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Anaerobic digestion of biomass and waste: current trends in mathematical modeling

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Abstract: Although anaerobic digestion is a widely applied technology, the process is not yet fully understood because of its high complexity, and an optimization of the current technology is still needed. The design and control of digester systems is still generally performed by rule-of-thumb since no tools are currently available for an accurate evaluation of performance. The application of mathematical models is a prerequisite to improve digester performance and hence much attention is focused on the development of accurate models. This paper critically reviews the current state of the art about mathematical modeling of anaerobic digestion models. Moreover, the main trends in optimization of the existing models and the development of new models are discussed.

Keywords: anaerobic digestion, ADM1, modeling

1. INTRODUCTION

The production of a huge amount of waste sludge is an inevitable drawback of waste activated sludge processes, and sludge handling and disposal already accounts for up to 50% of total treatment costs of wastewater purification (Neyens *et al.* (2004)). Anaerobic digestion is of particular interest in sludge treatment since it has the ability to reduce the overall amount of biosolids to be disposed by circa 40%, while producing an energy rich biogas (55-70% CH_4) that can be valorized energetically (Appels *et al*. (2008)). Other beneficial features include the stabilization of the sludge, the inactivation and reduction of pathogens, and the improvement of sludge dewaterability (Appels *et al*. (2010)). Although this technology has been applied for several decades, there is still a lack of fundamental knowledge on the mechanisms of anaerobic digestion, what is mainly due to the very high complexity of the process. As a result, the design of digester systems is still generally performed by rule-of thumb (De Baere (2006)).

The microbial communities responsible for the digestion process represent a "biological factor" that poses some particular challenges for modeling approaches. Specifically for microbial processes is the fact that the performance of a micro-organism is not solely dependent on the organism itself, but also on the environment it resides in. Due to changes in the digestion system, (e.g. feed composition, alkalinity, thermal disturbances, pollutants or accumulation of intermediate or end-products), the activity of certain communities may vary widely between not and fully active. This is reflected in models by the values of certain parameters that can vary greatly according to the specific application or even during the course of an experiment. One must realize that a full and completely deterministic model is an almost utopian idea because (*i*) the number of identified species in an anaerobic digester culture is very high (at least over 100 according to Deublein & Steinhauser (2008)), (*ii*) evolves dynamically between different levels of activity and (*iii*) some are not obligatory but facultatively anaerobic. An additional problem in modeling anaerobic digestion is the availability of data needed for system identification. The number of independent components found in a digester can be extremely large, and measurements are often time consuming and costly. Also, only a limited number of process variables can be measured on-line, which makes automated control even more troublesome. To overcome these monitoring problems, the use of software sensors can be very useful. These techniques will be dealt with in Section 4.

There is a general agreement in the literature that the application of mathematical models is a prerequisite to improve digester performance and hence much attention is currently focused on the development of accurate models. This paper critically reviews the current state of the art digestion models. Moreover, the main trends in optimization of the existing models and the development of new models are discussed.

2. DESCRIPTIVE MODELING

2.1 Early models

The first anaerobic digestion models already date back to the end of the sixties, early seventies with the models proposed by Andrews (1969) and Andrews & Graef (1971) which consider the methanogenesis performed by acetoclastic methanogenesis as the rate-limiting step and already include inhibition by substrate accumulation described by Haldane kinetics. Other initial models such as Gosset & Belser (1982)

and Pavlostathis & Gosset (1986) consider the hydrolysis step as rate-limiting for the digestion of activated sludge. Further development led to more realistic models that consider the process as a chain of reaction stages performed by distinct microbial populations: three according to Hill and Barth (1977) (solubilization of organics, acidogenesis and methanogenesis) and four according to Mosey (1983) (acidogenesis, acetogenesis and two methanogenic reactions). The latter was further elaborated by (*i*) Rozzi *et al.* (1985) who divided the system into a gaseous and liquid phase and a biological system, and (*ii*) Costello *et al.* (1991) and Perrier & Dochain (1992) who included the degradation of glucose. A flaw in these early models was that they considered the substrate to be homogenous or synthetic. Therefore, other models were also developed for specific substrates such as liquid manure (e.g. Hill (1982) and Angelidaki *et al.* (1993)), or sewage sludge (e.g. Siegrist *et al.* (1993)). Based on extensive experimental work, Angelidaki *et al.* (1999) proposed a general applicable model in which the substrate is expressed in terms of carbohydrates, proteins, lipids and intermediate degradation products. A more elaborate review on the history and evolution of model development lies beyond the scope of this paper and the reader is referred to Tomei *et al.* (2009), Appels *et al.* (2008) and Lübken *et al.* (2010).

