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Population dynamics at digester overload conditions

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ABSTRACT

Two different case studies concerning potential overload situations of anaerobic digesters were investigated and mathematically modelled by means of the Anaerobic Digestion Model No. 1 (ADM1). The first scenario included a digester failure at a municipal WWTP which occurred during revision works of the upstream digester within a two-step digestion system when the sludge was directly by-passed to the 2nd-step reactor. Secondly, the non-occurrence of a highly expected upset situation in a lab-scale digester fed with cattle manure was investigated. ADM1 was utilized to derive indicators which were used to investigate the relationship between digester stability and biomass population dynamics. Conventional design parameters such as the organic loading rate appeared unsuitable for process description under dynamic conditions. Indicators reflecting the biokinetic state (e.g. F_{net}/M_{net} or the VFA/alkalinity ratio) are more adequate for the assessment of the stability of reactors in transient situations.

1. Introduction

The degradation of organic matter in anaerobic digesters occurs through four basic phases, termed hydrolysis, acidogenesis, acetogenesis and methanogenesis. These phases are a series of interlinked reactions proceeding spatially as well as temporally in consecutive and parallel steps and hence, influence one another (Schink, 1997). Due to the highly sensitive interdependence of the different microbial groups involved, there is always a potential risk of process instability.

Previous research has found that around 70% of the methane produced in the digestion process comes from the transformation of acetate to methane (methanogenesis), usually by the aceticlastic methanogens (e.g. Tchobanoglous et al., 2003). When methanogenesis is not rapid enough due to some upset, volatile fatty acids (VFAs) accumulate, which may lead to a decrease in the pH and a cessation of the methane production. Returning to normal operating conditions can be costly and time-consuming. Remedy actions can include reducing the organic loading rate (OLR) to the point where the VFA production rate is less than their maximum consumption rate. This will allow for the consumption of the excess VFA and a return of neutral pH until stable conditions occur again. If this measure is not sufficient, decrease in loading must be coupled with the addition of appropriate chemicals for pH correction (Grady et al., 1999). In the worst case, it could be necessary to empty the complete reactor and start again, including a period with reduced gas production, and thus an associated loss of income.

In this paper, two different case studies concerning overload situations of anaerobic digesters were investigated and mathematically modelled by means of IWA's Anaerobic Digestion Model No. 1 (ADM1; Batstone et al., 2002). The first scenario included a digester failure at WWTP Salzburg (Austria) which occurred during revision works of the upstream digester within a two-step digestion system when the sludge was directly by-passed to the 2nd-step reactor. In the second scenario, the non-occurrence of an expected upset situation in a lab-scale digester fed with cattle manure was investigated. This experiment was part of a project dealing with different start-up options for agricultural biogas plants and is described in Schoen et al. (2008). Although a washout of methanogens was expected due to deliberately high feeding rates and a hydraulic retention time of only 3 days, a reactor breakdown failed to appear. This was attributed to a continuous re-seeding with methanogenic biomass stemming from the alimentary system of the livestock.

For deeper examination, mathematical modelling by application of ADM1 for both cases was utilized to derive indicators which were used to investigate the relationship between digester stability and biomass population dynamics.

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2. Methods

2.1. Case study 1: digester upset at WWTP Salzburg

The municipal WWTP Salzburg (Austria) is operated as a 2-stage system (high-rate/low-rate) for a design-load of 680,000 PE. Excess sludge from both stages is mixed together in one pipe and passes a pre-thickening unit before it is fed into two digesters connected in series. Both reactors have an operating volume of 8160 m^3 (effectively only 6860 m^3 due to sand deposits detected during revision) and a gas space of 920 m^3.

In the course of revision works, the upstream digester (FT1) was shut-down and the sludge was directly by-passed to the 2nd-step reactor (FT2) (day 34 in Fig. 1). After that there was remarkable breakdown of pH, gas production, and methane content in FT2. This was attributed to (i) a poor adaptation of FT2 to direct feeding from the pre-thickener, (ii) an average HRT of only 14 days and (iii) a yet unexplained slight pH decrease in the feeding sludge from the pre-thickener beginning about 10 days before. On day 40 it was decided to recover FT2 by inoculating the feed with sludge from FT1 that was withdrawn from there to a storage tank after the shut-down of FT1. However, the recovery was not the subject–matter of the present investigation.

2.2. Case study 2: non-occurrence of expected reactor failure during start-up experiment

In the context of a research project dealing with the development of novel concepts for agricultural biogas plants, a pilot-plant was constructed and commissioned at a cattle farm (Wett et al., 2006a,b). In order to investigate a proper start-up strategy for the plant, two different start-up approaches were investigated at a lab-scale for their adequacy to be applied at the pilot full-scale plant. This included the use of seed material from a biogas plant treating similar substrate as well as process acclimatization by gradual temperature and load increase, respectively. As reported in Schoen et al. (2008), these results determined the selection of the optimum start-up strategy for the pilot-plant with modifications of its control system in order to provide the best operation conditions. Furthermore, the data gained from the lab analyses served as a basis for the calibration of a numerical kinetic model (applying ADM1) which was setup in order to mathematically simulate the anaerobic processes during the start-up.

