and, consequently, biogas production to empirical data was dependent mainly on the amount of inerts. Most of the degradable COD is in the reactor long enough to be fully digested to CH₄ and CO₂. Initial biomass concentrations were also determined under these steady state conditions.

Logged sensor data of effluent flow, biogas flow, methane concentration, and reactor temperature were resampled by decimation using the *idresamp* function in MATLAB. Setting the new time interval to one hour reduced the number of data points to a few thousand. The code can be found in Appendix B:

Resampling code, which also creates a .txt file. AQUASIM is able to import this data as a list variable, which can be used as an input or simply plotted to compare with simulation results (e.g. methane concentration). The measured effluent flow is assumed to be equal to the feed flow. Therefore this data was decimated and used as the feed flow input for the simulation.

Some parameters, like reaction rates, have values as suggested by Page et al. (2008) and Zhang et al. (2009). The full list of relevant parameters can be found in Appendix A: Selected ADM1 parameters.

The time period used for adapting the ADM1 model was August 14 to November 21, 2011. In this span of one hundred days, new batches of manure were put into use on days 30 and 87. Feed flow and reactor temperature were manipulated during the study so the reactor's dynamic response could be observed. Simulations in AQUASIM were done with a step size of 0.005 d.

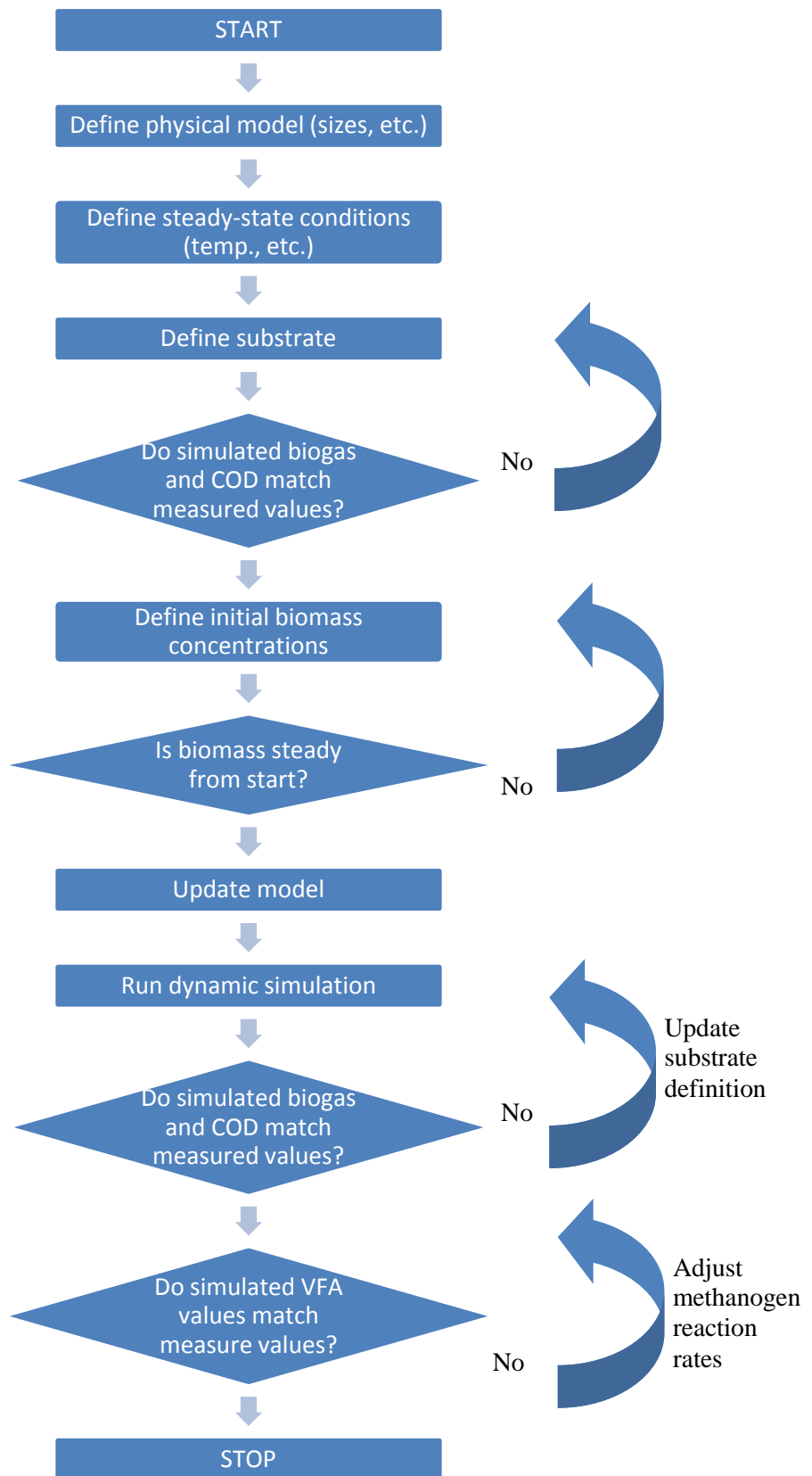


Figure 4.1: ADM1 AQUASIM model development process

5. Results

5.1 Reactor operation

Operational changes in feed flow and temperature during the study are presented in Figure 5.1 and Figure 5.2. The brief drops in feed flow are the result of clogged inlet pipes. The reactor temperature was increased from 24 °C to 30 °C on day 60, and to 35 °C on day 67.