2.2 Anaerobic Digestion Model No. 1 (ADM1)

The diversity and variety in models developed so far required a convergent action to consolidate the various approaches found in the different existing models. With this objective, the IWA Task Group on Mathematical Modeling of Anaerobic Digestion Process, founded in 1997, developed the Anaerobic Digestion Model No. 1 (ADM1), as a unified base for modeling of anaerobic digestion (Batstone *et al.* (2002)). The used nomenclature, units and model structure are consistent with the existing anaerobic modeling literature and the Activated Sludge Models ASM1, ASM2, and ASM3 (IWA Task Group on Mathematical Modeling for Design and Operation of Biological Wastewater Treatment (2000)) Implementations of ADM1 are available in Matlab and Simulink but also in specific water related simulation software such as WEST and Aquasim.

ADM1 describes the reactions occurring in anaerobic digestion, by assuming a perfect mixture. The components are expressed in terms of their Chemical Oxygen Demand (COD) (g O_2/g sludge). The model includes biochemical as well as physicochemical processes. The biochemical reaction pathway is depicted in Fig. 1 and includes: (*i*) an extracellular disintegration step converting composite particulate matter into carbohydrates, lipids and proteins, (*ii*) an extracellular enzymatic hydrolysis step converting the degradation products into their chemical building blocks, i.e. monosaccharides, long chain fatty acids (LCFA) and amino acids (AA), (*iii*) acidogenesis or fermentation of the building blocks into hydrogen, acetate and volatile fatty acids (VFA), i.e. propionate, butyrate and valerate, (*iv*) acetogenesis of VFA to acetate, (*v*) acetoclastic and hydrogenotrophic methanogenesis. All biochemical extracellular steps are assumed to be of first order, while the intracellular biochemical reactions use Monod-type kinetics for substrate uptake. Substrate uptake in the intracellular biochemical reactions is also accompanied with biomass growth. Death of biomass is represented by first-order kinetics with the dead biomass considered as a composite particulate matter. Inhibition of the biological activity by pH (all groups), hydrogen (acetogenes) and free ammonia (acetoclastic methanogenes) is included.

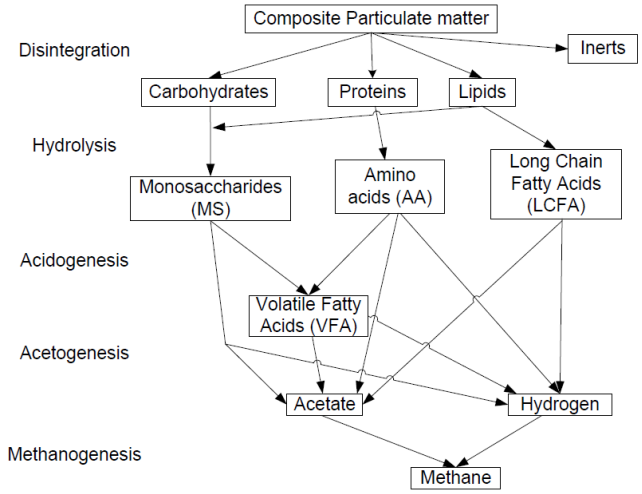

Fig. 1. The reaction paths described in ADM1 (Batstone et al. (2002))

ADM1 is expressed in 32 ordinary differential equations (ODEs) of which 12 describe the dynamical behavior of the particles and biomass, 10 ODEs the soluble components, 2 ODEs the inorganic nitrogen and carbon, 2 ODEs the cation/anion-balance in the liquid and 6 ODEs the acid-base reaction to determine the pH and the concentration of ionized forms of VFAs, NH_3 and CO_2.

2.3 Applications and extensions of ADM1

Due to the experience and prestige of the collaborators in the Task Group and due to the numerous successful validations, the ADM1 is considered as the current state-of-the art model. Applications are found in many occasions, e.g. digestion of grass silage (Koch *et al.* (2010)), co-digestion of municipal waste with activated sludge (Derbal *et al.* (2010)), olive mill wastewater with solid waste (Fezzani & Ben Cheikh (2008)) and blackwater (Feng *et al.* 2006). The application of ADM1 for the prediction of larger quantities of hydrogen seems to be more problematic (Peiris *et al.* (2005)).

