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Anaerobic digestion models for control purposes: a short survey

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Abstract
In the literature one can find two important types of models: (i) ADM1-like models, mostly dedicated to knowledge integration to come up with a real virtual anaerobic digestion (AD) process and (ii) simplified models of the AD including a limited number of steps, mostly dedicated to process optimization and control. In this paper, we go through these two types of models by presenting first, a state of the art of the ADM1 in terms of applications and modifications and then some examples of simple models of AD. We claim that the interest of complex ADM1-like models can be relevant only if their emergent properties are analyzed. A way to do so is to study simpler models and to infer what their properties imply to the so-called “complex” models.

Keywords
ADM1; Anaerobic digestion; process control and optimization; synthesis models

INTRODUCTION
The ADM1 developed by [Bat:02] is a generalized model proposed with the aim of integrating the extensive knowledge available at that time about AD process. It presents a number of important specific characteristics with regard to previous proposed models, namely i) the inclusion of disintegration with first order kinetics and ii) the use of COD unit for all components providing this model with the specific possibility of “closing” the mass balance. In addition, the three phases (solid, liquid and gaseous) and the dynamic of pH are modelled. It is claimed by its authors that the initial model proposed in 2002 has to be seen as a general framework and that it is expected to be piecemeal adapted depending on the specific context within which it is being used. Simpler models were proposed with the aims either i) of better understanding a specific step of the process or ii) of being used for control design or optimization purposes. They are either obtained through the reduction of more complex models, by using alternative modelling approaches or still in neglecting some dynamics or in restricting the model to a limited number of reactions steps. In this paper, we claim that parameterizing an ADM1-like model using real data is likely to provide useful information at the condition that model qualitative properties may be extracted from this model. We suggest simple models – which specific links are being to be established with the ADM1 – may provide us with a way of extracting such information.

PART 1: ADM1-like models

THE ADM1 MODEL AND ITS APPLICATIONS
The ADM1 for Anaerobic Digestion Model No. 1 developed by an IWA (International Water Association) task group in 2002 describes, in its basic version, 19 biochemical processes, 3 kinetic processes of gas-liquid transfer and 7 different bacterial populations. This model was widely successfully applied and has proved its usefulness in many works. For instance, in the work of [Gai:12], the authors used the ADM1 to estimate the internal states of AD. They stressed the importance of the optimization of full-scale biogas plant operation to make biomass a competitive source of renewable energy. Furthermore, their developed state estimator that can be implemented online to gain important information concerning the state of the plant. Another example is in the
work of [Bor:13], where the ADM1 was analyzed with respect to the dilution rate and the substrate concentration. This study proved the ADM1 ability to accept up to ten coexisting steady states for the same operational condition and provided important concepts for control improvement. In the same time, the ADM1 can hardly be applied in some particular cases. For example, for fermentation reactions involving carbon substrates with an oxidation state strongly different from biomass, the COD-based approach is not convenient, as stated by [Kle:06]. Furthermore, the authors showed that the total solids concentration in an anaerobic bioreactor treating glucose as a function of the SRT as calculated with ADM1, demonstrates that unrealistic biomass concentrations are achieved at high SRT-values. Another failing reported by [Bat:06], is that the ADM1 stoichiometry focuses on catabolism rather than anabolism, i.e., inorganic carbon can be used unrealistically as a carbon source during some anabolic reactions. In view of the forgoing, it is clear that the ADM1 need to be developed to lead to a new model that will better describe the physicochemical phenomena, the pH, etc, as suggested by [Bat:12].

**MODIFICATIONS/EXTENSIONS OF THE ADM1**

Considering that the ADM1 is not always adapted or sufficient in all cases, some authors proposed some modifications or extensions. In the literature, two other versions of the ADM1 are available: (i) the COST version ([Ros:06]) and (ii) the CEIT (University of Navarra) version for plant-wide modelling (PWM), i.e. ADM1-PWM. In (i), the stoichiometric coefficients, the equations of the degradation of the biomass and the composition of the parameters are adjusted in consequence to balance the COD, C and N, given that the use of the default parameters lead to an unbalance of inorganic C and N which can give bad predictions of the biogas composition. In (ii) six equations of conservation were introduced, to add additional transformations to the process. In BSM2 [Jep:07], the main difference with regard to the original ADM1, is the introduction of continuous inhibition functions for pH to avoid simulation problems related to discontinuities. Concerning the ASM1/ADM1 model interfaces, the original interface in BSM2 has been modified i.e., (i) $X_S$ and biomass fractions are treated differently, (ii) mapping no longer leads to composite material ($X_C$) in ADM1, and (iii) inorganic carbon can be calculated directly. Modifications and extensions have been also brought to the ADM1 to include new knowledge gained since 2002. [Bat:06] stated that the most commonly requested extensions are sulphate reduction, description of the behaviour of phosphorous and mineral precipitation. Other extensions have focused on specific issues. For example, ethanol oxidation was included to simulate the degradation of winery wastewater in an ASBR ([Bat:04]). In [Bat:12], they stressed the need and the fundamental approaches that can help to focus the effort of research groups to develop a physicochemical framework specifically in support of whole-plant process modelling. More recently, [Jim:14], adapted the ADM1 to include the bio accessibility of the substrates. The proposed approach showed a strong application potential for reactor design and advanced control of AD processes. In view of the foregoing, the ADM1 can be considered as a link between different research and engineering fields. However, its qualitative properties such as its equilibrium points, as a function of inputs and parameter values, have still not been established. Because it is important to extract all the information that the ADM1 can include and because it is too complex for being studied with standard analytical tools from mathematics, the development of procedure to systematically obtain simpler models from more complex ones are in this case very important mainly when dealing with controller synthesis.

