COMPUTATION AND IMPLEMENTATION ISSUES FOR BIODIVERSITY SIMULATIONS WITH EXTENDED ANAEROBIC DIGESTION MODEL NO 1 (ADM1_N) IN MATLAB/SIMULINK.

CONSIDERACIONES COMPUTACIONALES Y DE IMPLEMENTACIÓN PARA SIMULACIONES DE BIODIVERSIDAD CON EL MODELO DE DIGESTIÓN ANAEROBIA NO 1 EXTENDIDO (ADM1_N) EN MATLAB/SIMULINK.

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RESUMEN

El proceso de digestión anaerobia comprende toda una red de reacciones secuenciales y paralelas, de doble naturaleza: bioquímica y fisicoquímica. Los Modelos matemáticos diseñados con el objetivo de ayudarnos a comprender y optimizar este proceso, describen estas reacciones de forma estructurada. Siendo el modelo de digestión anaerobia Nº 1 (ADM1) el más extendido y bien establecido. Mientras que este y otros modelos distinguen diferentes microorganismos involucrados en diversas reacciones, a nuestro conocimiento ninguno de ellos describe la diversidad entre organismos con la misma función, es decir, que participan en la misma reacción. Sin embargo, la evidencia experimental disponible sugiere que la estructura y propiedades de una comunidad microbiana pueden estar influenciadas por las condiciones operacionales del proceso y a su vez también determinan el funcionamiento del reactor. Con el fin de describir adecuadamente estos fenómenos, los modelos matemáticos deberían considerar la diversidad microbiana subyacente. Así quedó mostrado en uno de nuestros trabajos anteriores, extendiendo ADM1 con objeto de describir la diversidad microbiana entre organismos de un mismo grupo funcional. El modelo resultante fue llamado ADM1_N. Debido a su complejidad y rigidez, la implementación del modelo no es una tarea sencilla y deben considerarse varios aspectos computacionales. En este trabajo, se presentan las experiencias obtenidas de algunas implementaciones en Matlab/Simulink de ADM1 y de ADM1 extendido (ADM1_N). Aspectos relacionados con las implementaciones en ecuaciones deferenciales ordinarias (EDO) vs Ecuaciones Algebraico diferenciales (EAD), la rigidez del sistema, las variables y constantes de tiempo, problemas algebraicos para el cálculo del pH y otras variables de estado problemáticas, algoritmos numéricos de solución y tiempos de simulación son discutidos. El modelo resultante ha sido comparado con el tradicional ADM1 para simular datos experimentales provenientes de un reactor piloto anaerobio hibrido de lecho fluidizado y filtro con flujo ascendente. Los resultados obtenidos muestran que el modelo extendido mejora el ajuste de datos experimentales.

Palabras claves: ADM1, ADM1_N, digestión anaerobia, biodiversidad, parámetros de funcionamiento del reactor, modelización, simulación, diversidad microbiana, UASFB.

ABSTRACT

The anaerobic digestion process comprises a whole network of sequential and parallel reactions, of both biochemical and physicochemical nature. Mathematical models, aiming at understanding and optimization of the anaerobic digestion process, describe these reactions in a structured way, the IWA Anaerobic Digestion Model No. 1 (ADM1) being the most well established example. While these models distinguish between different microorganisms involved in different reactions, to our knowledge they all neglect species diversity between organisms with the same function, i.e. performing the same reaction. Nevertheless, available experimental evidence suggests that the structure and properties of a microbial community may be influenced by process operation and on their turn also determine the reactor functioning. In order to adequately describe these phenomena, mathematical models need to consider the underlying microbial diversity. This was demonstrated in one of our previous work by extending the ADM1 to describe microbial diversity between organisms of the same functional group. The resulting model was called ADM1_N. Due to its complexity and stiffness, the implementation of the model is not a simple task and several computational aspects need to be considered. In this paper, the experiences gained from a Matlab/Simulink implementation of ADM1 into the extended ADM1 Model (ADM1_N) are presented. Aspects related to ODE vs. DAE implementations, system stiffness and varying time constants, algebraic solvers for pH and other troublesome state variables, numerical solvers and simulation time are discussed. The resulting model has been compared with the traditional ADM1 in describing experimental data of a pilot-scale hybrid Upflow Anaerobic Sludge Filter Bed (UASFB) reactor. The obtained results show that the extended model improves the fit of experimental data.

Keywords: ADM1, ADM1_N, anaerobic digestion, biodiversity, reactor performance parameters, modeling, simulation, Microbial diversity, UASFB.