A notable application of ADM1 is found in the Benchmark Simulation Model No 2 (BSM2) (Jeppsson *et al.* (2007)) in which control strategies are tested on a simulated water treatment plant facility comprising a primary and secondary clarifier, a nitrogen removal activated sludge system, an anaerobic digester, a thickener, a dewatering system and a storage system. The implementation of ADM1 is somewhat adapted: pH inhibition is described by continuous functions instead of threshold values, the nitrogen and carbon imbalance is straightened out and the fast evolving hydrogen state is implemented as an algebraic equation rather than a

differential one (Rosen *et al.* (2006)). The imbalance of N, P, and organic in ADM1 is also discussed by De Gracia *et al.* (2006).

Some efforts are made to include dispersion effects in the mixture in a distributed parameter model. Batstone *et al.* (2004a) for instance modeled a biofilm digestion system and Mu *et al.* (2008) an upflow anaerobic sludge bed (UASB) using a 1D discretisation. 2D and 3D discretisations were studied by Picioreanu *et al.* (2005).

Albeit ADM1 is a state-of-the-art model which has been validated in numerous applications, it also serves as a platform for further model elaboration. Some adjustments have been made specifically for certain substrates. Examples are the extensions on the degradation of phenols for olive mill wastes by Fezzani *et al.* 2009) and the inclusion of expressions for ethanol oxidation in winery wastewater, by Batstone *et al.* (2004b). Other extensions are more fundamental. Fedorovich *et al.* (2003) extended the model with sulfate reduction to hydrogen sulfide. Batstone & Keller (2003a) considered precipitation of $CaCO_3$, applicable as a template for other precipitation reactions. Isomeric forms of butyrate and valerate were included by Batstone *et al.* (2003b). Ramirez *et al*. (2009b) discussed the rather simple kinetic first order expression for disintegration and hydrolysis. A Contois-model is used for the disintegration, accompanied with a Hill-function for ammonia inhibition of acetoclastic methanogenes instead of a non-competitive function. Palatsi *et al.* (2010) made some suggestions to overcome the fact that inhibition by VFA is not included in ADM1. Finally, to address to the rather poor applicability of ADM1 in non-methanogenic systems, Penumathsa *et al*. (2008) made the stoichiometry for glucose degradation variable and dependent on the organic acid concentration.

Although large steps are made in the descriptive modeling of anaerobic digestion, a lot of issues remain. For instance the kinetics involving disintegration and hydrolysis are greatly simplified in ADM1 and most follow-up articles by assuming first order kinetics. The kinetic constant is then determined by calibration and acts as a summary of all the complex processes that are involved in those two steps. This approach is recommended by Batstone *et al.* (2002) as the default method and has been applied numerous times. However, Batstone *et al.* (2002) acknowledge that the use of surface-based kinetics gives better results, although they argue that results for first order-kinetics are comparable and are similarly good. This is rather striking as in almost all applications of ADM1 the disintegration and hydrolysis parameter results are considered the most important and subject to calibration by fitting to model to data. The majority of the other parameters are assumed constant to a reference value, given by the literature or by separate research.

Another problem is the development of accurate models for the anaerobic digestion of solid waste. This topic is even more challenging, as some issues arise that are not dealt with in the aforementioned models, mostly concerning the effects of mixing of the reaction mixture. For instance, Vavilin & Angelidaki (2005) have investigated the co-digestion of municipal household solid waste and digested manure in mesophilic conditions. They discovered that in situations where the methanogenic step is rate-limiting, a gentle mixing regime is beneficial for the methane production as in that case spatial methanogenic zones can develop. In case of hydrolysis as rate-limiting, an intense mixing regime leads to the highest degradation.

