

Parameters Analysis and Discussion of the IWA Anaerobic Digestion Model No.1 (ADM1) for the Anaerobic Digestion of Blackwater plus Kitchen Refuse

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Abstract

The IWA anaerobic digestion model No.1 (ADM1) had been successfully applied to the lab-scale mesophilic blackwater anaerobic digestion (BWAD) plant for both cases with only blackwater (BW) feeding and with BW plus kitchen refuse (KR) feeding. In this paper, the simulation results of BW + KR anaerobic digestion are presented and discussed, following by the analyses and discussion of the critical and important parameters as well as the performance of ADM1 based on these results. The raw BW can contain up to 30% short chain fatty acids (SCFA) which impacts to the performance of the model severely. The model proved that the disintegration/hydrolysis rate of BW is around 4.5 d^{-1} , which is about ten times higher than it of KR ($K_{\text{dis,KR}} = 0.5 \text{ d}^{-1}$). ADM1 is not sensitive to distribution ratio among carbohydrates, proteins and lipids. For BWAD the C4 metabolism can be integrated in the uptake of LCFA. The uptake delay phenomenon was observed and can not be simulated by ADM1, but it is tolerable. No unique $K_{\text{I,NH}_3,\text{ac}}$ is found out for all investigated ammonia concentration ranges. Meanwhile, ADM1 is not sensitive to K_{La} and k_{p} , so they can be easily set up.

Keywords

ADM1, blackwater (BW), kitchen refuse (KR), blackwater anaerobic digestion (BWAD), disintegration, hydrolysis, inhibition, K_{La} and k_{p} , mesophilic, Monod-type kinetics

INTRODUCTION

Being one of the oldest natural processes, anaerobic digestion (AD) is also among the oldest processes used for wastewater treatment and biosolids stabilization (Metcalf & Eddy 2003). AD is also an appropriate as well as an important waste and wastewater treatment method for Ecological Sanitation (ECOSAN) (Otterpohl *et al.* 1997). Therefore, due to its many advantages both European community and U.S. consider the anaerobic treatment as the most promising approach for future in sustainable development (Lema and Omil 2001, NRC 1995). The mathematical anaerobic digestion model (ADM) has been extensively investigated and developed during the last 3 decades (Gavala *et al.* 2003). As one of the most sophisticated and complex ADM, the IWA Anaerobic Digestion Model No. 1 (ADM1) was published by the IWA Task Group for Mathematical Modelling of Anaerobic Digestion Processes in 2002 (Batstone *et al.* 2002).

Based on ECOSAN concepts, blackwater (BW) (contains faeces, urine, toilet paper and flushing water) from vacuum toilet can be treated in biogas plant so that the energy is recovered as biogas and the fertilizer is generated (Otterpohl *et al.* 1999). One ECOSAN project was successfully realized in Lübeck-Flintenbreite, Germany (Otterpohl 2001). Correspondingly, in order to optimize the on-site biogas plant and find out control options and process variations, a lab-scale mesophilic blackwater anaerobic digestion (BWAD) plant was built up in the Institute of Municipal and Industrial Wastewater Management, Hamburg University of Technology, Germany. ADM1 was applied to simulate the performance of this lab-scale BWAD plant. The model successfully achieved three scenario studies, namely, (1) Reference Conditions, (2) Different Feeding Frequencies and (3) With High NH_4^+ Concentration. Meanwhile, two virtual scenario studies with kitchen refuse (KR) as

additional organic loading were executed by the model, and the model properly showed the tendency and provided usable suggestions (Feng *et al.* 2005). Hereby, KR was added into lab-scale BWAD plant. In this paper the simulation results of anaerobic digestion of blackwater plus kitchen refuse (AD of BW + KR) are presented and discussed, and the important parameters as well as the performance of ADM1 are analysed and discussed based on these simulation results.