INTRODUCTION

The world presently derives some 60% of its energy from fossil fuels. It is however widely recognized that the supplies of these are limited and, at projected future rates of consumption, are likely to be depleted well before the end of this century (1). One of the great challenges of the new century is therefore to obtain new sources of renewable energy, capable of replacing fossil fuels. In addition to renewable sources of energy such as solar, wind or hydroelectric energy, the use of solid, liquid and gaseous fuels from biomass-based raw materials is of importance. Biomass includes a broad range of materials (agriculture and forestry products and residues, fast-growing trees and grasses, farm and food wastes, municipal sludge and solid wastes, animal manure, marine and aquatic plants, industrial and manufacturing wastes) which are biological in nature and can be used to generate various forms of bio-energy. As such, biomass is a desirable source of renewable energy which can be converted by direct combustion or biological and/or thermo-chemical liquefaction or gasification into a variety of bio-fuels. Among these bio-fuels, biogas produced from anaerobic digestion of biomass is potentially a very important one.

Anaerobic Digestion (AD) is a complex series of biological processes that take place in the absence of oxygen and by which organic matter is decomposed and bioconverted on one hand into biogas, i.e., a mixture of carbon dioxide (CO_2) and methane (CH_4) as well as trace gases such as hydrogen sulfide (H_2S) and hydrogen (H_2) and, on the other hand, into microbial biomass and residual organic matter. Besides physicochemical reactions, the process comprises two types of biochemical reactions: extracellular (disintegration and hydrolysis) and intracellular ones. The latter type involves a variety of microorganisms, namely fermentative bacteria (i.e. acidogens, responsible for the uptake of sugar and amino acids), hydrogen-producing and acetate-forming bacteria (i.e. acetogens, degrading long chain fatty acids, valerate, butyrate and propionate), and archaea which convert acetate or hydrogen into methane (i.e. methanogens). Other types of anaerobes play important roles in establishing a stable environment at various stages of methane fermentation. An example of the latter is homoacetogens, which can oxidize or synthesize acetate depending on the external hydrogen concentration (2).

Several advantages are recognized to AD processes when used for waste and wastewater treatment: (i) high capacity to treat slowly degradable substrates at high concentrations, very low sludge production (5 to 10 ti-

mes less than in aerobic processes), (ii) potentiality for valuable intermediate metabolites production, (iii) low energy requirements (no aeration is required), (iv) reduction of odors in a closed system, (v) pathogens reduction and (vi) possibility for energy recovery through methane combustion. As a consequence, AD compares very favorably with activated sludge processes in terms of energy balance and sludge production (*Cf.* Figure 1) and this makes it very well adapted to highly concentrated wastewater and solid wastes. Last but not least, when carried out properly and thoroughly, the digestion process will transform toxic organic materials into clean fertilizers which are free of pathogens and weed seeds.

However, AD processes also have drawbacks: (i) the low sludge production is closely linked to the slow growth of micro-organisms. As a consequence, the start-up phase is often tedious and some time is required (e.g., 2-4 months or longer) before steady state conditions are obtained, (ii) AD micro-organisms are highly sensitive to overloads of the process and disturbances of several causes, (iii) AD is a complex process involving many different micro-organisms which is still not completely understood.

These drawbacks explain probably that AD processes are not more widely used at the industrial scale. In the past, the lack of knowledge concerning AD processes led indeed to breakdowns, ranging from minor to catastrophic, mainly due to organic overloads of various origins. They created some kind of suspicion towards this process and delayed its development at the industrial scale. This is why actual research aims not only to extend the potentialities of anaerobic digestion, but also to optimize anaerobic processes and increase their robustness towards perturbations.

In general, anaerobic reactors are affected by external changes, although the severity of the effect is dependent on the type, magnitude, duration and frequency of the imposed changes (3). Typical responses indicating reactor failure include a decrease in performance, accumulation of reaction intermediates such as volatile fatty acids (VFAs), drop in pH and alkalinity, change in biogas production rates and compositions, sludge washout and shifts in microbial community structure.

The availability of new molecular biological tools for studying microbial communities in bioreactors and other engineered systems without cultivation has resulted in remarkable insights linking microbial diversity and dynamics to process stability. Fernandez et al. (4), monitored the community dynamics of Bacteria and Archaea in a functionally stable, continuously mixed methanogenic reactor, fed with glucose, over a 605 day period. Even though the reactor maintained constant pH and COD removal during this period, they found differences in the levels of diversity and dynamics between the Bacterial and Archaeal domains, indicating that functional stability does not imply community stability, i.e. levels of individual populations fluctuate in a functionally stable community. Similar results were observed in another methanogenic reactor system, a fluidized bed reactor fed with vinasse (wine distillation waste) in which the biomass was immobilized on powder from porous volcanic stone (5).