As already stated in the introduction, caution has to be made on what can be expected from these descriptive models. When properly calibrated, they can be powerful tools for prediction. Especially, since the development of ADM1 and its descendants, the quality of descriptive models has stepped up to a new level. However, the increased descriptive power of the models comes with a price, namely the model complexity. Due to the many chemical, biological and physical effects to be taken into account, the number of parameters included model has increased significantly, e.g. 90 for ADM1 including the initial concentration of biomass. Calibration of ADM1 follows in most cases the following procedure: (*i*) data from an anaerobic experiment are gathered, (*ii*) a few parameters are selected for calibration, mostly concerning the disintegration or hydrolysis; other parameter values are taken from the literature, mostly from Batstone *et al.* (2002), and (*iii*) the selected model parameters are fitted to the data. A problem that arises with this procedure is the issue of identifiability, i.e. is it possible to define a unique set of values to the parameters to obtain the best fit. Due to the large number of parameters and the high model complexity, the answer is probably negative, with large confidence intervals accompanying the parameter values as a consequence. In all, the evolution to more complex models results in a paradoxical situation: the more correct the models are and the better they fit for prediction purposes, the harder it is to uniquely define the parameter values and make precise predictions, i.e. with small confidence intervals.

3. MODELS FOR CONTROL

With the technique of anaerobic digestion fully growing into its maturity and with large-scale plants already built, the development of efficient controllers has become a necessity. However, again due to the "biological factor" the realization of controllers is not as easily performed as in normal process industry since some major issues hamper a straight-forward implementation. Firstly, anaerobic digestion is a highly non-linear process that requires complex models for an adequate description (see above). Finding an appropriate control law for such processes is not easy. One should also realize that not all dynamics behind the process are fully understood, resulting in situations in which the digester will behave in an unexpected manner. A third issue is the feed of the digester. This is mostly some sort of waste and, as a consequence, a constant and non-polluted inflow in the digester cannot always be guaranteed. Another issue is the difficulty of obtaining sufficient and qualitative on-line measurement. This problem is discussed in Section 4. Finally, only a rather limited number of control actions is possible. These are mostly restricted to controlling the dilution rate or adding a

certain substrate to bring the digester into a 'safe-mode'. Because the digestion is performed by microbial processes, caution has to be made that the controllers do not lead to conditions in which the organisms wither or are being washed-out.

Two objectives are distinguished in control strategies for anaerobic digestion: stable operation and maximizing the yield for products such as hydrogen, ethanol, organic acids, or a biogas with sufficient caloric value. Because an anaerobic digestion culture can be rather fragile, until now most research efforts focused on maintaining stable operating conditions.

In general, distinction can be made between model free controllers and model-based controllers.

3.1 Model- free controllers

Model free controllers are controllers which ignore all knowledge on the process, but rather rely on retrieved data. This approach has the advantages that the implementation and accompanying calculations are rather simple. The first and simplest model free controllers are PI or PID controls. These are used to maintain the digester at a certain set point by adding for instance bicarbonate (Marsili-Libelli & Beni (1996)) to preserve the alkalinity, or altering the feed inflow (von Sachs *et al.* (2003)). A more advanced method of maintaining the stability of the reactor is through the use of fuzzy-controllers as described by e.g., Estaben *et al.* (1997). Another interesting approach is to develop an artificial neural network, trained on sufficient amount of data and use this for optimization purposes. Holubar *et al.* (2002) have applied this reasoning on the optimization of methane production. Obviously, the major disadvantage of model free controllers for both stabilization and optimization is the large amount of data they need, both online or offline.

3.2 Model-based controllers

Albeit the descriptive models presented in Section 2 are capable of presenting reasonable predictions on the output, they are not appropriate for control purposes. Due to their complexity they have an arguable identifiability and are hard to calibrate completely. Additionally, due to their complexity, the mathematical implementation is not straight-forward as is the derived automatic controller. As a result, most model based controllers are built on relatively simple models with an important example the two step (acidogenesis-methanogenesis) mass balance model of Bernard *et al.* (2001a). In this fully structurally identifiable model, the uncharted biological complexity is located in dedicated terms, namely the reaction rates. Its general model is of the form

$$d\mathbf{x}/dt = \mathbf{K}\mathbf{r}(\mathbf{x}) - \mathbf{D}\mathbf{x} - \mathbf{Q} + \mathbf{F} \tag{1}$$

with

$$\mathbf{x} = \left[X_1\ X_2\ Z\ S_1\ S_2\ C\right]^T \tag{2}$$

where X_1 and X_2 are the concentrations of the acidogenic and methanogenic biomass, Z the total alkalinity (mmole/L), S_1 (g/L) and S_2 (mmole/L) the amount of organic substrate and volatile fatty acids respectively, C the inorganic carbon (mostly bicarbonate) (mmole/L), **D** the dilution matrix for the components (in case of biofilm reactors the dilution rate of biomass will differ from the dilution rate of other components), **K** the yield matrix, **Q** the gaseous outflow, **F** the liquid feed and **r(x)** the reaction rates. The reaction rates are proportional to the associated biomass and are expressed as Monod and Haldane kinetics for the acidogenic and methanogenic reaction. The flow rates of CO_2 and CH_4 as well as the pH-value are described by algebraic equations.