MATERIALS AND METHODS

All experimental data were generated by three parallel lab-scale BWAD reactors, which were built up as the Continual Stirred Tank Reactors (CSTR). Each reactor has 10.0 l volume. 8.0 l blackwater (BW) and sludge were held in each reactor, where 2.0 l space was retained as the headspace. The reactors were operated at 38°C with discontinuous BW feeding, which were under the same conditions as the on-site biogas plant (Wendland *et al.* 2004). The reactors were fed 3 times per week. The hydraulic retention time (HRT) and the sludge retention time (SRT) were the same of 20 days. BW from vacuum toilets has relative high COD, which is normally in the range from 4,500 to 13,000 g COD/m³ with the average level of 6,500 g COD/m³. The biogas production and pH were measured on-line, where other parameters were checked once per week. The lab-scale BWAD reactors had been steadily operated for two years. More details about materials, equipments and experiments can be found from Feng *et al.* (2005). ADM1 was implemented by the software AQUASIM 2.1d, which is a computer program for data analysis and simulation of aquatic systems (Reichert 1994). AQUASIM 2.1d also provides two powerful tools: Sensitivity Analysis and Parameter Estimation, where the latter tool can be used for verifying the kinetic parameters.

Regarding KR, every time the grinded KR was mixed with BW firstly, and then the mixture was fed into the reactors. The feeding frequency was also 3 times per week, and HRT were kept the same as before, i.e. 20 days. The organic loading of KR was in the range of 7,000 to 13,5000 g COD/m³.

RESULTS

In this paper the simulation results of AD of BW + KR are presented and discussed, and the simulation of other five above-mentioned scenario studies can be found from Feng *et al.* (2005).

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The model has been calibrated based on the Reference Conditions scenario (see Feng *et al.* 2005). KR is added into the model considered as independent organic loading. The stoichiometric coefficients of KR ($f_{\text{product,KR}}$) and the disintegration rates of KR ($K_{\text{dis,KR}}$) were set up, respectively. In order to get better simulation results, the different $K_{\text{dis,KR}}$ were tested by the model, i.e. 0.8 d⁻¹, 0.5 d⁻¹ and 0.3 d⁻¹. Figure 1 shows the simulation results of biogas production rates (BPR) with different $K_{\text{dis,KR}}$. In the figure Y-axis is the specific BPR which is the absolute BPR divided by the reactor volume under the standard conditions.

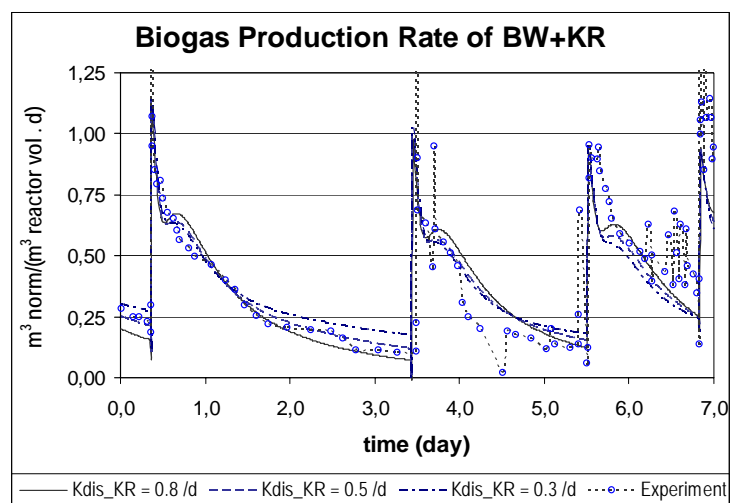


Figure 1: Biogas production rate (BPR) of BW + KR, with different $K_{\text{dis,KR}}$

Due to unknown reasons, the experimental data of day five and day seven are unstable. Except that,

the model is able to properly simulate AD of BW + KR in a general manner. It shows also that when $K_{dis,KR}$ is set up as 0.5 d^{-1} , the simulation curve is fitted with the experiment data better. It is also well coped with the suggested value by ADM1. This rate is about ten times lower than that of BW which is 4.5 d^{-1} . Meanwhile, under the reference conditions, the maximum BPR is around $0.2 \text{ m}^3 \text{ norm}/(\text{m}^3 \text{ reactor volume} \cdot \text{d})$ (see Figure 2). Therefore, BW + KR has around 4 times higher BPR than BW, which implicit that AD of BW + KR is a very promising method for waste and wastewater treatment. Other parameters were also appropriately simulated which are not shown here.