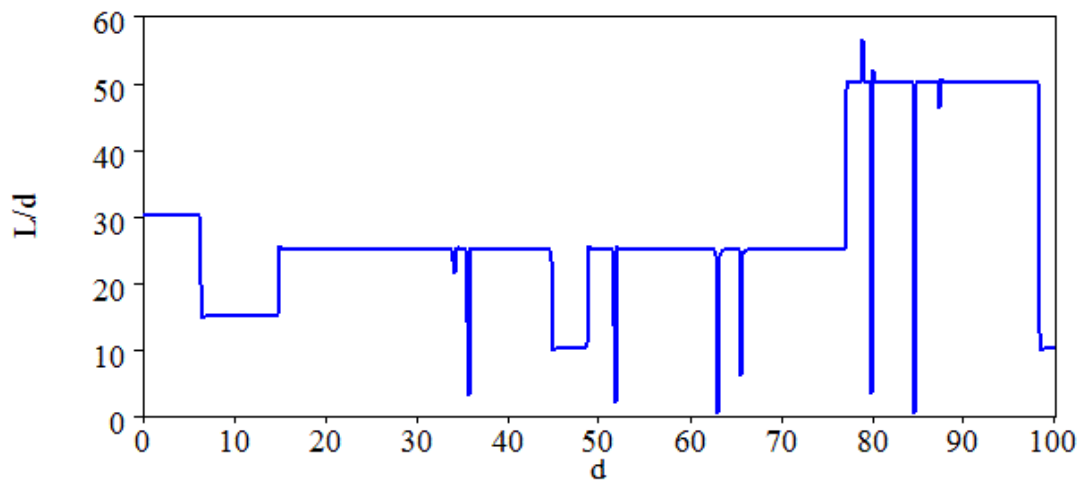


Figure 5.1: Feed flow used in the simulation

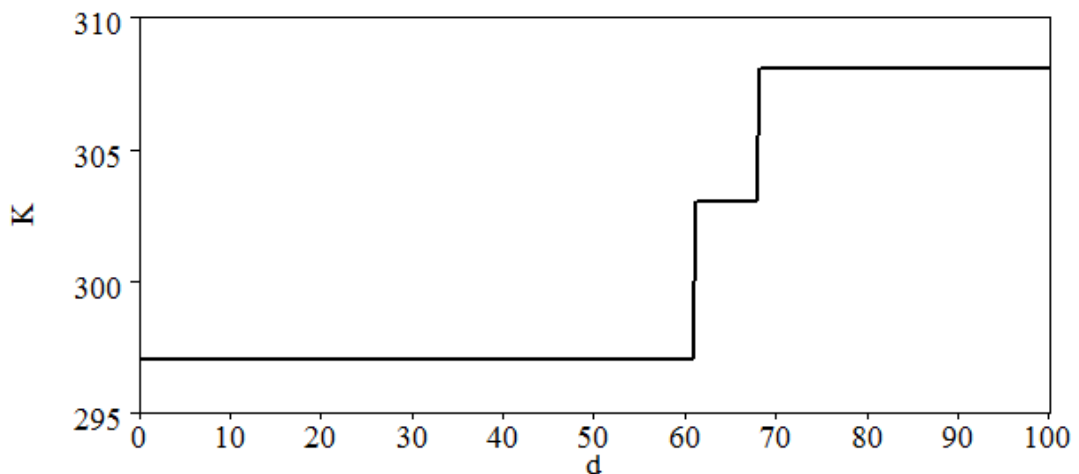


Figure 5.2: Reactor temperature used in the simulation

All of the plots presented below (until section 5.7) are from the same simulation with these operating conditions.

5.2 Manure composition

The influent to the reactor is defined in the model as presented in Table 5.1.

Table 5.1: Definition of the manure (feed) used in ADM1.

	Symbol	Fraction	Average ¹	Units
Soluble				
Amino acids	input_S_aa_in	0.31	4.23	gCOD/L
Fatty acids	input_S_fa_in	0.21	2.87	gCOD/L
Sugars	input_S_su_in	0.15	2.05	gCOD/L
Degradable sCOD		0.67	9.15	gCOD/L
Inerts	input_S_I_in	0.33	4.51	gCOD/L
Total sCOD		1.00	13.66	gCOD/L
Inorganic carbon ²	input_S_IC_in	-	0.005	M
Inorganic nitrogen ³	input_S_IN_in	-	0.065	M
Particulate				
Carbohydrates	input_X_ch_in	0.01	0.32	gCOD/L
Complex comp. particulates	input_X_c_in	0.01	0.32	gCOD/L
lipids	input_X_li_in	0.02	0.65	gCOD/L
proteins	input_X_pr_in	0.03	0.97	gCOD/L
Degradable pCOD		0.07	2.26	gCOD/L
Inerts	input_X_I_in	0.93	30.09	gCOD/L
Total pCOD		1.00	32.35	gCOD/L
Total Degradable COD		0.25	11.42	gCOD/L
Total COD		1.00	46.01	gCOD/L

1. Based on influent from 14.08.2011 through 18.11.2011.

2. Default value from UASB file.

3. Calculated average from lab measurements.

The substrate was defined in accordance with the screened values of dairy manure determined by Rico et al. (2007). Figure 5.3 shows that the unscreened values of Rico et al. are consistent with others studies that tested only raw manure. The 1.5 mm mesh sieve used by Rico et al. is comparable with the 1.4 mm mesh separator used at the farm. The ratios between soluble substrate components (amino acids, fatty acids, and sugars), and particulate substrate components (proteins, lipids, and carbohydrates) are roughly the same.

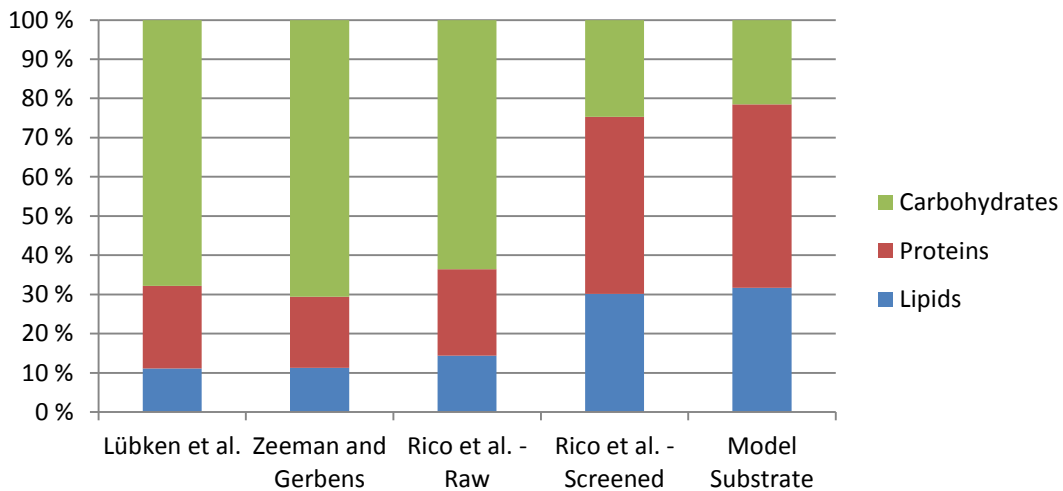


Figure 5.3: Model substrate breakdown compared to Lübken et al. (2007), Zeeman and Gerbens (2002), and Rico (2007).