In these experiments, four continuous stirred tank reactors (CSTRs) referred to as A1, A2, B1 and B2 were used. The 100 L (75 L operating volume + 25 L gas space) digesters feature mechanical mixers, insulation, heating jackets as well as analysis and measurement equipment. The focus in this paper is placed on "B1" which was inoculated with 15 L seeding sludge from an operating biogas reactor treating similar substrate as the pilot-plant (i.e. mainly cattle manure) plus 60 L of tap water prior to substrate addition. The reactor was operated at a constant temperature of 37 °C and fed once a day with cattle manure originating from the location of the pilot-plant with increasing feeding rates from 0.75 up to 24 L d^{-1} (Fig. 2).

The experiment was run for 42 days and the progression of important parameters (including gas production rate, gas quality, pH, COD, NH_4–N, organic acid content) was monitored and analyzed. The characteristics of the inoculum and the cattle manure used in B1 are presented in Table 1. The manure feeding rates of B1 can be expressed as an average organic loading rate (OLR) of 0.3 up to 9.1 kg VS m^{-3} d^{-1}, resulting in a hydraulic retention time (HRT) of 100 days down to 3 days.

Besides finding a proper start-up strategy, the purpose of steadily increasing the load was to investigate the lowest possible limit of HRT in order to avoid a reactor failure due to the washout of methanogens. However, despite a minimum HRT of 3 days, the expected failure did not occur (Fig. 4a) due to reasons discussed below.

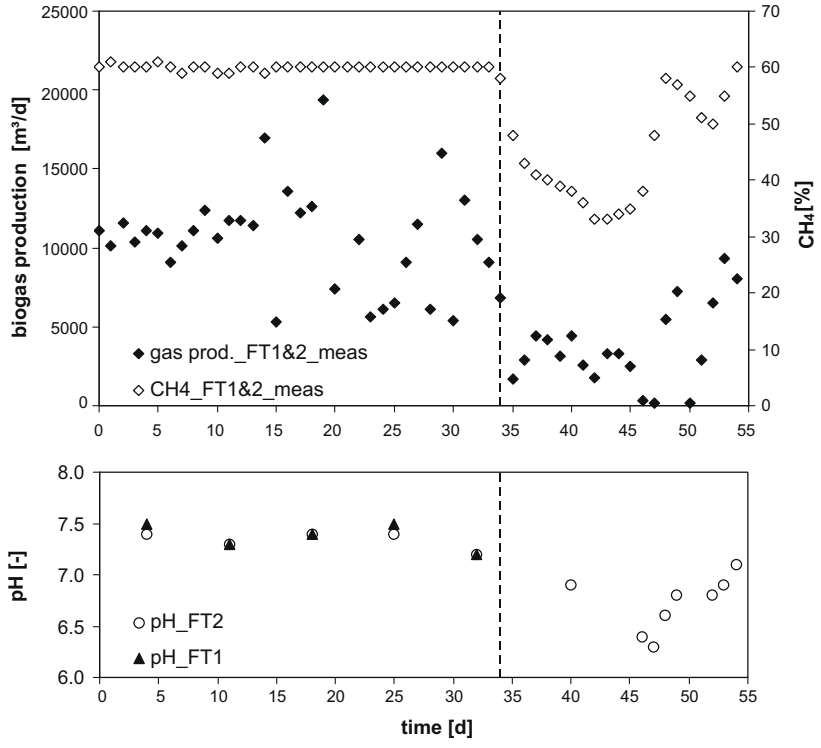

Fig. 1. Gas production rate, methane content and pH for both digesters (FT1 and FT2). Note that until day 34 (sludge by-pass to FT2; dotted line) gas production and CH_4 refer to an average value for FT1 and FT2; after day 34 it refers to FT2.

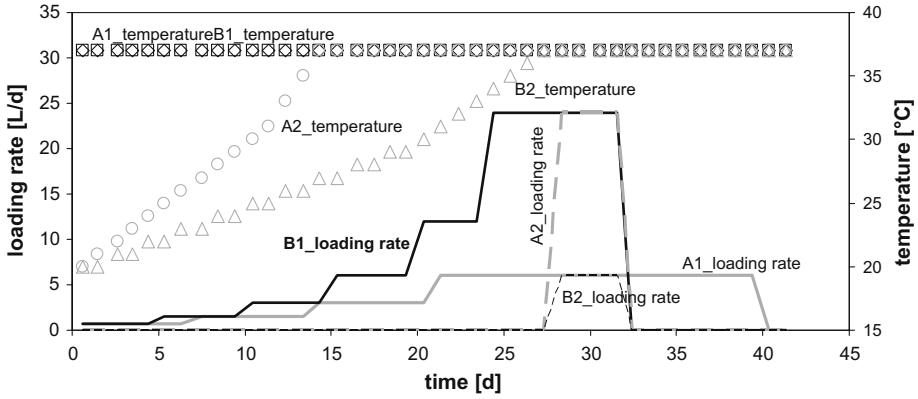

Fig. 2. Feeding rates and temperature progression in the lab-scale reactors.