DISCUSSION

Based on all these scenario studies, the important parameters as well as the performance of ADM1 are analysed and discussed as follows.

Characterization of the raw blackwater

As discussed in ADM1, the biodegradability of raw BW is one of the key issues. The analytical method from Pavlostathis and Gossett (1986) and Gossett and Belser (1982) are suggested. However, those methods mainly deal with the biodegradability of activated sludge from wastewater treatment plants, which is unlike BW, so the biodegradability of BW needs to be examined individually. From the medical description of faeces and the testing results by ADM1, the inert part of BW is around 20 to 30%. In our studies, 25.5% of total input COD was treated as the inert part which resulted in the very good simulations.

The biodegradable portion of input is further hydrolysed into three parts, carbohydrates (ch), proteins (pr) and lipids (li). The distribution ratio among three parts is regarded as the critical and difficult issue, as carbohydrates, proteins and lipids have different hydrolysis rates. It is, generally, necessary to determine this ratio in order to execute ADM1 accurately. However, it is found that the distribution ratio is not sensitive in BWAD, which might be caused by following reasons. Firstly, the hydrolysis rates of the BWAD are not critical. One observed phenomenon can prove this conjecture. For checking the hygiene conditions of BW after AD, one reactor was fed with cooked BW, which was heated at 70°C degree for an hour before feeding. This heating step can dramatically speed up hydrolysis rates. Nevertheless, cooked and uncooked BW have the same biogas products and BPR, which implicates that hydrolysis is not rate-limiting step for the BWAD. Secondly, in our case BW already contains around 25-30% short chain fatty acids (SCFA), which are mainly acetate. The existence of SCFA (especially acetate) in raw BW further diminishes the influence of hydrolysis step on the final output in the model.

By the performance of our model, it shows that the variation of this ratio can be 20 ~ 30%, whereas BPR and the biogas components are only slightly different. At the same time, the existence of SCFA in raw BW makes the model more sensitive to BW. Therefore, instead of knowing the distribution ratio, the amount of SCFA in BW must be determined. In our case, BW is characterized in Table 1.

Table 1. Characterization of the raw blackwater

Biodegradable						Inert
ch + pr + li (47.5 %)			SCFA (27 %)			25.5 %
carbohydrates	proteins	lipids	butyrate	propionate	Acetate	
14.5 %	14.5 %	18.5 %	2 %	5 %	20 %	

Disintegration and hydrolysis

As the first stage of anaerobic digestion processes, these two steps are often rate-limiting, so their reaction rates have been investigated extensively. These two steps are not separated in many literatures, and the processes are generally investigated by the term of hydrolysis.

The disintegration rates (k_{dis}) suggested by ADM1 are around 0.5 d^{-1} for mesophilic digestion.

However, k_{dis} of our BW is ten times higher than this value. After extensively testing by the model, it was found that k_{dis} has to be set around 4.5 d^{-1} . It is probably because the components of BW are mainly human faeces and BW is the liquid phase, which can be beneficial to disintegration and hydrolysis. Meanwhile, before BW was transported from the locale to the laboratory, it had been kept in the container for one or two days, and afterwards BW was stored at 4°C for about two weeks, which provides more time to perform disintegration and hydrolysis. This also can be the reason that BW contains such high amount of SCFA.

Normally, carbohydrates, proteins and lipids have different hydrolysis rates and falls into the range $0.01 \sim 1.0 \text{ d}^{-1}$. But their recommended values from ADM1 for mesophilic and thermophilic solids AD are set up as the same value of 10 d^{-1} . It is presumed that under certain situations the hydrolysis rates of three parts are not significantly different, so the same rate can be used and, consequently, they can be represented by the disintegration step. Hence, the adequately high values (e.g. 10 d^{-1}) are used in order to completely exclude the influence of hydrolysis step in the model. This also makes the model easier to be manipulated. When three components have the same hydrolysis rates, it further causes the model less sensitive to the aforementioned distribution ratio. In our case, the hydrolysis rates of three components are set up as 10 d^{-1} as recommended by ADM1.

