Parameter analysis of the IWA Anaerobic Digestion Model No. 1 for the anaerobic digestion of blackwater with 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 cases of only blackwater (BW) feeding and of BW plus kitchen refuse (KR) feeding. In this paper, the simulation results of BW + KR anaerobic digestion are presented and discussed, followed 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 severely impact the performance of the model. The model proved that the disintegration/hydrolysis rate of BW is around 4.5 d⁻¹, which is about ten times higher than that of KR (Kdis,KR = 0.5 d⁻¹). ADM1 is not sensitive to the 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 cannot be simulated by ADM1, but it is tolerable. No unique Kᵢ,NH₃,ac is found out for all investigated ammonia concentration ranges. Meanwhile, ADM1 is not sensitive to Kᵢₘ and Kᵢₜ, so they can easily be set up.

Keywords ADM1; blackwater; blackwater anaerobic digestion; disintegration; hydrolysis; inhibition; kitchen refuse; Kᵢₘ and Kᵢₜ, 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 and 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 the European community and U.S. consider the anaerobic treatment as the most promising approach for the 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 three 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 toilets can be treated in biogas plant so that the energy is recovered as biogas and a 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 control options and process variations, a lab-scale mesophilic blackwater anaerobic digestion (BWAD) plant was built at 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: (1) reference conditions, (2) different feeding frequencies, and (3) with

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Materials and methods

All experimental data were generated by three parallel lab-scale BWAD reactors, which were built as continual stirred tank reactors (CSTR). Each reactor has 10.01 volume. 8.01 BW and sludge were held in each reactor, where 2.01 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 three times per week. The hydraulic retention time (HRT) and the sludge retention time (SRT) were the same 20 days. BW from vacuum toilets has relatively high COD, which is normally in the range 4,500–13,000 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. (2006). 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 ground KR was firstly mixed with BW, and then the mixture was fed into the reactors. The feeding frequency was also three times per week, and HRT were kept the same as before, i.e. 20 days. The organic loading of KR was in the range 7,000–13,5000 g COD/m³. 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).

Anaerobic digestion of BW + KR

The model has been calibrated based on the reference conditions scenario (see Feng et al., 2006). KR is added into the model considered as independent organic loading. The stoichiometric coefficients of KR (f_{product,KR}) and the disintegration rates of KR (K_{dis,KR}) were set up, respectively. In order to get better simulation results, the different K_{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_{dis,KR}. In the figure the Y-axis is the specific BPR which is the absolute BPR divided by the reactor volume under the standard conditions.

Due to unknown reasons, the experimental data of day five and day seven were unstable. With that exception, the model is able to properly simulate AD of BW + KR in a general manner. It also shows that when K_{dis,KR} is set up as 0.5 d^{-1}, the simulation curves fit the experiment data better. It also coped well 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 m³ norm/(m³ reactor volume d) (see Figure 2). Therefore, BW + KR has around 4 times higher BPR than...
BW, which implies that AD of BW + KR is a very promising method for waste and wastewater treatment. Other parameters which were also appropriately simulated 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 BW
As discussed in ADM1, the biodegradability of raw BW is one of the key issues. The analytical methods 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

Figure 1 Biogas production rate (BPR) of BW + KR, with different Kdis,KR

Figure 2 Comparison of ADM1 with different sorts of degraders
testing results by ADM1, the inert part of BW is around 20–30%. In our studies, 25.5% of total input COD was treated as the inert part which resulted in 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 the 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.

**Disintegration and hydrolysis**

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

The disintegration rates (k_{dis}) suggested by AMD1 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 may also be the reason that BW contains such a high amount of SCFA.

Normally, carbohydrates, proteins and lipids have different hydrolysis rates and fall into the range 0.01–1.0 d^{-1}. But their recommended values from ADM1 for mesophilic and thermophilic solids AD are set at the same value of 10 d^{-1}. It is presumed that under certain situations the hydrolysis rates of the 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 the hydrolysis step in the model. This also makes the model

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<th>Table 1 Characterization of the raw blackwater</th>
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<td><strong>Biodegradable</strong></td>
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<td>Biodegradable ch + pr + li (47.5%)</td>
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easier to manipulate. When three components have the same hydrolysis rates, it further causes the model to be less sensitive to the aforementioned distribution ratio. In our case, the hydrolysis rates of the three components are set up as $10 \text{d}^{-1}$ 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 the 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., 2006). The parameter estimation tool offered by AQUASIM 2.1 d 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 found to be as $18, 14, 13 \text{d}^{-1}$, and the corresponding $K_S$ are $110, 120, 160 \text{g COD/m}^3$.

**Modification of the model.** As the intermediates with a relative low concentration, valerate and butyrate can be omitted in our case. Two more simulations were performed in order to check the influence from valerate and butyrate on BWAD, i.e. case one: omit only valerate from the model, and case two: omit 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 omitted. In the real situation, valerate concentration in the reactors remains at a low level, which is around 20–40 g COD/m$^3$ in BW, and in the reactors it is no longer detectable 3 hours 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.