5.3 Biogas flow and composition

Simulated and measured biogas flow during 100 days of reactor operation is presented in Figure 5.4. Even though the simulation's steady-state gas production levels are not exact, the model correctly predicts production changes resulting from step changes in operating conditions. Feed flow reductions on days 6 and 44 caused decreased biogas production that the model accurately predicts. However, when the feed doubles to 50 L/d at day 77, the simulated biogas production is about 25% lower than observed. The sharp spikes in production at days 60 and 67 are the result of temperature increases. The simulation predicts the initial rise but does not settle at a higher production rate like the measurements suggest. Simulated and measured methane content of the biogas can be seen in Figure 5.5. The simulated values are only slightly lower than observed and the effects of temperature increases on days 60 and 67 are accurately predicted by the model.

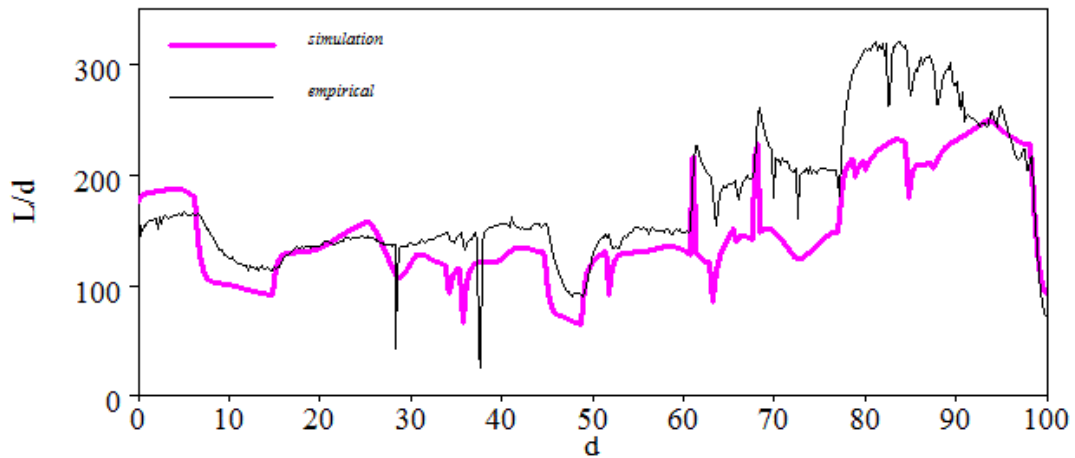


Figure 5.4: Biogas flow in the reactor

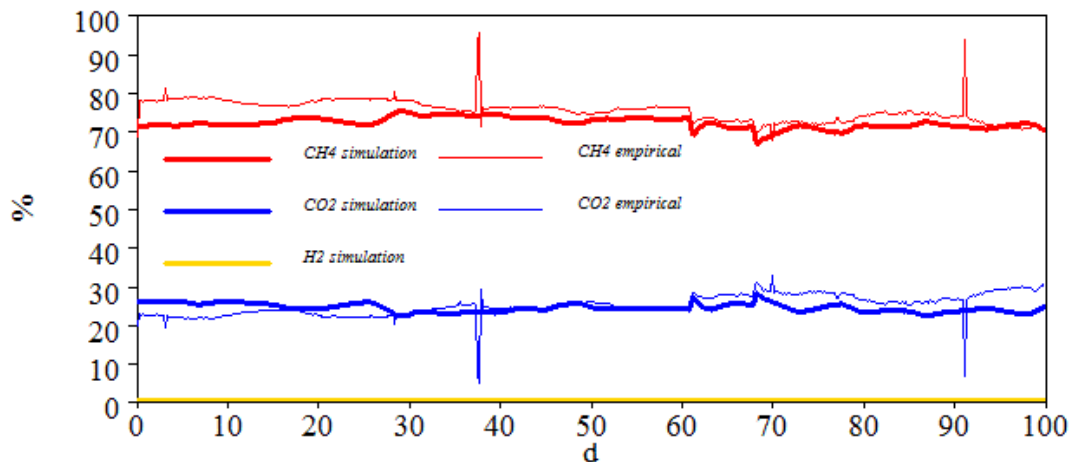


Figure 5.5: Biogas composition

5.4 COD

In Figure 5.6 the simulated COD concentrations are shown for the reactor and effluent. The high pCOD concentration in the reactor is expected because of the long solids retention time. The high feed flow from day 77 to 98 causes an accumulation of pCOD in the reactor. In contrast, the sCOD concentration in the reactor remains relatively constant and is the same as the effluent concentration. The sCOD concentration of the influent is plotted with simulated and measured values of the effluent in Figure 5.7. The same plot for pCOD concentrations is presented in Figure 5.8. It can be seen that it is mainly sCOD that is converted to biogas in the anaerobic digester. The average sCOD reduction is 62%, while pCOD changes by just 3%.¹ The simulated effluent pCOD exhibits large step

¹ average reduction = $\frac{\text{average change in COD}}{\text{average influent COD}}$

changes, but Figure 5.6 shows that this is just an outlet phenomenon and the effect on the conditions in the reactor are negligible.