Monod-type Kinetics

ADM1 includes 7 different sorts of degraders utilising 8 different substrates, where valerate and butyrate are utilised by the same degraders. Like most literatures, all kinetic parameters are figured out based upon their total concentrations in reactor, although Spieß (1991) proved that only undissolved SCFA can be utilised by microorganisms. In our work the same manner as ADM1 was used for uptake.

Estimation of kinetic parameters (k_m and K_S)

The batch experiments were executed in our studies in order to obtain the kinetic parameters of butyrate, propionate and acetate (Feng *et al.* 2005). The Parameter Estimation Tool offered by AQUASIM 2.1d was used to estimated the maximum uptake rates of acetate (k_m) and the corresponding half saturation concentration (K_S) of each substrate, respectively. In our studies, k_m of butyrate, propionate and acetate are testified as 18, 14, 13 d^{-1} , and the corresponding K_S are 110, 120, 160 g COD/m^3 .

Modification of the model

As the intermediates with a relative low concentration, valerate and butyrate can be skipped in our case. Two more simulations were performed in order to check the influence from valerate and butyrate on BWAD, i.e. case one: skip only valerate from the model, and case two: skip both valerate and butyrate. In both cases, the parameters were kept the same as the original model. The comparison of BPR is shown in Figure 2. It is clearly shown that BPR are nearly the same no matter with or without the utilization step of valerate, and no significant differences of other parameters were observed, either.

For the mesophilic BWAD the impact of valerate to the whole system is so small that it can be

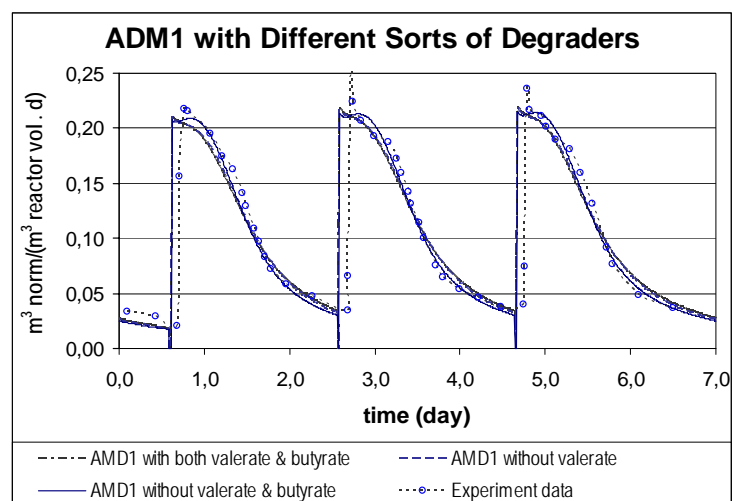


Figure 2: Comparison of ADM1 with different sorts of degraders

skipped at all. In real situation, valerate concentration in the reactors remains at a low level, which is around 20 to 40 g COD/m³ in BW, and in the reactors it is not detectable any longer 3 hours later after feeding. As to the second case, without the uptake steps of both valerate and butyrate the BPR was kept at highest rate for longer time comparing to the original one, but it is still tolerable. Furthermore, this distortion of BPR curve in the second case can be compensated by adjusting the uptake kinetics of substrates which have been successfully done.

Grounded on these two cases studies, one can say that the uptake of valerate and butyrate are optional steps for BWAD, and they can be included or excluded depending on their situations or the simulation purpose. Likewise, other intermediates can also be involved or skipped depending on their essentiality in the certain cases.