Although relatively simple, the model performed very well. Due to its simplicity, all parameters are identifiable (although the variability in the kinetic parameters was quite high due to the rough approximations of the biological reactions and changing feed conditions). It was also noticed that steady-state calibrated models, performed adequately in predicting transient behavior.

The model of Bernard *et al*. (2001a) is widely used in model-based controllers, especially by the *Laboratoire de Biotechnologie de l'Environnement LBE-INRA* under the supervision of J.-P. Steyer which is a progenitor of considerable research effort on the subject of control of anaerobic digesters. Steyer *et al.* (2006) have reviewed some of the most interesting research conducted on model-based controllers. For a more detailed description we refer to the respective papers, listed in Table 1.

Table 1. Review on model-based controllers (partially retrieved from Steyer *et al.* (2006)).

Linear model based controllers
Disturbance accommodating control (Harmand *et al*.(2000))
Non parametric adaptive control (Hilgert *et al.* (2000))
Non linear control with constraints handling (Antonelli *et al.* (2003))
Non-linear model based controllers
Adaptive control (Bernard *et al.* (2001b))
Interval based non linear control (Alcaraz-Gonzalez *et al.* (2005))
Robust non linear control (Mailleret *et al.* (2004))
Model predictive control (Aceves-Lara *et al.* (2010))

3.3 Developing more simple models

As already pointed out, the descriptive models described in Section 2 are too complex to apply for control purposes. However, if these models can be simplified while they still remain reasonably good predictors, they can form the basis for successful model-based controls. The reduction in model complexity can be based on knowledge of the process. For instance, some state-variables can be considered constant and can be excluded from the process (steady-state assumption). Also a pseudo-steady-state approximation can be applied to simplify matters. It is in that case assumed that concentrations of components that are rapidly consumed are

essentially constant and approximately equal to zero. If this reasoning of eliminating the fast evolving state variables is continued, the result would be a rate-limiting step model in which the dynamic behavior of the model is described by a single reaction. Because this approach, in most cases, presents no dynamic information on the variables defined in the scope of the control, it is not always desirable.

Bernard *et al.* (2006) and Bernard & Bastin (2005) propose an alternative way for developing simple models. In this approach, it is assumed that the process can be represented by a general mass balance model:

$$d\mathbf{x}/dt = \mathbf{K}\mathbf{r}(t) + \mathbf{v}(t) \quad (3)$$

with $\mathbf{x}=\{x_1, x_2, \ldots x_n\}$ the concentration of the various components inside liquid medium and the term $\mathbf{v}(t)$ representing the net balance between inflows, outflows and dilution effects. The reaction rates are given by the vector $\mathbf{r}(t) = \{r_1(t), r_2(t), \ldots r_p(t)\}$. The matrix $\mathbf{K}$ is the pseudo-coefficient matrix and links together the different components and reactions, and essentially represents the structure of the reaction network. In some cases the reaction network is already determined, i.e. $\mathbf{K}$ is known. In other cases no assumptions are made on the reaction network, i.e. $\mathbf{K}$ is unknown. In both situations, the aim is to obatin a simple model in which a small number of reactions are included that represent the main mass transfer within the process. This is achieved by using data obtained from the process. Consider a matrix U (n x N) obtained from a set of N estimates of $\mathbf{u}(t)$:

$$\mathbf{U} = \left[\mathbf{u}(t_1)\mathbf{u}(t_2)...\mathbf{u}(t_N)\right] \quad (4)$$

These estimates could be data, measured from experimental work or can be "virtual data" generated by an investigated complex process. The number of reactions included in the reduced model is determined by performing a principal component analysis on $\mathbf{U}$. In theory, the number of reactions necessary to reproduce the data set equals the number of non-zero eigenvalues. However, in practice none of the eigenvalues will be zero so the method consists in selecting the *p* first principal axis that explains a total variance in the data larger than a fixed threshold. Note that the technique is only valid if the number of state variables equals or exceeds the rank of $\mathbf{W}$, with $\mathbf{W}$ the matrix containing the reaction rates $\mathbf{w}(t_i)$**:**

$$\mathbf{W} = \left[\mathbf{w}(t_1)\mathbf{w}(t_2)...\mathbf{w}(t_N)\right] \quad (5)$$

Bernard *et al.* (2006) have applied the method both for data from a pilot-scale anaerobic digester and virtual data generated from the ADM1 model. The first set of data led to the identification of 1 reaction that accounts for 82.3% of the variability in the data while the second led to the identification of 1 or 2 reactions, explaining 87.1% and 98.7% respectively. Following the identification of the reaction network, expressions for the reaction rates are proposed.