Another aspect concerns the effect of operational disturbances on the underlying microbial community. Fernandez et al. (6) experimentally investigated the effect of substrate loading shocks on population dynamics. For continuously mixed methanogenic reactors that maintained two different communities, they found that the less stable community structure resulted in more stable functioning. These results were attributed to the

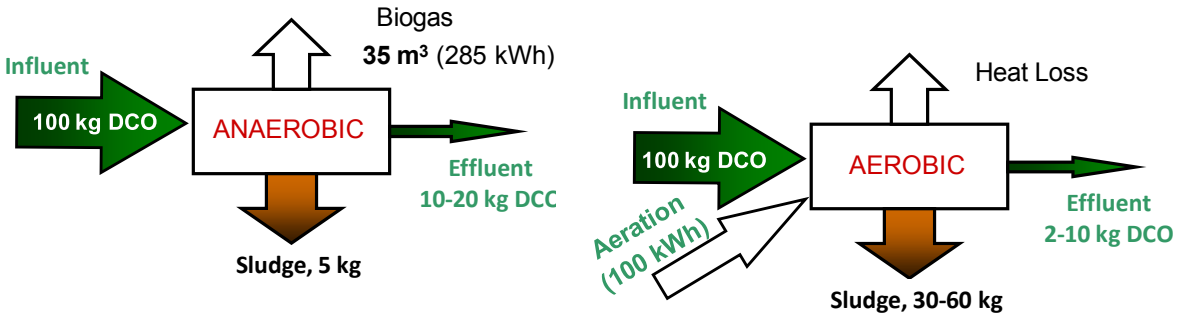

Figure 1. Comparison of anaerobic digestion with activated sludge processes

substrate processing structure that was developed in each reactor type prior to perturbation: substrate processing through parallel pathways was associated with a functionally more stable (resilient) system, in contrast to serial processing of substrate. An important outcome of these and other experiments is the realization that population diversity alone does not drive ecosystem stability. The positive relationship between the presence of multiple pathways towards a product (parallel processing of substrate) and functional stability parallels theoretical concepts in higher ecological organization (7). Ecosystem stability is not the outcome of population diversity as such, but of functional redundancy, which is ensured by the presence of a reservoir of species able to perform the same ecological function. Recognizing the diversity and the links within each key functional group of a system can lead to better ways to model diversity and functioning, and can help to improve process stability (8).

It is our belief that the engineering of wastewater treatment systems would be improved if one could predict and manipulate the associated microbial diversity. Mathematical models, in which data on micro-scale molecular diversity has been incorporated to more closely represent wastewater treatment processes, can provide a useful tool to reach this goal. Such models can be used to gain insight in the influence of process conditions on the selection of certain types of bacteria. In a later stage, these models can also be used to develop efficient control strategies adapted to model-based population optimization. In this contribution, this approach is demonstrated for two different wastewater treatment applications. With respect to anaerobic digestion, the Anaerobic Digestion Model No. 1 (ADM1, (9)), developed by the corresponding International Water Association (IWA) Task Group, has become widespread and generally accepted. However, ADM1 does not distinguish between microorganisms performing the same reaction – which implies all of them are assumed to have the same properties – and can therefore not adequately represent or predict experimental results concerning this type of interspecies diversity. The need for incorporation of detailed micro-scale data into current wastewater treatment models was also indicated previously by Yuan and Blackall (10), regarding the influence of plant design and operation on microbial community structure and microbial properties in activated sludge systems.

Although a thorough discussion of an appropriate definition of species is beyond the scope of the current work, we feel that it is important to provide the ‘‘species concept’’ used throughout this manuscript. In our model, species are defined as groups of like individuals that share a common set of kinetic and stoichiometric characteristics. This may or may not correspond to species as defined by 16S ribosomal DNA sequence comparisons (11) nor species as defined by operational taxonomic units (OTU) based on molecular fingerprinting assays (12). This contribution presents an approach for modeling microbial diversity in the anaerobic digestion process, applied to the standard ADM1 which has been extended with multiple species for each reaction. Experimental results will be used to compare classical models such as ADM1 with an increased complexity model and further simulations will show that microbial diversity can lead to different results and different conclusions about some experimental results. The extended model has subsequently been applied to handle microbial diversity in both normal conditions, not leading to process imbalance, and abnormal situations, characterized by the presence of inhibiting ammonia levels in the reactor.