Delay phenomenon

When the organisms enter the new environment, they need certain time to adapt this change before they start functioning. This kind of delay phenomenon was limpidly observed in our lab-scale AD plant. The simulated BPR peak is always about 1 hour earlier than reality (Figure 2). This delay can not be represented by Monod-type kinetics anyhow. Batstone *et al.* (2003) observed the similar uptake delay of valerate, and tried compensating it by increasing decay rate and increasing k_m . The conjectural reasons of delay are also given by Batstone *et al.* (2003). In our case, the uptake delay can not be totally overcome by adjusting k_m , K_s or decay rates.

Inhibition

The inhibition is one of the most important aspects of anaerobic processes. Here the ammonia and pH inhibition are discussed according as the performance of ADM1 in our studies.

Ammonia inhibition

It is widely accepted that high levels of free ammonia nitrogen (FAN) are more inhibitory to the anaerobic processed than the ammonium ion itself, and the inhibitory effects of FAN influence mostly only on *methanogenesis* (e.g. Stronach *et al.* 1986). Nonetheless, many literatures reported the ammonia inhibition as total ammonium nitrogen (TAN). Meanwhile, the *methanogens* can be acclimated in the higher TAN concentration. It is reported that after acclimation to higher level of TAN, the *methanogens* become less sensitive to the change of both TAN and pH (Liu and Sung 2002). This kind of acclimation can not be simulated by ADM1.

Back to our simulation, normally TAN in BW is around 1,000~1,200 NH₄⁺-N/m³ due to the existence of urine. In order to understand the impacts of ammonia to BWAD, step by step TAN was artificially increased from 1,000~1,200 to 2,000~2,200 g NH₄⁺-N/m³ in the reactors. Correspondingly, FAN is around 45 and 70 g NH₃-N/m³, respectively. The ammonia inhibition was clearly observed and appropriately simulated (Figure 3). When TAN was increased 2 times higher, the maximum BPR was decreased 30%.

ADM1 uses the non-competitive inhibition equation to describe the ammonia inhibition, and the half inhibitory coefficient $K_{I,NH_3,ac}$ is employed.