On the basis of 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 omitted depending on their essentiality in the specific cases.

**Delay phenomenon.** When the organisms enter the new environment, they need certain time to adapt to 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 cannot be represented by Monod-type kinetics. Batstone et al. (2003) observed the similar uptake delay of valerate, and tried compensating it by increasing the decay rate and increasing $k_m$. The conjectured reasons for the delay are also given by Batstone et al. (2003). In our case, the uptake delay cannot be totally overcome by adjusting $k_m$, $K_S$ or the decay rates.
Inhibition

Inhibition is one of the most important aspects of the 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 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 cannot be simulated by ADM1.

Returning to our simulation, normally TAN in BW is around 1,000–1,200 NH₃⁺–N/m³ due to the existence of urine. In order to understand the impacts of ammonia on BWAD, step by step TAN was artificially increased from 1,000–1,200 to 2,000–2,200 g NH₃⁺–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 K₁,NH₃,ac is employed. When TAN is 1,000–1,200 g NH₃⁺–N/m³ (FAN is around 45 g NH₃-N/m³), K₁,NH₃,ac has to be set around 250 g NH₃-N/m³; however, when TAN is 2,000–2,200 NH₃⁺–N/m³ (FAN is around 70 g NH₃-N/m³), K₁,NH₃,ac has to be decreased to 50 g NH₃-N/m³, 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 g NH₃-N/m³. When FAN is lower than the threshold, K₁,NH₃,ac has to be set high enough in order to eliminate the ammonia inhibition from the model. Furthermore, the recommended K₁,NH₃,ac value from ADM1 is 25.2 g NH₃-N/m³, which seems a bit too small. With this value, the methanogenesis will be 70% inhibited when TAN is 1,000–1,200 g NH₃⁺–N/m³ (FAN is around 45 g NH₃-N/m³), which does not reflect the reality.

![Figure 3](https://iwaponline.com/wst/article-pdf/54/4/139/431808/139.pdf)

Figure 3 Comparison of biogas production rate
In ADM1, two empirical equations are introduced for pH inhibition. One considers 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 at high pH level the higher concentration of ammonia will be formed, so the inhibition will be presented by the ammonia inhibition term. This could also be the reason that $K_{I,NH_3,ac}$ from ADM1 is relatively small. For our simulation since $K_{I,NH_3,ac}$ was modified, the first equation with both upper and lower pH inhibition was used and 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, $NH_4^+/NH_3$ was implemented by these two methods in two independent models. In order to make the results comparable, other acid-base processes were kept to one method ($CO_2/HCO_3^-$ and $HCO_3^--CO_2$ 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 is there an almost invisible difference (Figure 4). The differences of other parameters between the two methods are so small that they can be ignored. Meanwhile, the simulating speeds of the two methods are similar on a normal PC. The same test results were achieved for $CO_2/HCO_3^-$ and $HCO_3^-/CO_2$, which resulted in the same conclusion, as well. Thus, two methods can be arbitrarily chosen for implementing 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 $k_{l,a}$ of CH$_4$ and H$_2$ with the different types of reactors, and reported $k_{l,a}$ of H$_2$ and CH$_4$ as 3.84 ± 0.48 and 2.16 ± 0.24 d$^{-1}$ for anaerobic processes in CSTR, respectively. Siegrist et al. (2002) found that $k_{l,a,CO_2}$ was above 100 d$^{-1}$ in their lab.
In ADM1 $k_{La}$ is not sensitive anyhow. The values of $k_{La}$ from 1.0 to 1,000 d$^{-1}$ result in the same BPR that all can fit with the measurements. Only when it is smaller than 1.0 d$^{-1}$, does BPR start to be impaired. Therefore, $k_{La}$ can easily be set up. As also suggested by ADM1, $k_{La}$ for all three kinds of gases can have the same value in the normal case. In our model, $k_{La}$ 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. Only when $k_p$ is smaller than 0.5 is the biogas flowrate 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 m$^3/(d\cdot bar)$.

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 strongly influence pH due to the charge balance. However, the determination of $S_{Cat^+}$ and $S_{An^-}$ is difficult and sensitive.

Conclusions

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 us to implement supplementary substrates like KR as additional organic loading. The calculation time of the model is in a tolerable range (using AquaSim 2.1 d on a 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 cannot 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 ($K_{I,NH3,ac}$) 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 be partly 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 $k_{La}$ and the pipe resistance coefficient $k_p$ proved not sensitive to the mathematical model. Cations and anions can influence the 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 though nearly all biological status (e.g. high food to biomass ratio (F/M), low F/M and starving phase, etc.), it is stricter with the mathematical model. Meanwhile, if a large amount of acetate exists in the input, it also requires a 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.
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