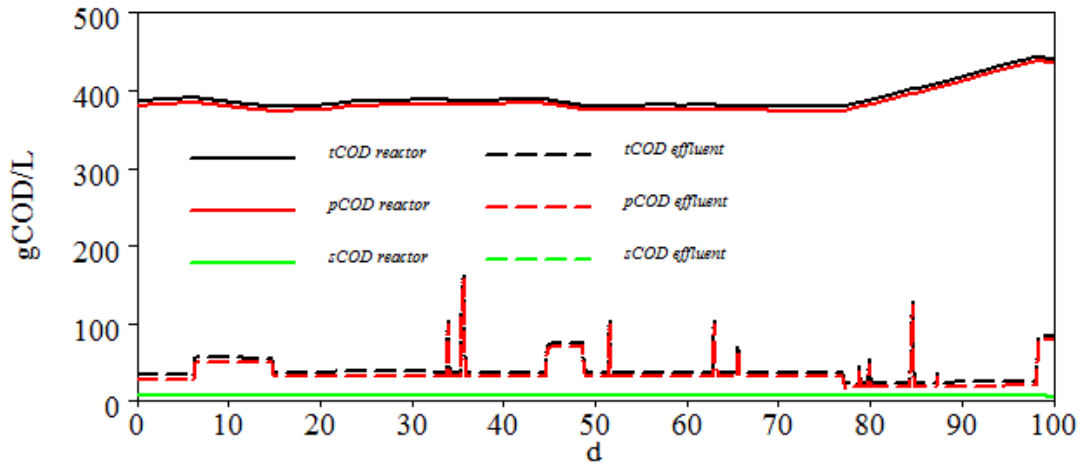


Figure 5.6: Simulated COD values in the reactor and effluent

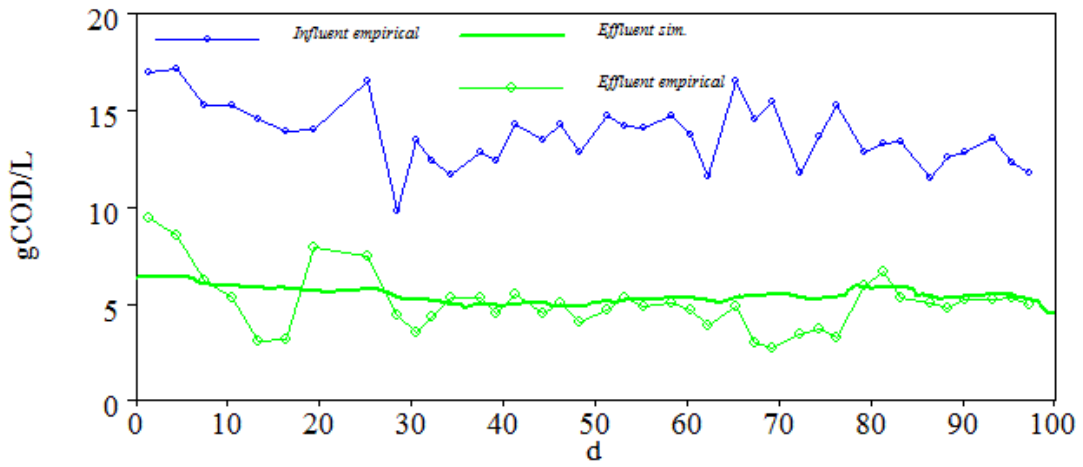


Figure 5.7: Soluble COD at inlet and outlet

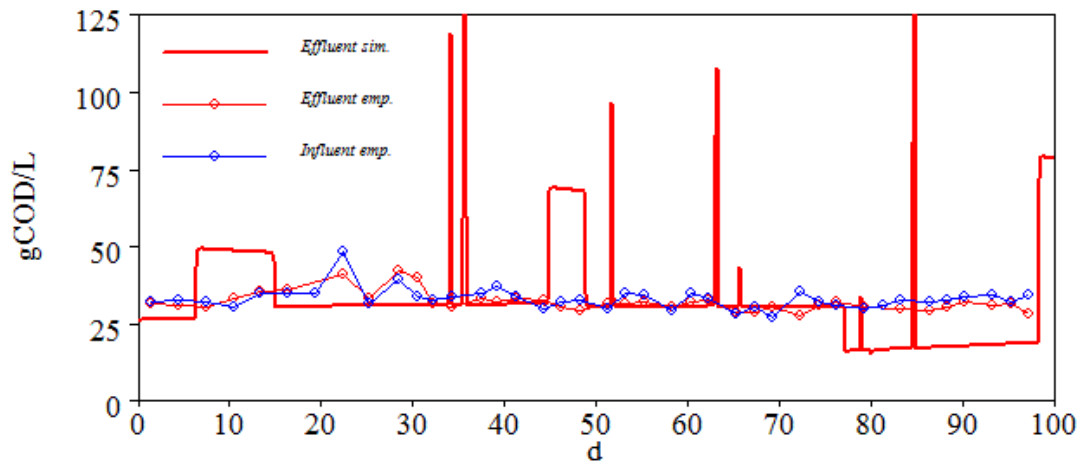


Figure 5.8: Particulate COD at inlet and outlet

5.5 VFA

Volatile fatty acids are an intermediate state of anaerobic digestion. Their relative concentrations can indicate if processes are unbalanced. Simulated and measured total VFA concentrations of the effluent are presented in Figure 5.9. The measured values show much larger variations than the simulation. Figure 5.10 shows that acetic and propionic acids are the main components in both the simulation and empirical data. The shape of the simulated acetic acid concentration is very similar to the simulated biogas flow, which is logical because it is a precursor to methane. The high simulated acetic acid concentration in the effluent explains the lower than expected biogas production in the last 23 days. Acetate is being produced by acidogenesis faster than acetoclastic methanogenesis can convert it to methane.