When TAN is 1,000~1,200 g

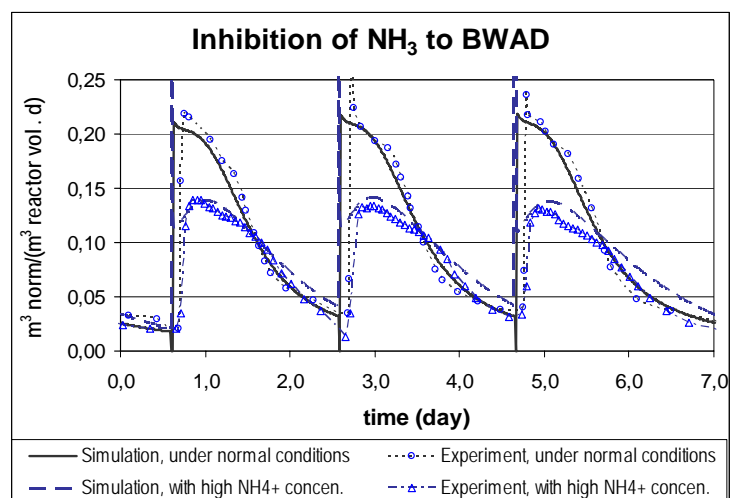


Figure 3: Comparison of biogas production rate

$\text{NH}_4^+-\text{N}/\text{m}^3$ (FAN is around $45 \text{ g NH}_3\text{-N}/\text{m}^3$), $K_{I,\text{NH}_3,\text{ac}}$ has to be set nearby $250 \text{ g NH}_3\text{-N}/\text{m}^3$; however, when TAN is $2,000\sim 2,200 \text{ g NH}_4^+-\text{N}/\text{m}^3$ (FAN is around $70 \text{ g NH}_3\text{-N}/\text{m}^3$), $K_{I,\text{NH}_3,\text{ac}}$ has to be decreased to $50 \text{ g NH}_3\text{-N}/\text{m}^3$, otherwise the measurement data can never be matched by simulation. It is assumed that there is a threshold of ammonia inhibition, which could be around $50 \text{ g NH}_3\text{-N}/\text{m}^3$. When FAN is lower than the threshold, $K_{I,\text{NH}_3,\text{ac}}$ has to be set up higher enough in order to eliminate the ammonia inhibition from the model. Furthermore, the recommended $K_{I,\text{NH}_3,\text{ac}}$ value from ADM1 is $25.2 \text{ g NH}_3\text{-N}/\text{m}^3$, which seems a bit too small. With this value, the *methanogenesis* will be 70% inhibited when TAN is of $1,000\sim 1,200 \text{ g NH}_4^+-\text{N}/\text{m}^3$ (FAN is around $45 \text{ g NH}_3\text{-N}/\text{m}^3$), which does not reflect the reality.

pH inhibition

In ADM1, two empirical equations are introduced for pH inhibition. One deliberates both upper and lower pH inhibition (Angelidaki *et al.* 1993), and the other considers only lower pH inhibition (Ramsay 1997). ADM1 suggests that the second equation (with only lower pH inhibition) should be used when the ammonia inhibition is included. It is probably because that at high pH level the higher concentration of ammonia will be formed, so the inhibition will be presented by the ammonia inhibition term. This also could be the reason that $K_{I,\text{NH}_3,\text{ac}}$ from ADM1 is relative small. For our simulation since $K_{I,\text{NH}_3,\text{ac}}$ was modified, the first equation with both upper and lower pH inhibition was used and the reasonable simulation results were gained.

Physicochemical processes

Comparison of equilibrium and dynamic processes

Acid-base processes can be implemented as either equilibrium or dynamic processes. For checking their reliabilities, $\text{NH}_4^+/\text{NH}_3$ was implemented by these two methods in two independent models. In order to make the results comparable, other acid-base processes were stuck to one method ($\text{CO}_2/\text{HCO}_3^-$ and $\text{HCO}_3^-/\text{CO}_3^{2-}$ as dynamic processes, and organic acids as equilibrium processes). Results are shown in Figure 4.

The same NH_3 concentration in the reactor was obtained by both methods. pH is nearly the same in two methods, and only after each input there is an almost invisible difference (Figure 4). The differences of other parameters between two methods are so small that they can be ignored. Meanwhile, the simulating speeds of two methods are similar on normal PC. The same tested were achieved for $\text{CO}_2/\text{HCO}_3^-$ and $\text{HCO}_3^-/\text{CO}_3^{2-}$, which resulted in the same conclusion, as well. Thus, two methods can be arbitrarily chosen for implementing acid-base processes.

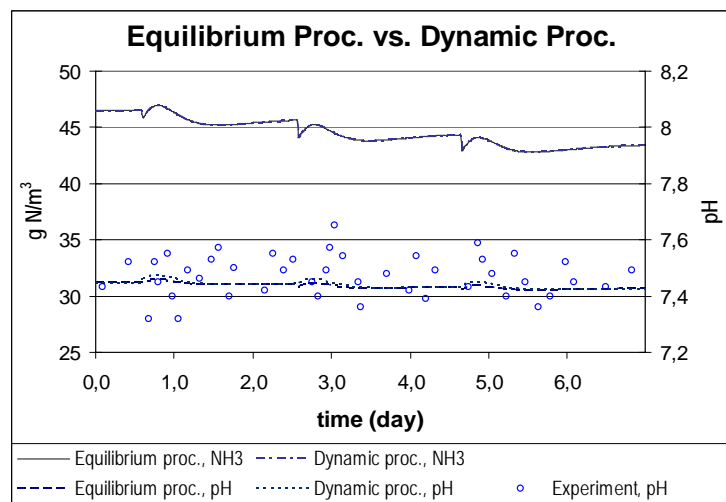


Figure 4: Comparison of the different implementation methods for acid-base processes