MATERIALS AND METHODS

Experimental setup

The schematic diagram of the laboratory scale Up-flow Anaerobic Sludge Filter Bed (UASFB) reactor (diameter 12 cm; height 117 cm; effective volume 9.8 L) used in this study is shown in Figure 2. The reactor column was made up of Plexiglas and constituted of two compartments: the bottom part was operated as a UASB reactor whereas the top part was operated as an anaerobic filter. The top portion of the UASFB reactor was randomly packed with 90 pieces of small cylindrical, buoyant polyethylene packing media (height: 29 mm; diameter: 30–35 mm; density: 0.93 kg/m^3), and baffled with 16 partitions. Fifty percent of the reactor volume (excluding the headspace of 30 cm height) was filled with the packing media.

The reactor, operated at 33±1°C, was equipped with a continuous internal recirculation system from top to the bottom (recirculation rate: 9 L/h). Recirculation was done mainly to eliminate the possibility of high organic loading close to the feed port and to favor better wastewater/sludge contact. The digester was seeded with granules (15% by total volume) originating from a UASB digester treating cheese wastewaters. This hybrid UASFB reactor was operated for a total period of

232 days. Continuous feeding of the reactor was started with an initial OLR of 3.1 gCOD/L d. OLR was then increased stepwise by increasing the substrate concentration from 3.1 to 21.7 g/L (around 95% of the total COD was soluble), while maintaining a constant HRT of 1.15 days. A CODs removal efficiency of 80% was considered as the threshold level in the present study for the operation of the UASFB reactor. The OLR was progressively increased by 20–30% once or twice a week until the CODs removal dropped below 80%. The feed was supplemented with nutrients to attain a COD: N: P ratio of 400:7:1 in the wastewater. The feed pH was adjusted to 6–6.5 using a 6 N sodium hydroxide. The following measurements are available on-line: input and recirculation liquid flow rates, pH in the reactor and in the input wastewater, temperature, biogas output flow rate, CO_2, CH_4 and H_2 composition in the gas phase, total organic carbon, soluble chemical oxygen demand, VFAs and bicarbonate concentrations and total and partial alkalinity in the liquid phase. More details on the process can be found in Rajinikanth et al. (13).

The experiments were performed with distillery vinasse (wine residue after distillation), which was obtained from a local distillery around Narbonne, France. In this type of wastewater, soluble COD is mainly present as monosaccharides (Ssu in ADM1) and little as amino acids (Saa) and long chain fatty acids (Sfa). Particulate COD is mainly present in the form of carbohydrates (Xch), besides some composites (Xc), proteins (Xpr) and lipids (Xli).
The input VFA values were calculated from measured concentrations of acetate (Sac), propionate (Spro), butyrate (Sbu) and valerate (Sva). The initial pH resulted from the ionized forms of VFAs, bicarbonate, ammonia and cation/anion concentrations. Ammonia (SIN) and bicarbonate (SIC) were measured by Keljdahl's method and using a TOC meter, respectively. Anion concentration (San) was taken equal to SIN and cation concentration (Scat) was adjusted in each case according to the initial experimental pH. The concentrations of these individual components used in the model as process inputs are shown in Table 1.

Model structure

The IWA Anaerobic Digestion Model No. 1 (ADM1, Batstone et al., 2002) was extended to handle microbial diversity within functional groups. In the traditional ADM1 model, one microbial population is associated to each reaction. Seven functional groups of microorganisms are distinguished, corresponding to the degradation of sugar (by Xsu), amino acids (by Xaa), LCFA (by Xfa), valerate and butyrate (by Xc4), propionate (by Xpro), acetate (by Xac) and hydrogen (by Xh2) and one microbial population is associated to each reaction. In order to account for microbial diversity, the traditional ADM1 model was extended in such a way that multiple species are associated to each functional group.
Whereas the original ADM1 possesses 24 state variables, of which 7 biomass species (7 functional groups, 1 species per functional group), the extended model includes 7.N different biomass species (7 functional groups, N species per functional group), of 17+7.N state variables in total. The number of associated reactions is extended from 19 to 15.N+4. The resulting model will further be denoted as ADM1_N, where 'N' refers to the extension of the original model for microbial diversity with N species for each group. Within each functional

Table 1. Input concentrations of the wine distillery wastewater used during the experiments

Constituent	Values	Constituent	Values
Sugars	0.420*CODt_in	Carbohydrates	0.90*CODp_in
Amino acids	0.020*CODt_in	Proteins	0.07*CODp_in
Long Chain Fatty acids	0.010*CODt_in	Lipids	0.03*CODp_in
Total Valerate	0.035*CODt_in	Inorganic Nitrogen	0.05/18*CODt_in
Total Butyrate	0.181*CODt_in	Inorganic Carbon	0.003/18*CODt_in
Total Propionate	0.128 *CODt_in	Total input COD	CODt_in*
Total Acetate	0.152*CODt_in	Input particulate COD	CODp_in*

** variable input signals*

group, species may differ in terms of their yield coefficient Y as well as Monod maximum specific uptake rate km and half saturation constant Ks.