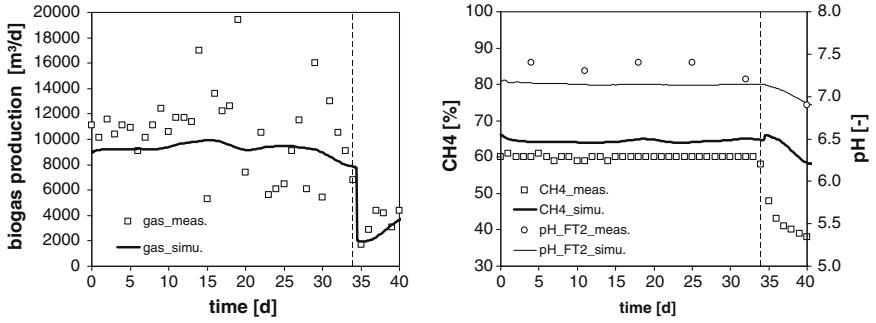

Fig. 3. WWTP Salzburg simulation results and measured values for gas production, pH and methane content. Note that on day 34 digester FT1 was shut-down and sludge was by-passed to FT2.

Table 1
Characteristics of the feeding substrates.

	TS [%]	VS [% TS]	pH [−]	COD_{tot} [mg L^{-1}]	COD_{sol} [mg L^{-1}]	NH_4–N [mg L^{-1}]	Organic acids [mg L^{-1}]
Inoculum[a]	4.9	66.9	8.7	49589	11789	2232	1702
Manure[b]	4.1	68.6	8.4	36672	12403	1035	3312

[a] Before dilution with tap water.
[b] Average values of four batches.

2.3. Methanogenic population

In order to quantify the methanogenic community composition in reactor B1, the ANAEROBECHIP microarray (Goberna et al., 2009) was hybridised with sludge DNA from B1 which was extracted using the PowerSoil™ DNA isolation kit (MO BIO Laboratories Inc., California). Six genera of methanogens were detected, which were then targeted using real time quantitative PCR as described by Franke-Whittle et al. (2009). After quantification of the number of 16S rRNA gene copies per μL^{-1} DNA in the samples, the results were converted to grams of methanogenic cells per gram sludge. These calculations were based on several broad assumptions: (1) DNA extraction efficiency is equivalent among samples, (2) methanogens have an average of 2.5 copies of the 16S rRNA gene per cell (Klappenbach et al., 2001) and (3) most methanogens in the reactor (mesophilic *Methanosarcina* sp.) have an average 1.9 μm diameter (Kendall and Boone, 2006) a spherical shape and a cytosolic density of 1 g cm^{-3}.

2.4. Biokinetic modelling tools

By means of the Matlab/Simulink based simulator SIMBA, numerical models of both case studies were set up and data sets from the lab-scale experiments and from the WWTP were used for model calibration. SIMBA applies IWA's Anaerobic Digestion Model No. 1 (ADM1; Batstone et al., 2002) for its calculations of the biokinetic processes involved in anaerobic digestion. ADM1 is a universally applicable biokinetic model which allows for the mathematical description of the anaerobic digestion of different types of organic substrates. ADM1 describes digestion of particulate composites as a 5-stage process involving disintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis. In the disintegration step, composite solids (Xc) and cells of microorganisms are degraded to their principal constituents including carbohydrates, proteins and fats. Additionally, inert particulate and soluble matter emerge which are not affected by the subsequent reactions. Thereafter, the macromolecular products are subject to enzymatic decomposition and transformed to monosaccharides, amino acids and long chain fatty acids. Further anaerobic digestion finally leads to biogas production via acetogenesis and methanogenesis.

Model calibration was accomplished mainly by manually fitting the simulated values to the measurement data (gas production, pH and COD) to an acceptable match by an appropriate choice of the model parameters and coefficients. For both investigated cases, an almost uniform parameter set regarding kinetic and stoichiometric