This approach of a reduced pseudo-stoichiometric matrix is ideal for simplifying a model, while still retaining a large portion of its predictive characteristics. However, care must be taken as the method is also prone to some perturbations as a result of the simplified model (1), measuring noise, numerical implementation and time-alignment of the data. Finally, one must not expect to describe all the variables that were expressed in the full model by the reduced models, This can be circumvented by assuming a fixed ratio in reaction products, albeit this is rather susceptible to errors.

4. SOFT SENSORS

A major problem in modeling and control of anaerobic digestion is the availability of data. For the majority of the components that are described by common models such as ADM1 (Batstone *et al.* (2002)), off-line methods exist. However, these are costly in both money and time. Additionally, some variables that are essential for a realistic description of the system are virtually immeasurable. e.g. biomass determinations. If the model only includes one type of biomass, which could be estimated by, e.g., the turbidity of the sludge, but devices or measurement protocols that can distinguish between different kinds of microbial organisms are practically impossible due to the enormous cost that accompanies them. A common way to calculate the unknown parameters is to consider the initial biomass as a parameter and determine it by calibration on measured data.

Albeit off-line composition measurements are satisfactory for model, calibration and validation, effective control of the digestion process requires on-line measurements. Available methods are gas chromatography, Total Organic Carbon (TOC) analyzers, Titrimetric sensors, UV- and FT-IR-spectrometers to determine alkalinity, TOC, dissolved CO_2 and H_2, VFA-concentrations, acetate, bicarbonate, nitrogen and phosphorus (Steyer *et al*. (2006)). An approach to extend this number of on-line measurements is the use of software sensors, i.e. *softsensors* or *inferential sensors.* Softsensors can be categorized in model-based softsensors and data-based softsensors.

Data-based softsensors apply a black-box approach for estimating the unknown measurements with the most popular techniques being: (i) Principle component regression (PCR) (Martens & Naes (1992)) (ii) Partial least squares (PLS) (Wold *et al.* (2001)), (iii) Artificial neural networks (ANN) (Bishop (1995)), (iv) Neuro-fuzzy systems (Jang & Sun (1995)) and (v) Support Vector Machines (SVM) (Vapnik (1999)). Successful applications of data-based softsensors are found in Holubar *et al.* (2002) (ANN). As for the weaknesses of these softsensors: *Nomen est omen;* data-based softsensors need data for model training. As already pointed out, these data can be costly to acquire or unavailable. In the rest of this section, model-based softsensors are elaborated.

Four types of model-based softsensors are found in current research: (*i*) extended Kalman filters (EKF), (*ii*) Extended Luenberger observers (ELO), (*iii*) adaptive observers, and (*iv*) asymptotic observers (AO).

4.1 Extended Kalman filters

Consider the general continuous non-linear system model (6) describing the state variables **x** of which frequent discrete-time measurements $\mathbf{z_k}$ of the output $\mathbf{y}_k$ are taken.

$$d\mathbf{x}/dt = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t)) + \mathbf{w}(t) \quad (6)$$

$$\mathbf{y}_k = \mathbf{g}(\mathbf{x}_k) + \mathbf{v}_k \quad (7)$$

where **f** the state-transition model, **g** the observation model, *k* the index of discrete time step t_k, **w**(t) the process noise due to the mismatch between the model and the reality and **v** the measurement noise. Column vectors are denoted in bold. Both the process noise as the measurement noise are considered multivariate Gaussian noises with covariances **Q**(t) and $\mathbf{R}_k$ respectively:

$$\mathbf{w}(t) \sim (\mathbf{0}, \mathbf{Q}(t)) \quad (8)$$

$$\mathbf{v}_k \sim (\mathbf{0}, \mathbf{R}_k) \quad (9)$$

In the EKF, the prediction of the unknown state is done by an alternating sequence of a prediction phase and an update phase. In the prediction phase, a first estimate of the states $\hat{\mathbf{x}}$ and its covariance error matrix **P** are made, based on the values of the states in the previous time step.