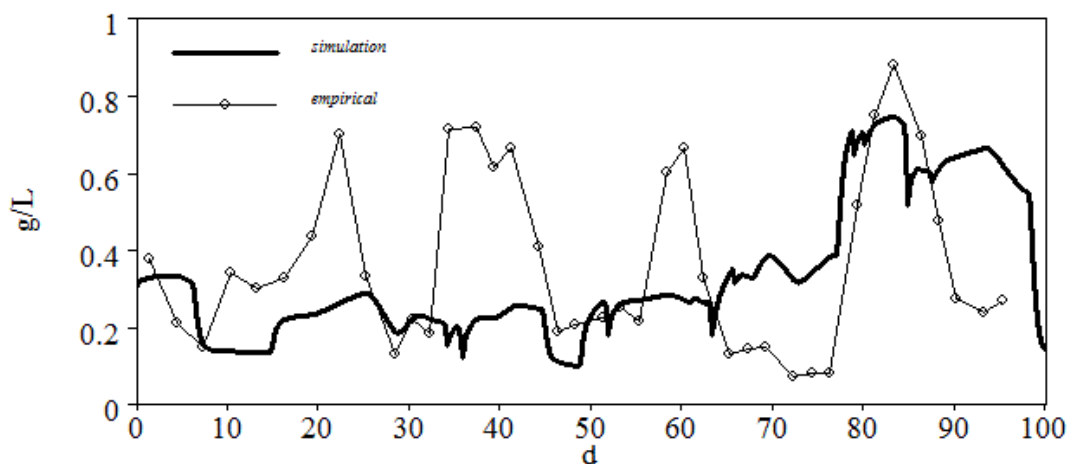


Figure 5.9: Total effluent VFA concentration

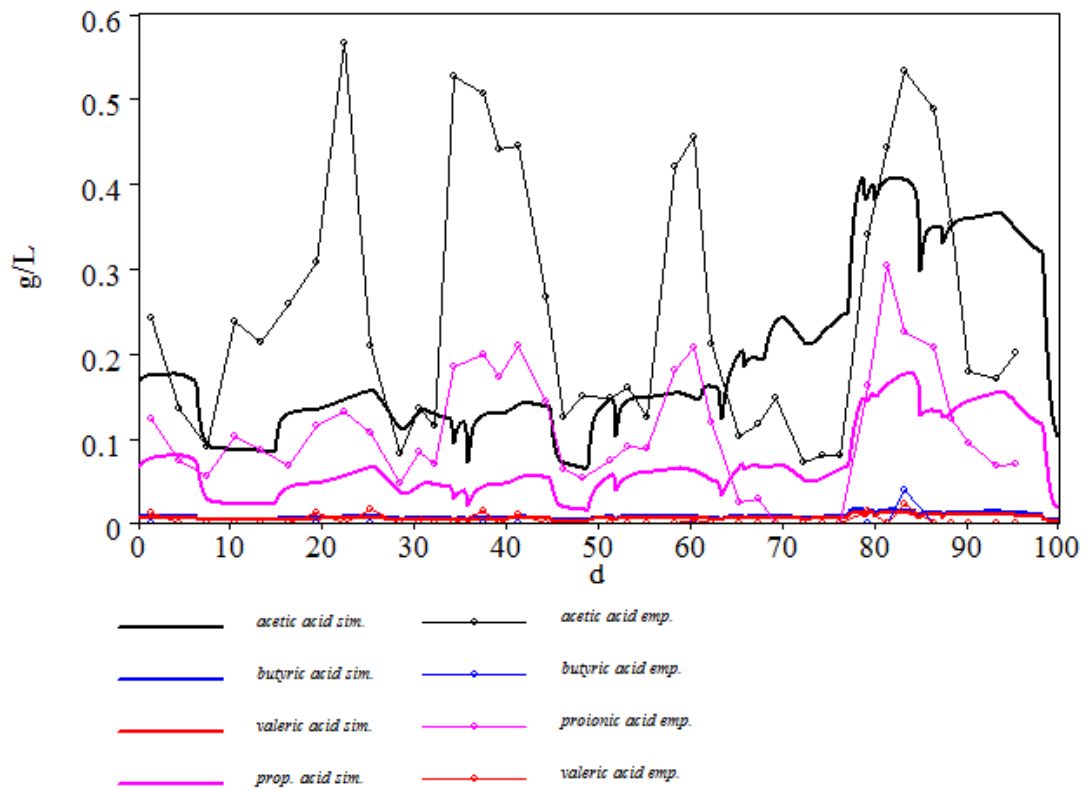


Figure 5.10: Comparison of different VFA concentrations in the effluent

5.6 Biomass

Simulated concentrations of acidogens and methanogens in the reactor are presented in Figure 5.11. As expected, the increase in feed flow at day 77 brings more substrate, which increases the number acidogenic organisms. The relatively slow response of methanogenic organism growth seen in Figure 5.11 can explain the increase in VFA concentrations at the same time.

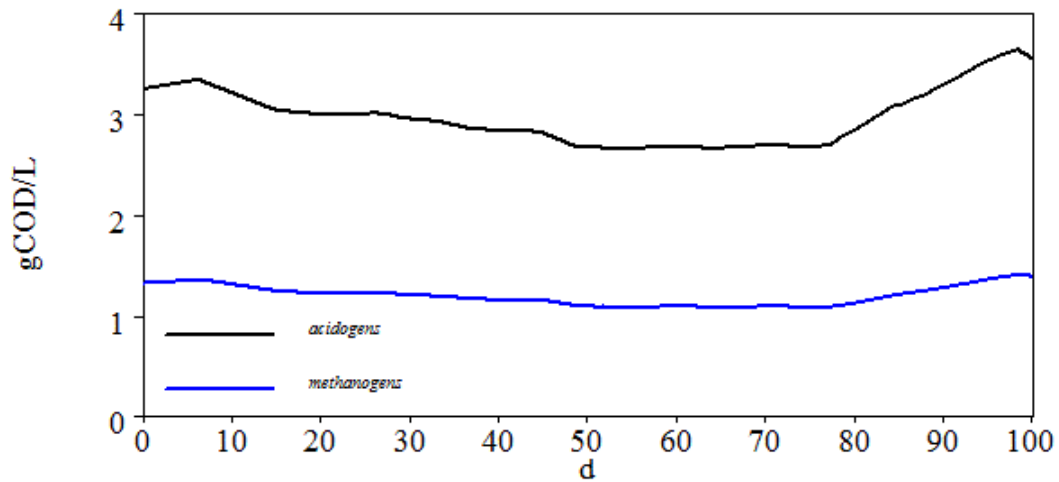


Figure 5.11: Reactor concentrations of acidogens (amino acid and monosachharide degrading organisms) and methanogens (acetic acid and hydrogen degrading organisms).

5.7 Inhibition and pH

The ADM1 model contains several inhibition factors that affect kinetic uptake and growth. Simulated values of these factors in the reactor are presented in Figure 5.12, where “1” means zero inhibition. Ammonia inhibition of aceticlastic methanogenesis increases on days 60 and 67, which coincides with the temperature increases and lower than expected biogas production. Hydrogen inhibition of organisms degrading propionate, butyrate, and valerate is stronger when flow rates are higher.