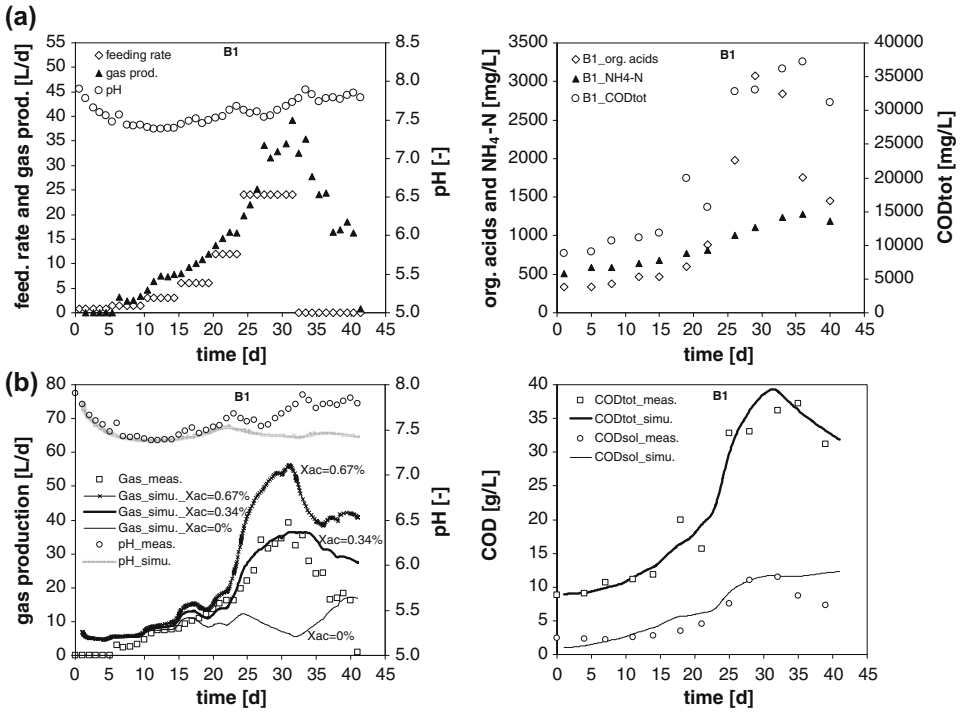

Fig. 4. (a) Feeding and gas production rates, pH, organic acids, NH_4–N and total COD progression in lab-scale reactor B1; (b) simulation results and measured values for gas production, pH, total and soluble COD in the start-up experiment. Simulated gas production curves include different ratios of additional biomass (XB).

coefficients could be determined and applied. For both models an appropriate, reasonable and detailed inflow characterisation had to be found especially when ADM1 is used for heterogenous substrates like liquid manure. This was done by determination of the proportional distribution of carbohydrates, lipids, proteins and inert constituents within the substrate. In a first step, values from the literature reviewed served as a starting basis followed by a detailed calibration protocol based on COD-, carbon- and nitrogen-mass balances.

In case study 1, average concentration values as given in Table 2 were extracted from routine WWTP operating data for the use with ADM1 simulations. Based on the relative sludge contributions from the high-rate and the low-rate stage, influent COD was estimated by a typical relationship between total solids content and COD of 1.2 and 1.0 kg COD kg TS^{-1} for the high-rate and the low-rate stage, respectively (Wett, 2004).

2.5. Determination of key indicators for digester stability

The stability and efficiency of the overall digestion process depends on the stability of the individual biochemical processes involved. Process upsets can result from temporarily high loadings, deviations in the environment provided, or the presence of toxic or inhibitory materials in the bioreactor influent (Grady et al., 1999). Also, any significant increase in the concentration of intermediate substrates (e.g. VFAs) may inhibit directly, through toxicity and energetics, the kinetics of other biochemical processes and lead to digester instability (Batstone et al., 2002). Since the ADM1 provides a particularly suitable generic model structure and is sufficiently complex to characterise digester dynamics under various reactor configurations and feeding protocols (Batstone et al., 2006; Straub et al., 2006), it was utilized to investigate the relationship between digester stability and biomass population dynamics. For this purpose, the calculation of different key indices for digester stability were implemented into the models in order to gain a comparable basis for both cases.

According to Switzenbaum et al. (1990), an ideal indicator would have intrinsic meaning as it must reflect the current metabolic status of the system. However, this indicator is difficult to obtain due to the fact that microbial ecosystems developed in a particular anaerobic reactor are unique to that particular system (reactor hydraulics, feeding pattern, composition, etc.). There is considerable debate in the literature on finding the best way to monitor digester stability and includes the following widely recognised parameters: (1) pH, (2) gas production rates and gas composition (methane and carbon dioxide), (3) gas phase hydrogen concentration, (4) volatile acids to alkalinity ratio, and (5) the acetate capacity number (ACN). In general, the first three mentioned indicators together with individual measurements of VFAs and alkalinity are good for detecting gradual changes but, however, none of them can determine how close a digester is to failure (Conklin et al., 2008; Switzenbaum et al., 1990). Both experience and theoretical analysis indicate that pH is not a good indicator of process upsets. Because of the buffering capacity inherent in the system, the pH changes very slowly and by the time noticeable decline in pH occurs, the upset may be well under way (Grady et al., 1999; Zickefoose and Hayes, 1976). The gas production rate, and more specifically the methane yield, can potentially be a good

Table 2
Average values for sludge fed from the pre-thickener to the digesters at WWTP Salzburg as used for ADM1 simulations. Note that only direct feeds from the pre-thickener to the digesters were used (not taking into account feeds of FT1 to FT2 on day 0–34 and 40–54).

Day	TS [g L^{-1}]	COD [mg L^{-1}]	NH_4–N [mg L^{-1}]	Q [m^3 d^{-1}]
0–9	43.9	52315	1949	606
10–19	42.3	55044	2043	567
20–29	44.7	54034	2008	562
30–34	41.0	40709	1548	591
35–39	45.4	44577	1681	472
40–49	41.3	44914	1693	567
50–54	48.8	53769	1999	374

indicator of the metabolic status of the digester. Lowering of methane yield, when compared to the influent organic loading rate, can be a warning sign for the accumulation of soluble acid products in the liquid phase. Unfortunately, this is again the result of an imbalance rather than a warning of it. Regarding the applicability of hydrogen concentrations as reactor stability indicators, ambivalent results can be found in literature. In a review, Switzenbaum et al. (1990) state that although a change in hydrogen concentration may be rapid for an upset situation, it is not always apparent why this change has occurred and thus limits the application of hydrogen as a stand-alone indicator.