K_{La} and k_p

K_{La} describes the transfer rates of gases between liquid phase and gas phase. It is affected by many boundary conditions, such as temperature, gas pressure, liquid quality, reactor type and stirring methods, and so on. Pauss *et al.* (1990) investigated k_{La} of CH_4 and H_2 with the different types of reactors, and reported k_{La} of H_2 and CH_4 as 3.84 ± 0.48 and $2.16 \pm 0.24 \text{ d}^{-1}$ for anaerobic processes in

CSTR, respectively. Siegrist *et al.* (2002) found the k_{L,a,CO_2} was above 100 d^{-1} in their lab. In ADM1 $k_{L,a}$ is not sensitive anyhow. The values of $k_{L,a}$ from 1.0 to 1000 d^{-1} result in the same BPR that all can fit in with the measurements. Only when it is smaller than 1.0 d^{-1} , BPR starts to be impaired. Therefore, $k_{L,a}$ can be easily set up. As also suggested by ADM1, $k_{L,a}$ for all three kinds of gases can have the same value in the normal case. In our model, $k_{L,a}$ of H_2 , CH_4 and CO_2 is 20 d^{-1} .

k_p is the pipe resistance coefficient for calculating the gas flow, when the pressure of headspace is variable (Batstone *et al.* 2002). It is not sensitive in the mathematical model, too. Only when k_p is smaller than 0.5 , the biogas flowrate is diminished. In our reactors, the pipe resistance is quite small, so it can be set up optionally as well. In our model, k_p is $100\text{ m}^3/(\text{d}\cdot\text{bar})$.

Cations and anions

Cations (S_{Cat^+}) and anions (S_{An^-}) represent ions of strong base and acid salts in liquid phase. Though they do not contribute any H^+ or OH^- , they still influence on pH strongly due to the charge balance. However, The determination of S_{Cat^+} and S_{An^-} is difficult and sensitive.

CONCLUSION

The mathematical model is an effective, efficient and economic method to design and control systems. ADM1 was successfully implemented and applied to the mesophilic BWAD plant. The model is able to provide valuable solutions and suggestions for operation and control of BWAD plant by simulating the virtual scenarios. It also allows to implement supplementary substrates like KR as additional organic loading. The calculation time of the model is in a tolerable range (using AquaSim 2.1d on normal PC)

Based on our studies, it is found that the distribution ratio among carbohydrates, proteins and lipids is not sensitive, whereas the percentage of SCFA in the input is more important instead. Fortunately, SCFA are much easier to be characterised than the composition of composite particulate material. Meanwhile, it is found that in mesophilic digestion of BW, the disintegration and hydrolysis are not the rate-limiting step (at least not the sole rate-limiting step), the disintegration rate of BW is ten times higher than that of KR. For BWAD the C_4 metabolism can be integrated in the uptake of LCFA. Moreover, the uptake delay occurred and it can not be simulated by ADM1, but it is tolerable.

A notable inhibitory effect of ammonia is observed and appropriately simulated by ADM1. But no unique half inhibitory coefficient ($K_{I,NH_3,ac}$) is found out for all investigated ammonia concentration ranges, where with higher level of FAN the smaller inhibition coefficient has to be used. pH inhibition can partly be explained by using HAc and HPr as substrate. The empirical approach for the pH-inhibition can be changed to an enzymatic approach.

As to physical-chemical processes, it is verified that equilibrium process and dynamic processes result in the same simulation, so they can be arbitrarily chosen. The mass transfer coefficient $k_{L,a}$ and the pipe resistance coefficient k_p proved not sensitive to the mathematical model. Cations and anions can influence on pH value significantly, but they are difficult and sensitive to determine in BW.

In addition, because each cycle of the batch experiment (or discontinuous feeding operation) goes through nearly all biological status (e.g. high food to biomass ratio (F/M), low F/M and starving phase, etc.), it is stricter with mathematical model. Meanwhile, if large amount of acetate exists in input, it also requires more functional and precise model. Therefore, these two kinds of circumstance can be the very good benchmarks or the higher criteria for examining mathematical models.

ACKNOWLEDGEMENTS

The first author acknowledges Mr. Damien John Batstone for providing him invaluable information and help even only contacted by email.

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