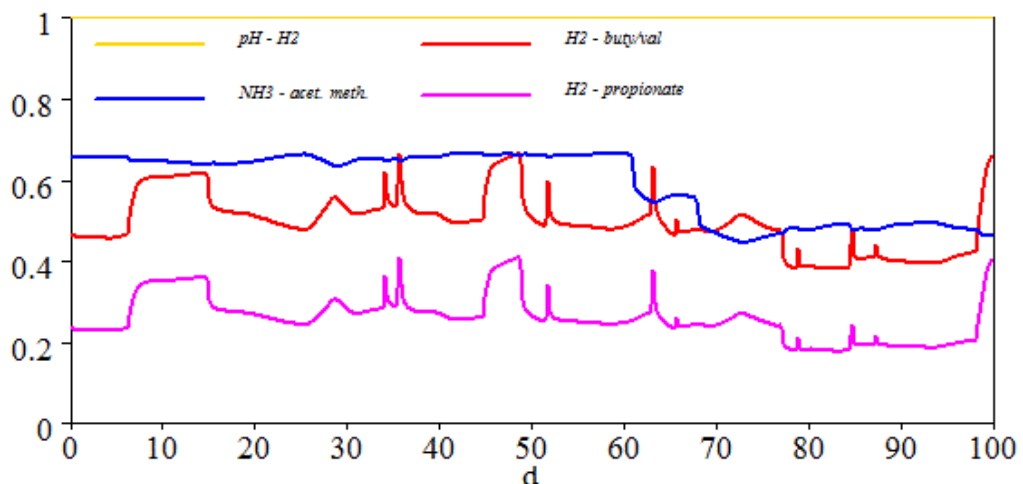


Figure 5.12: Simulated inhibition factors. pH-H2: pH inhibition of hydrogen degrading organisms, NH3-acet. meth.: NH3 inhibition of aceticlastic

methanogenesis, H₂-buty/val: hydrogen inhibition of butyrate and valerate, H₂-propionate: hydrogen inhibition of propionate.

Simulated and observed pH levels in the reactor are presented in Figure 5.13. It is assumed that pH measurements of the effluent are representative of the reactor contents. The simulated pH in the reactor is consistently lower than the measured values.

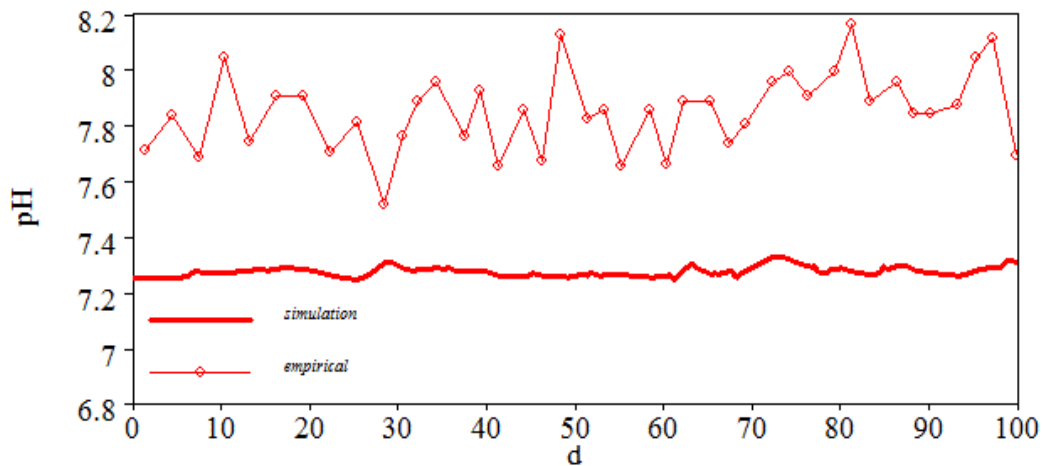
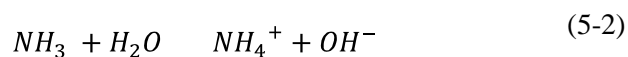


Figure 5.13: pH in the reactor

A simulation was conducted to observe the possible impact of this difference by “forcing” the pH in the model to the observed levels. The AQUASIM model was modified by changing the definition of hydrogen ion concentration (the basis of pH) from a state variable to a formula variable referencing the measured pH values as shown in equation (5-1).

$$S_{h_ion} = 10^{(-exp_pH)} \quad (5-1)$$

Figure 5.14 shows increased ammonia inhibition and that its shape is opposite to that of measured pH. This effect is consistent with equation (5-2), the dissociation when ammonia is dissolved in water. As pH increases the reaction shifts to the left, increasing ammonia levels and thus inhibition. The influence of this ammonia inhibition on biogas production can be seen in Figure 5.15. The simulated gas composition also changed, showing 10-15% more methane (figure not shown).



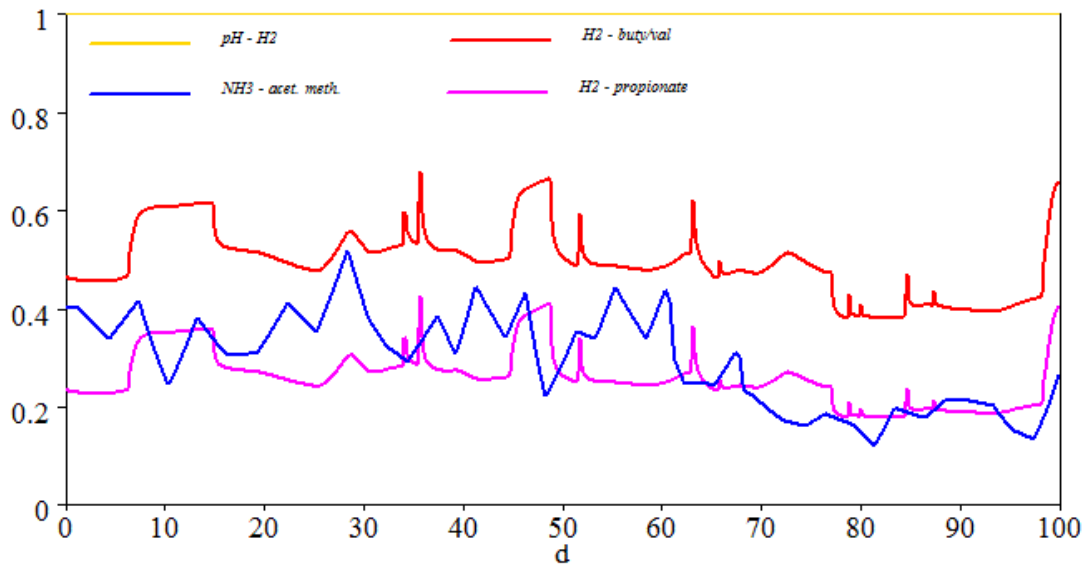


Figure 5.14: Simulated inhibition factors when pH in reactor set to measured values. pH H2: pH inhibition of hydrogen degrading organisms, NH3-acet. meth.: NH3 inhibition of acetoclastic methanogenesis, H2-buty/val: hydrogen inhibition of butyrate and valerate, H2 propionate: hydrogen inhibition of propionate.