For the early detection of upcoming process deterioration and reactor failure due to organic or hydraulic overloads as well as toxic events, more sensitive indicators are required. In this study, the VFA/alkalinity ratio and the acetate capacity number (ACN) were utilized for this purpose and implemented into the simulation models. The ratio of volatile fatty acids to alkalinity indicates the relative proportion of compounds acting to lower the pH and of buffering capacity to maintain it. The alkalinity represents the ability of a digester to neutralize the acids formed during digestion or present in the influent material. The accumulation of VFAs reflects a kinetic uncoupling between acid producers and consumers and is typical of stress situations. Accumulation of VFA can also be a cause of subsequent problems if the system lacks enough buffering capacity to avoid a drop in the pH (Grady et al., 1999; Switzenbaum et al., 1990). The VFA/alkalinity ratio is expressed in equivalents of acetic acid/equivalents of calcium carbonate and generally, values between 0.1 and 0.4 are considered to indicate favourably operating conditions without the risk of acidification (de Haas and Adam, 1995; Sánchez et al., 2005; Switzenbaum et al., 1990; Zickefoose and Hayes, 1976). Increases above 0.4 indicate upset and the need for corrective action. If the ratio exceeds 0.8, pH depression as well as inhibition of methane production can occur and the process can fail (Zhao and Viraraghavan, 2004). However, each plant has its own characteristic ratio for efficient digestion.

For the implementation into ADM1, VFAs were calculated as the sum of total valerate, butyrate, propionate and acetate including both the dissociated (HVa^-, HBu^-, $HPro^-$ and HAc^-) and non-ionised forms (valeric, butyric, propionic and acetic acid). The numbers were converted to mol L^{-1} and multiplied by 60 to gain g HAc-equivalents L^{-1} (Eq. (1)).

$$\mathrm{VFA} = \left[\frac{S_{\mathrm{Ac}}}{64} + \frac{S_{\mathrm{Pro}}}{112} + \frac{S_{\mathrm{Bu}}}{160} + \frac{S_{\mathrm{Va}}}{208}\right] \cdot 60 \quad [\text{g HAc-equivalents } \mathrm{L}^{-1}] \tag{1}$$

Alkalinity was assumed to be mainly due to bicarbonate and VFA. The alkalinity simulation results were calculated by a charge balance summing the bicarbonate, all ionised forms of VFA as well as ions from the influent (Scat and San) scaled to equivalents L^{-1}. Finally it was multiplied by 50 which equals the equivalent weight of calcium carbonate in order to gain g $CaCO_3$-equivalents L^{-1} of alkalinity (Eq. (2)).

$$\mathrm{Alk} = \left[\begin{array}{c} S_{\mathrm{An}}^- + S_{\mathrm{HCO_3}}^- + \frac{S_{\mathrm{Ac}}^-}{64} + \\ + \frac{S_{\mathrm{Pro}}^-}{112} + \frac{S_{\mathrm{Bu}}^-}{160} + \frac{S_{\mathrm{Va}}^-}{208} - S_{\mathrm{Cat}}^+ \end{array}\right] \cdot 50 \quad [\text{g } \mathrm{CaCO_3}\text{-equivalents } \mathrm{L}^{-1}] \tag{2}$$

However, under certain circumstances these numbers may need further conversion to represent total VFAs and total alkalinity taking into account that other influences may contribute to alkalinity and total organic acids. Koch et al. (2009) conducted digestion experiments with pure maize silage and found corresponding correction factors for maize digestion through statistical evaluation of gas chromatography and titration measurement data. For the purposes of this paper, however, corrections not applied.

As mentioned above, the acetate capacity number (ACN), defined as:

$$\mathrm{ACN} = \frac{\text{maximum acetate utilization rate}}{\text{acetate production rate}} \quad [-] \tag{3}$$

was used to index digester instability. Critical to stability under varying loading and environmental conditions, however, is not the acetate concentration but rather the acetate utilization capacity of the acetoclastic community beyond the steady-state production rate. The ACN is a measure for this excess acetate capacity and the lower the number, the less excess substrate utilization capacity exists in the digester and thus the greater the instability. Values of less than 1.0 under steady-state conditions indicate impending digester failure (Conklin et al., 2008; Straub et al., 2006).

In the simulation models, the maximum acetate utilization rate of the microbial community was calculated as.

$$\rho_{11,\max} = \mathrm{km\_ac} \cdot \mathrm{Xac} \cdot I_{\mathrm{pH\_ac}} \cdot I_{\mathrm{NH_3,Xac}} \cdot I_{\mathrm{IN}} \quad [\text{kg COD m}^{-3}\text{ d}^{-1}] \tag{4}$$

where km_ac is the maximum specific substrate utilization constant [kg COD_S kg COD_X^{-1} d^{-1}], Xac the biomass concentration of acetate degraders [kg COD m^{-3}], $I_{\mathrm{pH\_ac}}$ and $I_{\mathrm{NH3,Xac}}$ [−] are inhibition terms accounting for pH and free ammonia inhibition and I_{IN} [−] is an uptake-regulating function to prevent growth when inorganic nitrogen (ammonium and ammonia) is limited. For the Monod term, it was assumed that Sac/(KS_ac + Sac) = 1 when the rate is at maximum. The acetate production rate was determined from the sum of biochemical processes producing acetate:

$$\begin{aligned} &\sum_{j=5}^{10} \rho_{j=5-10} \cdot v_{i=7,j=5-10} = \rho_5 \cdot (1 - Y_{\mathrm{su}}) \cdot f_{\mathrm{AC\_SU}} + \rho_6 \cdot (1 - Y_{\mathrm{aa}}) \cdot f_{\mathrm{AC\_AA}} \\ &+ \rho_7 \cdot (1 - Y_{\mathrm{fa}}) \cdot f_{\mathrm{AC\_FA}} + \rho_8 \cdot (1 - Y_{\mathrm{c4}}) \cdot f_{\mathrm{AC\_VA}} \\ &+ \rho_9 \cdot (1 - Y_{\mathrm{c4}}) \cdot f_{\mathrm{AC\_BU}} + \rho_{10} \cdot (1 - Y_{\mathrm{pro}}) \cdot f_{\mathrm{AC\_PRO}} \end{aligned} \quad [\text{kg COD m}^{-3}\text{ d}^{-1}] \tag{5}$$

with denotations according to ADM1 terms given in (Batstone et al., 2002): ρ_j are the kinetic process rates [kg COD m^{-3} d^{-1}], Y_i the biomass yields [kg COD_X kg COD_S^{-1}] and $f_{\mathrm{AC\_S}}$ the fractions of acetate yield from substrate S [kg COD kg COD^{-1}].

3. Results and discussion

3.1. Case study 1

Fig. 3 shows measured values and simulation results of the numerical model for gas production, pH and methane content for WWTP Salzburg. The model outputs for gas production and analytical data corresponded well. However, there were deviations for pH and methane content due to unknown reasons.

3.2. Case study 2

In the lab-scale start-up experiments, biogas production increased up to a peak value after an initial lag phase, and then sharply decreased after the feeding was stopped (Fig. 4a). As mentioned previously, there was no pH drop or other reactor failure in digester B1 although a washout of methanogens was expected due to a HRT of only 3 days at maximum feeding rate. This was attributed to incoming methanogenic archaea stemming from the alimentary system of the cattle. Since many of the methanogenic organisms identified in anaerobic digesters are similar to those found in the stomach of ruminant animals, the reactor was continuously inoculated from the feedstock. This outweighed the loss of biomass due to short retention times (Boe, 2006; Tchobanoglous et al., 2003).

Fig. 4b depicts the comparison between measured and simulated results of the numerical model for digester B1. It can be seen

that the model predicted reasonably well the dynamic behaviour of the start-up process in lab-scale, especially COD was predicted accurately. Following the assumption made above that the non-occurrence of a methanogen washout was due to incoming archaea, an additional influent of biomass was introduced within the model. It was implemented as an adjustable portion of the particulate COD which is fed to the model reactor and was calibrated to an optimized value of 1%. Within that flux of additional biomass, the portion of acetate degraders (Xac) was set to a value of 33.5% (hence, Xac = 0.34%). Biomass portions of 2% and 0% in feed COD (corresponding to 0.67% and 0% of acetate degraders) led to overestimated and underestimated gas productions, respectively (Fig. 4b).

3.3. Methanogenic population

The methanogenic community found in B1 was mainly composed of *Methanosarcina* (>95%). Fig. 5 displays the measured relative portion of methanogens in the sludge in reactor B1 as well as the corresponding simulation results for the start-up experiment. It should be noted that the model produces continuous results whereas there are only four points of measured data between day 12 and 33 as well as one value for the feeding materials manure and inoculum, respectively. Both graphs have similar trends indicating a gradual washout due to decreasing HRT, although there are differences in the order of magnitude since the cell water content is unknown and thus, the measured values are not directly convertible.

However, when comparing the quantitative proportion of methanogens in the feeding substrate and in the reactor sludge (P_{fr}), both measured and simulated results show values in the same order of magnitude. Given approximately 1.0E-5 g cell g sludge^{-1} in the feeding (Fig. 5), P_{fr} amounts to a mean percentage of 31% for the measurement data points. In the simulation the value averages out at 22%. This reveals that there is already a relevant quantity of biomass in the feed to prevent a digester upset.

3.4. Biokinetic modelling

In the models, particulate COD is distributed to the ADM1 compounds in the disintegration step and thus, the fractionizing factors (fxx_Xc) for the particulate composites (Xc) as well as the carbon and nitrogen contents of Xc play an important role in model performance, determining a characterisation of the input substrate. Table 3 shows these factors as well as the parameters which turned out to be sensitive for the behaviour of both models. Many parameters, principally those with low or no sensitivity on model outputs, have been applied without any optimization as compared to the standard values given in ADM1.

For the WWTP Salzburg model, the biodegradable fractions of Xc (fCH_XC, fPR_XC and fLI_XC) are similar to values reported in literature (e.g. Huete et al., 2006). Also, the kinetic parameters (km_su and km_ac) were within the range of literature values (e.g. Batstone et al., 2002; Blumensaat and Keller, 2005), whereas the decay rate of acetate degraders (kdec_Xac) had to be increased by an order of magnitude to meet satisfying simulation results.