In our case, the yield coefficient was assumed constant as in reality the variability of this parameter is low. Within a functional group, the kinetic parameters km and Ks were randomly chosen from a statistical distribution. The distribution type and their parameters values could be found following a curve-fitting process using experimental data from each reactor type i.e., with the experimental data and the model, we first select the distribution type (among others normal, uniform or unimodal, bimodal), next their parameters (mean and standard deviation). We run the simulations and if the model does not fit experimental data, we change distribution parameters in first instance. If the misalignment persists, we change modal type and in last trial, we change the distribution type.

This approach adds a stochastic component to ADM1_N, compared to the deterministic ADM1. It is clear that many other approaches to define the microbial properties within functional groups can be thought of. They are all likely to be stochastic since microbial properties cannot be defined with certainty. In order to maintain comparable conditions for simulations, the initial biomass concentrations in ADM1 will be distributed equally among the corresponding microbial populations in ADM1_N.

Biomass retention in the UASFB reactor has been modeled in the simplified way suggested in the ADM1 report (9), with a term including the residence time of solids (tres,x) in the biomass mass balance equation to account for the difference between hydraulic retention time (HRT) and solid retention time (SRT). The resulting model has been implemented in MATLAB®/Simulink. Its applicability has first been tested by Ramirez and Steyer (14) to model anaerobic digestion in a fixed bed reactor. In this contribution, a thorough model validation has been performed on experimental data for UAFSB reactor. It is important to note that the presented modeling approach is generic and can also be applied to other processes. Volcke et al. (15) demonstrated the applicability of a model including different species performing the same reaction, describing experimental nitrification data through a model with two types of ammonium oxidizers.

Developing and tuning mathematical models in normal situations are nowadays a well defined procedure that can be easily performed, even with complex models such as ADM1. However, developing and tuning a model to adequately represent abnormal situations is still a difficult and challenging task. In particular, when facing inhibition by a toxicant, anaerobic digestion processes may experimentally present different behaviors that are still not fully understood: one process can indeed show high robustness with respect to the presence of a toxicant while another similar process is much more sensitive to this toxicant. It is indeed likely that different species will exhibit different behaviors towards these substances. The effect of nonreactive toxicant affecting all species has been examined by Ramirez and Steyer (14). Other non-reactive toxicant such as ammonia inhibits a specific population, in this case methanogens.

Computation and implementation issues

The availability of faster, more powerful computers allows for more complex models to be simulated but it is clear that a biodiversity model, which includes many species (e.g. ADM1_N), requires significant computational power. For steady-state simulation (constant inputs), the computational burden is relatively acceptable but for dynamic simulations (changing inputs), simulation time becomes extensive when the evaluation period is long.

Moreover, dynamic and especially stochastic inputs in

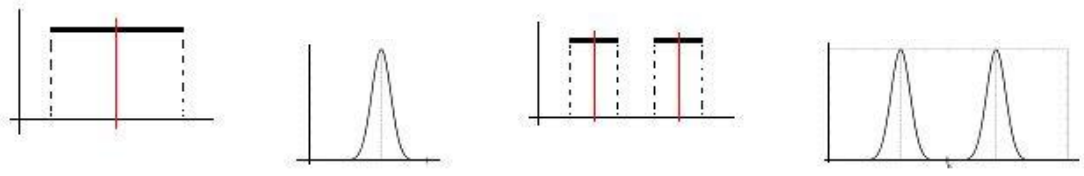

Figure 3. Model's Parameters distribution types

combination with the inherent structure of the ADM1_N further complicate the simulations due to numerical considerations and restrictions. In this section, we discuss the implementation of the Extended Anaerobic Digestion Model no 1 (ADM1_N) in Matlab/Simulink. This includes computational aspects encountered in the implementation of the model and some solutions in order to improve the simulation speed. The effort to improve the simulation speed of the ADM1_N is incited by the need to reduce the simulation time for biodiversity model. However, the results presented in this section are general and other users of the general ADM1 should also benefit from these results.

A system is called stiff, when the range of the time constants is large. This means that some of the system states react quickly whereas some react sluggishly. The ADM1_N is a very stiff system with time constants ranging from fractions of a second to months. This makes the simulation of such a system challenging and in order to avoid excessively long simulation times, we need to be somewhat creative when implementing the model.