$$d\hat{\mathbf{x}}^{(1)}/dt = \mathbf{f}(\hat{\mathbf{x}}(t), \mathbf{u}(t)) \quad (10)$$

$$d\mathbf{P}^{(1)}/dt = \mathbf{F}(t)\mathbf{P}(t) + \mathbf{P}(t)\mathbf{F}(t)^T + \mathbf{Q}(t) \quad (11)$$

$$\mathbf{F}(t) = \partial\mathbf{f}/\partial\mathbf{x}_{\hat{\mathbf{x}}(t),\mathbf{u}(t)} \quad (12)$$

In the update phase, the predictions of the states and covariance error matrix on time step *k*, $\hat{\mathbf{x}}_k^{(1)}$ $\mathbf{P}_k^{(1)}$ are corrected by the measurements.

$$\mathbf{K}_k = \mathbf{P}_k^{(1)}\mathbf{G}_k^T(\mathbf{G}_k\mathbf{P}_k^{(1)}\mathbf{G}_k^T + \mathbf{R}_k)^{-1} \quad (13)$$

$$\hat{\mathbf{x}}_k^{(2)} = \hat{\mathbf{x}}_k^{(1)} + \mathbf{K}_k(\mathbf{z}_k - \mathbf{g}(\hat{\mathbf{x}}_k^{(1)})) \quad (14)$$

$$\mathbf{P}_k^{(2)} = (\mathbf{I} - \mathbf{K}_k\mathbf{G}_k)\mathbf{P}_k^{(1)} \quad (15)$$

$$\mathbf{G}_k = \partial\mathbf{g}/\partial\mathbf{x}_{\hat{\mathbf{x}}_k^{(1)}} \quad (16)$$

An application of a Kalman Filter for anaerobic digestion is found in the research of Aubrun *et al.* (2001).

An implementation of an EKF is achieved quite easily, but has some issues concerning the stability of the estimator because of the linearization done in (7) and (11). The proper choice of the initial estimates of the states and the covariance matrix is, for this reason, critical. Another problem is that the linearized model is required to be locally observable. This requirement is rather restrictive in real-life situations and has led to few practical applications of EFK in the field of biotechnological processes (Dochain & Perrier (1998)).

4.2 Extended Luenberger observers

Consider the following non-linear state system model describing the state variables **x** and output **y(t)**.

$$d\mathbf{x}/dt = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \quad (17)$$

$$\mathbf{y}(t) = \mathbf{g}(\mathbf{x}(t)) \quad (18)$$

An ELO is designed, based on the linearization of the output function

$$d\mathbf{x}/dt = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{K}[\mathbf{y}(t) - \mathbf{g}(\hat{\mathbf{x}}(t))] \quad (19)$$

with **K** the gain matrix.

For more information on the ELO, the reader is referred to Zeitz (1987). Mendez-Acosta *et al.* (2010) have applied an ELO as part of a robust control of an anaerobic digester. In this control, the composition of the inflow in the digester is not known, which gives rise to uncertain terms. These uncertainty functions can be dealt with by including augmented state vectors that are estimated with an ELO.

4.3 Adaptive observers

This technique consists of a joint state and parameter estimation:

$$d\hat{\mathbf{x}}/dt = \mathbf{f}(\hat{\mathbf{x}}(t), \mathbf{u}, \hat{\mathbf{k}}) + \mathbf{K}_1(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}(t), \hat{\mathbf{k}}) \quad (20)$$

$$d\hat{\mathbf{k}}/dt = \mathbf{K}_2(\mathbf{M} - \mathbf{g}(\hat{\mathbf{x}}(t), \hat{\mathbf{k}}) \quad (21)$$

with $\mathbf{K_1}$ and $\mathbf{K_2}$ design parameters of the observer which have to be defined in such a way to ensure estimation convergence. The main advantage of an adaptive observer is that it does not require the analytical description of the specific growth rate. This is simply considered as an unknown time-varying parameter. For a full review, we refer to Bastin & Dochain (1990)

4.4 Asymptotic observers

EKF and ELO are both based on a linearized model of the process, the stability and convergence properties are essentially local and valid around an equilibrium point. Another problem of EKF and ELO is that they require a perfect knowledge of the system parameters and the kinetics in particular. This problem is not present for adaptive observers as the parameter values are continuously estimated. However, one may way wish to assign a unique value to the parameter or decouple the state estimation from the parameter estimation. This can be achieved by an asymptotic observer, which can be considered as an intermediate between EKF and ELO on the one side and an adaptive observer on the other. Estimation of the states with AO does not require knowledge of the reaction rates (and their kinetics) and is a global method that does not suffer from instability in convergence due to the linearization around an equilibrium point.