For the start-up experiment, the given substrate ratios indicate a relatively high portion of carbohydrates (CH) compared to proteins (PR) and lipids (Li) with proportions of CH/PR = 1.9 and CH/Li = 5.0. This is in agreement with reported compositions of cattle manure in the literature (e.g. Møller et al., 2004). Within the kinetic parameters, the maximum uptake rate of sugars (km_su) revealed a remarkable influence on the simulation results. It had to be reduced from an initial value of 30–8 d^{-1} to avoid an overestimation of gas production. Obviously, there is a poor adaptation of the degradation of sugars within the start-up process. In Schoen et al. (2008) it was revealed that this phenomenon was not observable in the long term which could be seen from applying the

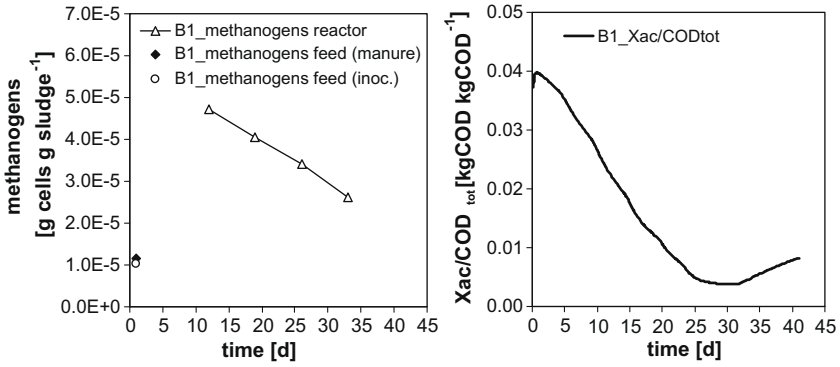

Fig. 5. Measured relative portion of methanogens in reactor B1 and in the feed (per g sludge; left) and simulation values for acetate degraders (Xac) (per kg COD; right) in reactor B1.

Table 3
Calibrated ADM1 model parameters including influent characterisation.

Parameter	Description	Value		Parameter	Description	Value	
		SBG[a]	SU			SBG	SU
fSI_XC [−]	Fraction SI from Xc	0.016	0.050	C_Xc [kmol C kg COD^{-1}]	Carbon content Xc	0.0280	0.0299
fXI_XC [−]	Fraction XI from Xc	0.101	0.240	N_Xc [kmol N kg COD^{-1}]	Nitrogen content Xc	0.0025	0.0022
fCH_XC [−]	Fraction Xch from Xc	0.165	0.350	kdis [d^{-1}]	Disintegration rate	1.0	0.1
fPR_XC [−]	Fraction Xpr from Xc	0.144	0.180	km_su [d^{-1}]	Uptake rate sugars	30	8
fLI_XC [−]	Fraction Xli from Xc	0.277	0.070	km_ac [d^{-1}]	Max. uptake rate acetate	20	30
fXP_XC[b] [−]	Fraction Xp from Xc	0.297	0.100	kdec_Xac [d^{-1}]	Decay rate Xac	0.131	0.020

[a] SBG:Salzburg WWTP, SU:start-up experiment.
[b] fXP_XC considers inert products from biomass decay in Xc as introduced in Wett et al. (2006a,b).