Some of the solvers in Matlab/Simulink are so called stiff solvers and, consequently, capable of solving stiff systems. However, a problem common to all stiff solvers is the difficulty to handle dynamic input - including noise. The more stochastic or random an input variable behaves, the more problematic is the simulation using a stiff solver. The reason for this is that in stiff solvers, prediction of future state values is carried out. However, predictions of future state values affected by stochastic inputs will result in poor results, slowing down the solver by limiting its ability to use long integration steps. Simulation of ADM1_N is, thus, subject to the following dilemma: ADM1_N model is a very stiff system and, consequently, a stiff solver should be used. However, if we use the model for control simulation purpose, noise must be included, calling for an explicit (i.e. non-stiff) solver.

When the states of a system are described only by ordinary differential equations, the system is said to be an ODE system. If the system is stiff, it is sometimes possible to rewrite some of the system equations in order to omit the fastest states. The rationale for this is that from the slower state's point of view, the fast states can be considered instantaneous and possible to describe by algebraic equations. Such systems are normally referred to as differential algebraic equation (DAE) systems. By rewriting an ODE system to a DAE system, the stiffness can be decreased, allowing for explicit solvers to be used and for stochastic elements to be incorporated. The drawback is that the DAE system is only an approximation of the original system and the effect of this approximation must be considered and investigated for each specific simulation model.

As already mentioned, ADM1_N model includes time constants in a wide range; from milliseconds for pH to weeks or months for the states describing various fractions of active biomass. Since most control actions affecting the anaerobic digester are fairly slow, it makes sense to investigate which fast states can be approximated by algebraic equations. In Batstone et al. (2002), it is suggested that the pH (S_{H+}) state is calculated by algebraic equations. However, this will only partially solve the stiffness problem. There are other fast states and a closer investigation suggests that the state describing hydrogen (S_{h2}) also needs to be approximated by an algebraic equation.

As mentioned above, stiffness of the ADM1 can be reduced by approximating the differential equations of the pH and S_{h2} states by algebraic equations. An implicit algebraic equation for the pH calculation is given in Batstone et al. (9). It has been suggested to calculate the S_{H+} and, consequently, the pH from the sum of all charges, which is supposed to be zero. To do so, the ion states are replaced in terms of SH+ and total concentrations. The differential equation for the Sh2 state, explicitly given in Rosen and Jeppsson (16), can be approximated by an algebraic equation in a similar way as was the case for the pH state, simply by setting its differential to zero (assuming fast dynamics). The obtained implicit algebraic equations are non-linear and therefore can be solved only by an iterative numerical method. In this case, the Newton-Raphson method used in Volcke et al. (17) for calculation of the pH and equilibrium concentrations was implemented. By using this method the new value of the unknown state is calculated at each iteration step as:

$$S = S_0 - \frac{E(S_0)}{\left(\frac{dE(S)}{dS}\middle|S_0\right)}$$

Where S_0 is the value of the state obtained from the previous iteration step and $E(S_0)$ is the value of the implicit algebraic equation that has to be zero for the equilibrium. The gradient of the algebraic equation dE(S)/dS is also needed for calculation of the new state value. The iteration is repeated as long as $E(S_0)$ remains larger than the predefined tolerance value, which in our case

is set to 10^{-12}. Normally only two or three iterations are required to solve the equation at each time step.

RESULTS AND DISCUSSION

The behavior of the modified anaerobic digestion model, ADM1_N, has been compared to the one of the standard ADM1 and to experimental results in simulating the behavior of a pilot-scale UASFB reactor operated under varying input OLR. The number of species per reaction is arbitrary and in this study has been set to 10, to keep a reasonable computation speed. It was shown (18) that it is not sufficient to describe only pH as an algebraic state. Also the hydrogen state must be approximated by an algebraic equation to obtain satisfying results. The reformulation of the model results in a decrease in simulation time of the ADM1_10 simulation period from approximately a day to less than an hour. Within a functional group, the kinetic parameters km and Ks were chosen from a normal bimodal distribution, with means of μ_1=0.6k ,μ_2=1.4k and standard deviations of $\sigma_{1,2}$=0.125k, where k is the value of the corresponding standard ADM1 parameter (See Figure 4). The results are described in what follows.

Simulation of UASFB with varying OLR: ADM1 vs. ADM1_10

Previous experience in simulating the behavior of a reactor fed with the same wine distillery wastewater (14) led to the identification of the main ADM1 parameters which need to be modified in order to reasonably reflect the experimental data. Only the maximum specific substrate uptake rate (km) and the half saturation constant (Ks) for acetate and propionate were calibrated to fit the data (See Table 2). The resulting values were used in all simulations, with ADM1 as well as ADM1_10 (in the latter case as center values).

Table 2. Main estimated parameters to fit the experimental data.