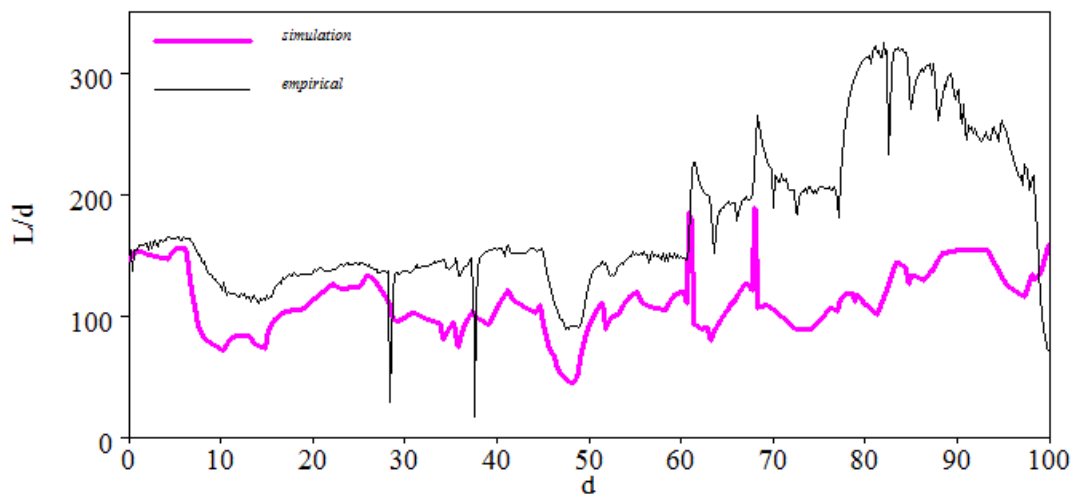


Figure 5.15: Biogas flow in the reactor using measured pH values in the model

5.8 Temperature effect

A simulation was conducted to isolate the effect of temperature increases and the biogas production is presented in Figure 5.16. The model used for the simulation above was modified to have constant, average sCOD and pCOD influent, as well as a flow rate of 25 L/d. Temperature started at 24 °C and increased to 30 °C at day 10, and to 35 °C at

day 60. Biogas production went from 155 L/d to 161 L/d to 166 L/d. These are clearly less dramatic than the observed increases.

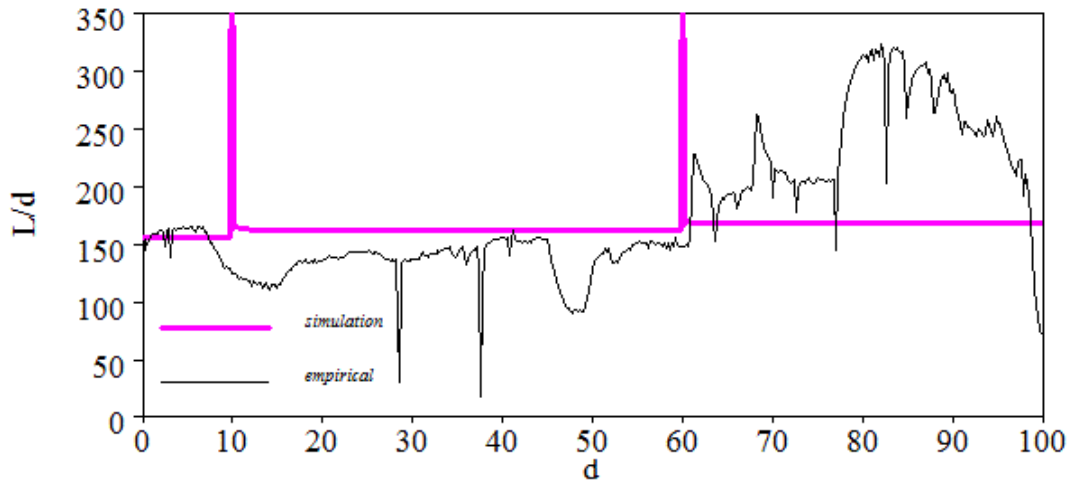


Figure 5.16: Temperature effect on biogas production (24 °C, 30 °C, 35 °C).

5.9 Feed flow and washout

Even though the granular sludge in the reactor is dense enough to remain in the reactor under high loading conditions, they are still susceptible to washout. A simulation was done in an attempt to find the maximum possible loading of the pilot plant. When the feed flow was increased step-wise to an extremely high level (10 000 L/d) the biogas production increased congruently without dropping off. This signals that the model is unable to predict washout and therefore cannot be used to determine maximum loading conditions.

In the model, solids are defined to remain in the reactor longer than the fluid, given by equation (5-3). The constant variable $tres_x$ represents the number of days difference between solids retention time (SRT) and hydraulic retention time (HRT). To model the granular sludge in the AD, $tres_x$ was set to 100 days. This is the reason the model is unable to predict washout even when HRT was extremely low.

$$SRT = HRT + tres_x \quad (5-3)$$

Another simulation was done setting $tres_x$ to 0.1 (the equivalent of 2.4 hours) and increasing feed flow. In this scenario biogas production eventually crashed, indicating that washout conditions had occurred and were possible to predict with a different definition of $tres_x$.

6. Discussion

Despite the thorough method used to define the influent, it is still an estimated average. The actual feed composition will vary between batches and constantly throughout the day.

The simulated biogas production fits observed data best between days 15 and 60. This is expected because operating conditions during that time are similar to the steady-state conditions when many parameters were determined. Feed flow and temperature increases after day 60 cause the simulation to deviate from measured values. This is most likely because the model's reaction rates (uptake, growth, etc.) are defined independent of temperature. In the description of ADM1, Batstone et al. (2002) state that reaction rates increase with increasing temperature as predicted by the Arrhenius equation. Furthermore, van Lier et al. (1997) suggest that mesophilic methanogens grow twice as fast at 35 °C than at 24 °C. Figure 5.11 shows the slow growth of methanogens that limits biogas production. This growth (and that of other microorganisms) accounts for the consistent, low effluent sCOD even though the biogas production has not increased proportional to the feed rate.

The two spikes in biogas production at days 60 and 67 are because of the temperature increase. The solubility of methane and carbon dioxide in water decreases with increasing temperature. As the temperature rises, gases dissolved in the reactor fluid are released to the headspace and increase the measure biogas flow. The drop in methane concentration and increase in carbon dioxide concentration is because the solubility of CO₂ drops more (percentage-wise) than methane, therefore the relative amount of CO₂ released is greater.