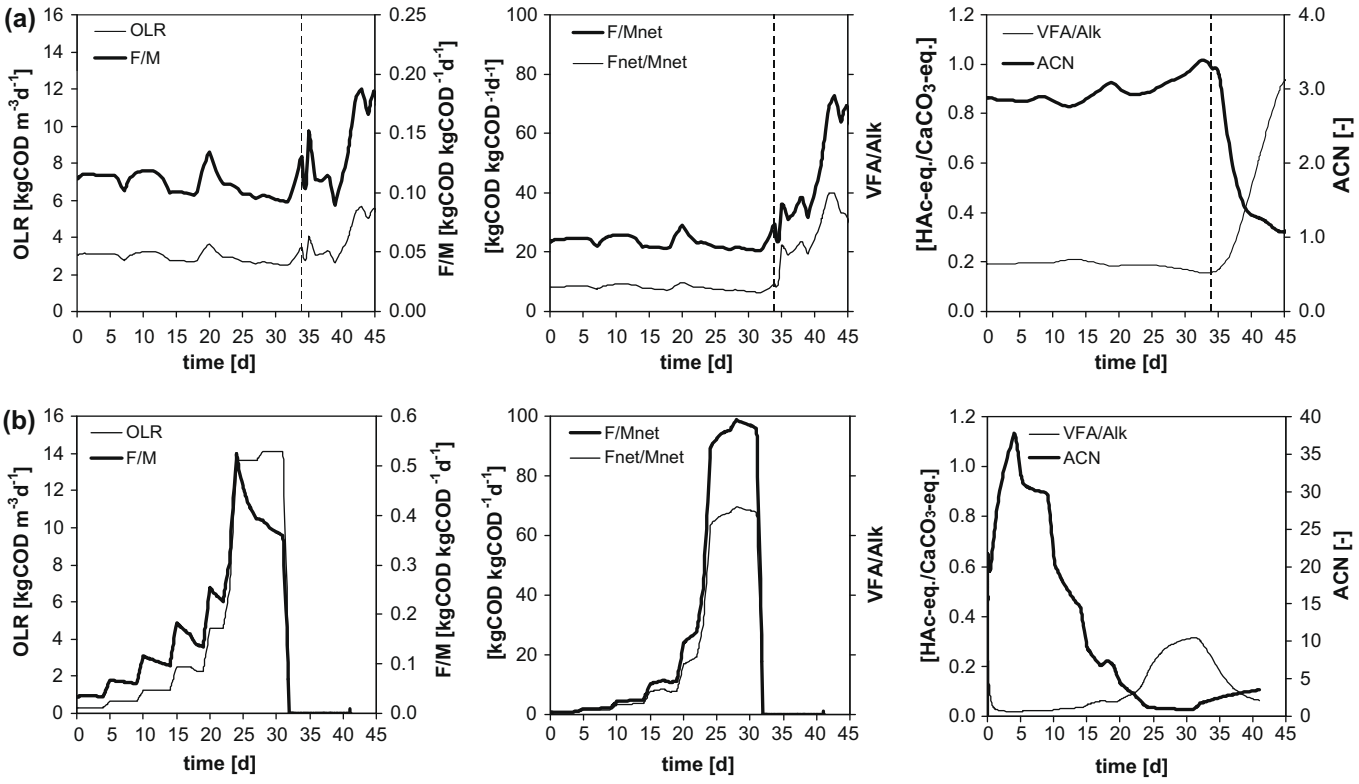

Fig. 6. (a) Simulation results of key indicators for Salzburg WWTP and (b) start-up experiment. Note that different *y*-axis scaling was used for *F*/*M* and ACN.

parameters to a model of the farm-scale pilot-plant. This is in accordance with findings of Page et al. (2008) where biogas production in bench-scale digesters was overpredicted by ADM1 but with correct results for full-scale systems.

3.5. Discussion of results for digester stability indicators

For both models, the VFA/alkalinity ratio and the ACN were calculated as described above. Additionally, the organic loading rate (OLR), the food to microorganism ratio (*F*/*M*), the food to net microorganism ratio (F/M_{net}), and the net food to net microorganism ratio (F_{net}/M_{net}) were assessed according to the equations given below:

$$OLR = COD_{input} \cdot Q/V \quad (6)$$

$$F/M = COD_{input} \cdot Q/(COD_{reactor} \cdot V) \quad (7)$$

$$F/M_{net} = COD_{input} \cdot Q/(Xac \cdot V) \quad (8)$$

$$F_{net}/M_{net} = COD_{degr} \cdot Q/(Xac \cdot V) \quad (9)$$

where COD_{input} is the COD concentration in the influent of the digester [kg COD m^{-3}], Q is the volumetric flow rate [$m^3\ d^{-1}$], V is the digester volume [m^3], $COD_{reactor}$ is the COD concentration in the digester [kg COD m^{-3}], COD_{degr} is the concentration of degradable COD in the digester [kg COD m^{-3}] and Xac is the concentration of acetate degraders in the digester [kg COD m^{-3}]. For the sake of uniformity with the other indicators, the OLR is expressed on a COD basis. For conversion to commonly used units for the OLR such as kg VSS $m^{-3}\ d^{-1}$, values must be divided by 1.4, which represents a rough approximation of the COD/VSS ratio of biomass (Tchobanoglous et al., 2003).

When examining the results for the digester failure at WWTP Salzburg in Fig. 6, it can be seen that there is a remarkable upward shift in F/M_{net} and F_{net}/M_{net}. The values of both loading indicators nearly doubled, reflecting the overload situation as soon as the sludge was directly by-passed to digester FT2 (day 34). This occurred parallel to the reactor breakdown, which is clearly indicated by the VFA/alkalinity and ACN results. Both reactor state indicators indicated impending failure as they exceed the range of a normal reactor status and approach values of >0.9 and <1.0, respectively. In contrast, failure was not indicated by the OLR as it increased insignificantly within its normal range of variation. The same is true for the *F*/*M* ratio. Thus, although the OLR is commonly used as a steady-state design parameter, it appears not to be suitable for the design under dynamic conditions.

Given the experiences from case study 1, a digester breakdown would appear likely for the start-up experiment due to *F*/*M* and OLR values that are more than double and F/M_{net} and F_{net}/M_{net} values that are 1.5 times higher compared to the Salzburg case (Fig. 6). The actual non-occurrence of a reactor failure supports the assumption of continuous re-inoculation from the feedstock as described above and is confirmed by the values for VFA/alkalinity and ACN. However, by the end of the experiment ACN values approached ≈1.0 and it is possible the digester would have failed if feeding had been continued.

4. Conclusions

The feasibility of predicting WWTP reactor upsets via stability indicators by modelling with ADM1 was shown. The net *F*/*M* ratio, the VFA/alkalinity ratio and the ACN clearly indicated impending failure. However, the OLR turned out to be unsuitable for reactor design under dynamic conditions. Instead, the utilization of indicators reflecting the biokinetic process state is more adequate for the assessment of the stability in transient situations.

Regarding the non-occurrence of a highly expected manure digester breakdown due to short HRT, the assumption of failure prevention due to a continuous methanogen re-seeding from the livestock was proved correct by modelling.

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