Parameter	Acetate	Propionate
km (kg_{COD}/kg_{COD}.day)	1.93 (8)	1.41 (0.15)
K_S (kg_{COD}/kg_{COD}.day)	2.51 (13)	1.41 (0.10)

Values in parenthesis are the recommended values in STR

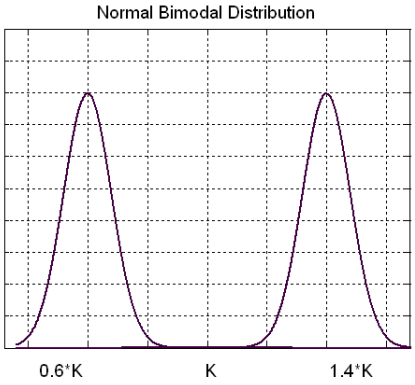

Figure 3. Kinetic parameters in ADM1_10

Figure 4 compares the experimental data with the simulation results obtained with both models for the UASFB reactor operated at a varying input loading rate by varying the influent concentration while maintaining a constant HRT. As it is seen both models can simulate nicely the dynamic evolutions of the main variables, in the liquid and also in the gas phase. As a consequence, assessing the most appropriate model among ADM1 and ADM1_10 is a tedious, not to say impossible, task. Note that the main purpose of this study was not to perfectly fit these data but to evaluate the ability of both models to adequately predict the behavior of this particular digestion process. Soluble COD, VFAs and biogas production values are higher in ADM1 than in ADM1_10 since the amount of biomass from ADM1 is lower than the biomass from ADM1_10. This is in agreement with the diversity–productivity hypothesis of Tilman et al. (19) and the phenomenon is known as "over-yielding".

Between day 100 and 200, both models over-predicted VFA concentrations. It appeared that the simulated rate at which acetate was converted to methane under the load imposed was somewhat under-estimated. This may have resulted from either under-estimation of the substrate consumption coefficients for aceticlastic methanogenesis or an over-estimation of the inhibition of this activity by ammonia. The models predict well the dynamics of the biogas production rate and composition as a response of the load imposed. Small deviations in predicting the biogas production and quality have been found, which may be attributed to the fact that the standard ADM1 uses the same gas/liquid transfer coefficients for all gases (CO_2, CH_4, H_2), while this is not the case in reality. Besides, also the dependence of these coefficients on the specific reactor configuration applied has been neglected.

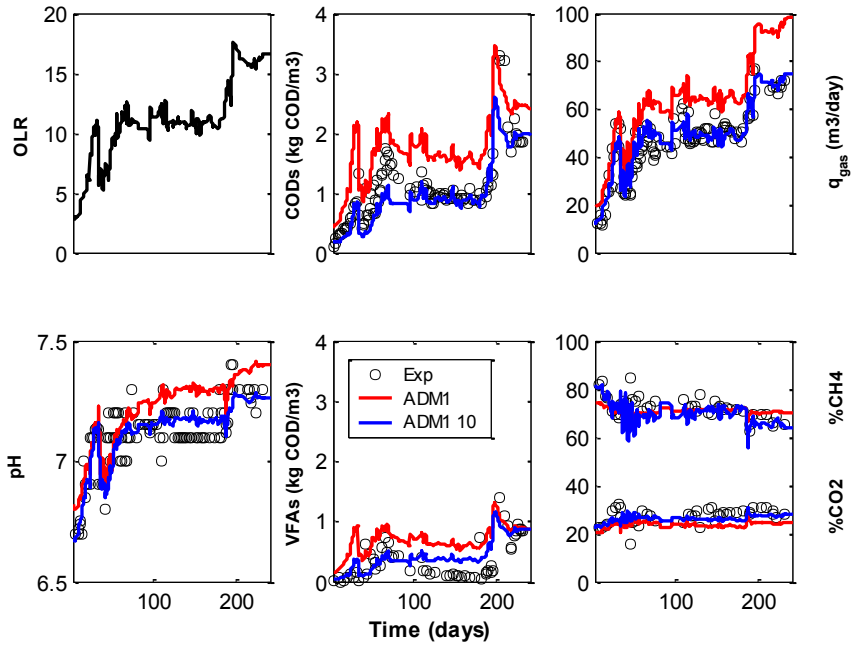

Figure 4. Behavior of a UAFSB reactor: experimental data versus simulation results with ADM1 and ADM1_10

The pH was also quite accurately simulated and the models were able to reflect the trends that were observed in experimental data. The pH prediction is closely related to the cation and anion concentrations in the reactor, and actually, the difference between the two concentrations. Since the ion concentrations were not measured, it was then calculated using the pH value and taking into account the concentration of ammonia, alkalinity and VFA concentration in the reactor. The value of the input cation from the reactor minus the input anion concentration in the feed was arbitrarily increased in the models, so that the pH values were calibrated. On day 35, about 300 mL of sludge were accidentally discharged out of the reactor (connection failure at the bottom of the reactor) and hence the performance of the UASFB was disturbed. This disturbance was not included in the simulations and may be this explains the differences mainly in CODs and VFAs between the simulated and experimental data during the period 35–57 days.