**PART 2: Simple models**

Alternative simpler descriptions of AD have been proposed over the last 30 years. Clearly limited by computer simulation power before 1980, they are largely preferred by a large engineering community for optimization and control design purposes. The main characteristics of such models are their ability to capture the main input-output causality links of processes under interest. In
addition, their parameters can be identified with known and well characterized confidence. Their relatively simple mathematical formulation (depending on the level of complexity included) is used to test their operation and robustness under different conditions and to synthesize stabilizing - possibly optimal - control laws using systematic synthesis methodologies. In this paper, we restrict our attention to mass-balance-like models that can be used for nonlinear control design. We claim that the systematic study of such reduced models and the search for their links with more complex models like the ADM1 may help us to highlight the main characteristics of such complex models.

EXISTING DESIGN MODELS OF ANAEROBIC DIGESTION
To use anaerobic digestion in industry in avoiding instability that may arise during treatment operation, several simple models can be used. They are characterized by different properties as those summarized in [Bas:90] that present how simple models of CSTR can be used for control design. It was subjected to disturbances that obligate [Mai:04] to use adaptive command to maintain process stability. Analogously, [Bay:13] developed optimal control to a model describing two coupled bioreactors treating micro-algae. In contrast, [Sim:03], considered just the organic substrate and biomass with nonlinear and uncertain parameter for synthesizing CRMFC (Compared Recursive Model Free Controller) in order to optimise biogas production, when for the same purpose ([Ang:07]) use the previous model with addition of temperature variable for controlling leachate influent by a feedback linear control combined to an on-line estimator.

By side of simple one stage models described above, there are simple models with two or three stages. They include in general organic substrate, VFA, acidogenic and methanogenic bacteria like in [Ant:03] or [Bas:83]. They were exposed to noises and had uncertain parameters respectively. In these two cases, a robust and an adaptive control were applied for optimising bioreactor yield. Likewise, another simple model was proposed by [Pet:08], this time after the reduction of tenth order anaerobic digestion model. This model includes as substrates glucose, acetate, inorganic carbon dynamics and was used to design an adaptive control to maintain pollution at low level. A three-step model was proposed by [Mar:96], including both the hydrolysis, acidogenesis and methanogenesis steps. It considers the organic substrate, the VFA, carbon dioxide and its partial pressure, in order to study the behaviour of the process, during overload.

In view of previous detailed description, it is obvious that control models are only interested in methanogenesis phase (first step model), and in some cases, this final phase can be accompanied by acidogenesis (two steps model) for analysis of process inhibition. However, what is often underestimated is the role of these models in the understanding of more complex models dynamics. Indeed, the manipulation of certain parameters during control allows us i) to deduce the behavior of component and then its important or negligible effect on AD and ii) to govern the level of inhibition. Also, if we see their synthetic structure in another way, we conclude the dominant effect of acidogenesis and methanogenesis step commonly used, and so, we could classify the component of digestion by their level of influence and justify some phenomenological knowledge of complicated models. Moreover, the introduction of another component to simpler models can be a helpful way to understand, predict and deduce ADM1 behavior in the presence of new dynamics.

SIMPLE MODEL FOR OPTIMIZATION
Even if the ADM1 was widely used in the literature, very little is known about it from its mathematical property point of view. A way to extract some knowledge could be to reduce the ADM1 and to analyse the reduced models obtained. This is a delicate task since after the reduction, it is expected to obtain reduced models maintaining the physical meaning of the variables and keeping the sensitivity of the states with regard to some parameters. However, besides the qualitative properties, one must ensure that the quantitative properties are preserved in the reduced models. This can be made by studying in what extent the properties of simple models (cf.
can have a sense in view of the ADM1’s knowledge. Moreover, another approach can be adopted, based on adding a new dynamics to simple models as in [Wee:12]. Otherwise, borrowing digital tools can be a key to finding a synthetic mathematical structure of a new model based on ADM1 simulation. That was used by [Bo:13], who indent the MatCont software to synthesize model accounting the possible inhibitory factors. The forgoing and other models are listed in Table 3.

Table 3. Simple models

<table>
<thead>
<tr>
<th>Author</th>
<th>Reference model</th>
<th>Variable introduced</th>
<th>Objective of the study</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Ben:13a]</td>
<td>AM2</td>
<td>SMP</td>
<td>Modelling the SMP in MBR</td>
</tr>
<tr>
<td>[Wee:12]</td>
<td>AM2</td>
<td>Heavy metals</td>
<td>Effect of toxic substance</td>
</tr>
<tr>
<td>[Bo:13]</td>
<td>ADM1</td>
<td>-</td>
<td>Define washout inlet concentration</td>
</tr>
<tr>
<td>[Kre:88]</td>
<td>Chemostat</td>
<td>-</td>
<td>Describe biodigester bi-stability with an organic influent toxicity</td>
</tr>
</tbody>
</table>

These models can be used to solve some anaerobic digestion problems that remain open, including those related to the control and the state observation. Thus, it can help to develop a new model by slightly modifying existing models according to the search field or by synthesizing a simple mathematical model with an understandable structure from a practical point of view. This will allow us to avoid anaerobic digestion instabilities and optimize the biological pathways and/or biogas.

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