The large step changes in simulated effluent pCOD are not supported by the lab analysis. They are, however, inversely proportional to the feed flow. When the feed rate drops from 30 to 15 L/d on day 6, HRT doubles while SRT increases by only 7%. In other words, solids such as pCOD are leaving the reactor at basically the same rate, while the amount of liquid leaving is half. For this reason the simulation shows that the concentration of pCOD in the effluent is nearly double. In reality, the retention time of pCOD is closer to HRT. In an earlier version of the model, simulated VFA concentrations were an order of magnitude below the measured values. Decreasing the yield of degradation (Y_{ac}) and increasing the half saturation constant of acetate utilization ($K_{s_{ac}}$) increased simulated concentrations of acetic and propionic acid. These changes reduce the rate and extent to which methanogens grow. As a result it also lowered simulated methanogen concentration, and is part of the reason the model underestimated biogas production after day 60.

The fluctuating measurements of effluent VFA may not be correct. There are known instances of overdue liner (filter) changes on the gas chromatograph that may have caused inaccurate measurements.

The ammonia inhibition of aceticlastic methanogenesis in Figure 5.12 changes with temperature. This is because the temperature dependence of the ammonium ion acid constant is included in the model. This inhibition contributes after day 60 to simulated biogas production that is lower than observed.

The reason for the discrepancy between simulated and observed reactor pH values is not known, nor are its consequences fully understood. One explanation may be that the lab analysis is done on samples stored at 4 °C, and the pH of most solutions increase as temperature decreases.

The model's inability to predict washout is because of the definition of SRT. As described above, SRT will be at least 100 days with the current model definition.

7. Conclusion

The ADM1 model developed in this project simulates the anaerobic digestion process at Foss farm quite well. Correct description of the influent is necessary for the model to predict reactor operation accurately. This is especially important when the model is to be used for process control and optimization. The model is able to accurately predict methane, effluent COD and VFA concentrations in steady-state and dynamic operating conditions. Simulations at reactor temperatures greater than 24 °C underestimate biogas production because the model's reaction rates are not functions of temperature. Redefining rates to be temperature dependent will allow the model to better predict the process over a wider range of operating conditions.

Additional research could be done to better understand pH levels in the model and their relation to measured values. Another area of work could be to redefine SRT so the model can simulate washout. For example, SRT could be defined as a constant unless (using the 'if' statement) the vertical velocity was greater than a recommended maximum value, where the velocity can be calculated from feed flow and reactor geometry.

In conclusion, ADM1 is a valuable tool for the design and operation of anaerobic digesters with dairy manure substrate. ADM1 simulations provide information on many states in the reactor that can help identify limiting factors in the anaerobic digestion process. This can be used to improve operating conditions or assist in reactor design. At the same time, the sheer number of inputs and parameters that must be specified make it time-consuming and cumbersome to use.

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Appendix A:

Selected ADMI parameters

<i>Parameter</i>	<i>Symbol</i>	<i>Value</i>	<i>Unit</i>	<i>Ref.</i>
Disintegration constant	kdis	0.4	1/d	1
Hydrolysis rate of carbs	khyd_ch	0.25	1/d	2
Hydrolysis rate of lipids	khyd_li	0.1	1/d	2
Hydrolysis rate of proteins	khyd_pr	0.2	1/d	2
Max uptake rate of amino acid degrading organisms	km_aa	50	gCODS/gCODX	3
Max uptake rate of acetic acid degrading organisms	km_ac	7.927	gCODS/gCODX	4
Max uptake rate of but. and val. degrading organisms	km_c4	20	gCODS/gCODX	1
Max uptake rate of LCFA degrading organisms	km_fa	6	gCODS/gCODX	3
Max uptake rate of hydrogen degrading organisms	km_h2	140	gCODS/gCODX	4
Max uptake rate of propionic acid degrading organisms	km_pro	13	gCODS/gCODX	1
Max uptake rate of monosaccharide degrading organisms	km_su	30	gCODS/gCODX	3
Yield of biomass on uptake of amino acids	Y_aa	0.08	gCOD/gCOD	3
Yield of biomass on uptake of acetate	Y_ac	0.03	gCOD/gCOD	5
Yield of biomass on uptake of valerate or butyrate	Y_c4	0.06	gCOD/gCOD	1
Yield of biomass on uptake of long chain fatty acids	Y_fa	0.06	gCOD/gCOD	3
Yield of biomass on uptake of elemental hydrogen	Y_h2	0.02	gCOD/gCOD	5
Yield of biomass on uptake of propionate	Y_pro	0.04	gCOD/gCOD	3
Yield of biomass on uptake of monosaccharides	Y_su	0.1	gCOD/gCOD	3

References:

1. Default value from original UASB file
2. Batstone et al. (2002)
3. Page et al. (2008)
4. Zhang et al. (2009)
5. Estimated in this study from experimental results

Appendix B: Resampling code

```
%Resampling Biogas Flow Rate- here to obtain fewer data points
(i.e. decimation)
%A filter is used by default on the original data
%The order of the filter is 8. Probably not necessary to change
order
%but can be done using an additional argument in function
idresamp.
%Functions iddata and idresamp belongs to System Identification
Toolbox.
%Get info about these functions, incl. additional arguments, with
Help in
%Matlab.
%Alternatively, the resample function in Signal Processing TB can
be used.
%Modified by Benjamin Lyseng 22.10.2011

Tsampling=1/24/60/2; %Sampling time of original data. 30 sec
expressed in unit of day.
iddata_logdata=iddata(biogasflow_bronkhorst_filt,[],Tsampling);
%First input is file to be filtered
resamp_factor=120; %120 gives hourly data.
iddata_logdata_resamp=idresamp(iddata_logdata,resamp_factor);
%Resampling is executed.
logdata_resamp=iddata_logdata_resamp.y; %y is an element in the
struct iddata_logdata_resamp.
for i=1:length(logdata_resamp)
    t_data(i,1)=Tsampling*resamp_factor*(i-1); %Time indexes the
data in days
    t_data(i,2)=logdata_resamp(i);
end
save('biogasflow_resamp.txt','t_data','-ascii'); %Saving data to
text-file.
```

**The code for resampling other data (e.g. feed flow) is almost identical and not presented here.