The main difference between the ADM1 and ADM1_10 models lies in the biomass evolutions. Figure 5 shows the obtained specific growth rates and the dynamic evolution of acetate degraders during these simulations. Similar results were obtained for other degraders (not shown). The specific growth rate in terms of substrate concentrations (Monod curves) are depicted too.

As it is seen in Figure 5c we have two biomass groups: k-strategists (species 1–5) vs. μ-strategists (also known as R-strategists, species 6–10) which is related to the fact that we have combined high K_S values with high μ values and low K_S values with low μ values. After an initial decrease of all species, related to a decrease of total biomass, from day 150 on, species 6–10 outcompete species 1–5, (Figure 5d), which is attributed to their higher growth rate (see Figure 5c). At the same time, acetate concentration switches from low values to high ones (data not shown), leading to a competitive advantage of the biomass group of m-strategists. This competitive advantage is also maintained for a longer simulation period: even after 3000 days, species 6–10 all survive (data not shown).

CONCLUSIONS

A methodology to account for microbial diversity in complex but structured models such as the anaerobic digestion model ADM1 has been presented. This approach consists of extending the number of mass balances for an arbitrary number of species having the same function (performing the same reaction), while using a stochastic mechanism to select the corresponding microbial parameters. The resulting model remains powerful in representing macroscopic experimental data, but is moreover able to get insight in underlying microscopy

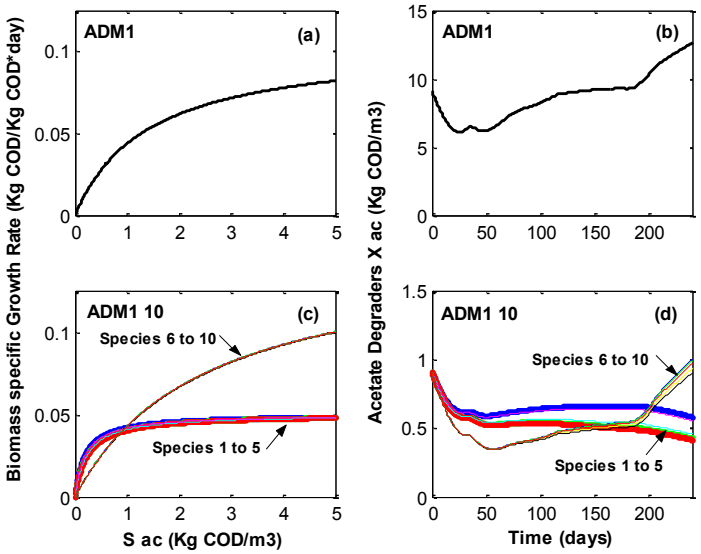

Figure 5. Acetate degrading biomass evolution and corresponding specific growth rates: ADM1 vs ADM1_10

To deal with microbial diversity, the number of species considered for each biological reaction is arbitrary and in this study was set to 10, which is sufficient to demonstrate the potential of modeling microbial diversity. Besides, the number of species considered may differ between different functional groups (reactions). Moreover, handling a very high number of species per reaction (e.g. 100–1000) can be seen as a way to reduce efforts required for parameter estimation. Indeed, only a "global" value of the model parameters such as in ADM1 would be required, microbial diversity being later accounted for by the high number of species handled with random kinetic parameters centered around the average values found to fit ADM1.

In this paper, several computational aspects of the Matlab/Simulink implementation of the ADM1 for use in the Biodiversity Model were discussed. It is shown that optimizing the computational efficiency of the ADM1_N implies that the stiffness of the ADM1 must be overcome so that fast simulation is achieved for dynamic input data, using a solver that handles stochastic inputs. This means that the stiff solvers provided by Matlab/Simulink cannot be used. Instead, rewriting the system as a DAE system is the only possibility. It is shown that it is not sufficient to describe only pH as an algebraic state. Also the hydrogen state must be approximated by an algebraic equation to obtain satisfying results.

Application of the presented methodology to represent – but not predict or engineer – biodiversity in other structured models, such as activated sludge models (ASMs) is straightforward. This offers wide perspectives not only in terms of modeling but also in terms of control objectives since microbial population appears nowadays to be a major component that drives process performances.

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