The following subsection is derived from Dochain & Perrier (1998).

Consider a general dynamic model:

$$d\mathbf{x}/dt = -D\mathbf{x} + \mathbf{K}\mathbf{r} + \mathbf{u} - \mathbf{q} \quad (22)$$

with D the dilution rate, **K** (n x m) the yield coefficient matrix, **r** (m x 1) the reaction rate vector, **u (**n x 1) the feed rate vector and **q** (n x 1) the gaseous outflow rate vector. The states $\mathbf{x_a}$ (p x 1) are measured on-line, the states $\mathbf{x_b}$ (n-p x 1) are unmeasured

Consider following assumptions:

- The number of on-line measured components (p) is larger than the number of reactions (m)
- The reaction rate vector **r** is unknown
- The yield coefficient matrix **K** is known.
- The feed rate **F**, the dilution *D* and the gaseous outflow rate **q** are known by measurement or by control.
- The m reactions are irreversible and independent

A state transformation is applied:

$$\mathbf{z} = \mathbf{A}_1\mathbf{x}_a + \mathbf{A}_2\mathbf{x}_b, \quad (23)$$

so that (17) becomes

$$d\mathbf{z}/dt = -D\mathbf{z} + \mathbf{A}_1(\mathbf{u}_a - \mathbf{q}_a) + \mathbf{A}_2(\mathbf{u}_b - \mathbf{q}_b) \quad (24)$$

The equations (23) and (24) form the basis of the derivation of the asymptotic observer: the transformed state z is estimated on-line with (24) followed by a back-transformation according to (23) to retrieve the unknown measurements.

$$d\hat{\mathbf{z}}/dt = -D\hat{\mathbf{z}} + \mathbf{A}_1(\mathbf{u}_a - \mathbf{q}_a) + \mathbf{A}_2(\mathbf{u}_b - \mathbf{q}_b) \quad (25)$$
$$\hat{\mathbf{z}}_2 = \mathbf{A}_2^{-1}\left[\mathbf{z} - \mathbf{A}_1\mathbf{z}_1\right] \quad (26)$$

The most straightforward and most used choice for the state transformation is the following:

$$\mathbf{A}_2 = I_{n-p} \quad (27)$$
$$\mathbf{A}_1 = -\mathbf{K}_2\mathbf{K}_1^{-1} \quad (28)$$

Note that the estimation of **z** is independent of the reaction rate.

5. INCLUDING MICROBIOLOGY?

As already mentioned in the introduction of this paper, the great diversity in microorganisms residing in an anaerobic digester greatly complicates the development of deterministic models. To our knowledge, no models exist that incorporate individual species or genera. However, efforts have been made by Ramirez *et al*. (2009a) to mimic the diversity by expanding each of the 7 microbiological groups in ADM1. Each group is partitioned into subgroup each with slightly different characteristics randomly chosen from a normal bimodal distribution. The prediction results tend to be more realistic in comparison to the original ADM1 which does not distinguish between microorganisms performing the same reaction.

Promising is, however, the rapid development of molecular techniques that monitor the microbial activity and will make studies of the structure of microbial communities economically more viable. Examples of these techniques are polymerase chain reaction (PCR), DNA sequencing of PCR amplified genes, fluorescent *in situ* hybridisation (FISH), DNA stable isotope probing (DNA SIP), temperature and denaturing gradient gel electrophoresis (TGGE and DGGE), terminal restriction fragment length polymorphism (tRFLP), etc. (Justé *et al.* (2008)). These techniques applied on anaerobic digesters provide a deeper insight on the phenomena that occur. A good example is given by Shin *et al.,* (2010) who monitor the shifts in the microbial community in a batch digestion using DGGE and real-time PCR. More specifically, we believe that identification of specific genera and a characterization of the kinetic parameters that define their activity (kinetic constants, yield coefficients) may become possible and will give impetus to more accurate and complex models.

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