Assessment of Characterization Procedures for the Implementation of Anaerobic Digestion Model No.1

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Abstract

In this paper, comparison were made among the characterization processes, designed for influent characterization in Anaerobic Digestion Model No.1 (ADM1) to choose one of the best available. The two procedures chosen are elemental analysis and conversion of Activated sludge Model (ASM) output to ADM1 input variables (ASM2ADM interface) given by John B. Copp, 2003. The Matlab code for elemental analysis was developed to facilitate computation and a c-file of the ASM2ADM interface was provided by the department of Industrial Electrical Engineering and Automation, Lund University Sweden. Both of these methods have been used in the collection of wastewater data from various locations and the demand for chemical oxygen (COD) after separation compared to experimental results. In almost all cases total fractionated COD from ASM2ADM interface was approximately equal to experimental COD. While as fractionation by elemental analysis shows variation from experimental value. Linear curve fitting was done between experimental COD and fractionated COD to check their equivalency. The elemental analysis method has lower value of coefficient of determination ($R^2=0.5468$) than ASM2ADM interface ($R^2=0.9453$). Based on the model requirements, it was concluded that ASM2ADM interface is the best option for influent characterization. Apart from obtaining good correlation with experimental COD, it provides all input variables for implementation of ADM1. While elemental analysis provide fewer fractionation and hence assumption of other input variables is must leading to deviation from actual model features. Features of both methods are also discussed in the paper.

Keywords: Anaerobic Digestion, ADM1, Characterization, Elemental Analysis, ASM2ADM interface

1. Introduction

Anaerobic digestion is the process of converting organic matter into a gas mixture mainly composed of methane and carbon dioxide by the combined action of the bacterial community. The process is usually used for solid pollutant and wastewater management, but the process is also used as a source of energy due to methane production. The energy requirements of a digester facility can be measured by using the gas produced in the power plant and thus minimizing the environmental damage resulting from the release of methane into the atmosphere. Optimization of methane production in anaerobic digestion will lead increase in power generation assets and hence improvement in economy of digestion facilities. This can be achieved by using mathematical models. One can predict process factors such as methane production rate, substrate utilization rate, pollution levels etc. It also helps to avoid process situations that could lead to digester instability and subsequent failure. Basic models are a complex that describes the anaerobic digestive process developed over the past forty years. The previous models were much simpler and assumed of a step-by-step measurement [1]. However, the growing need to use this process as an alternative energy source requires the development of more complex models to understand and control the process. Also, advances in computer technology have encouraged the development of dynamic process models, by providing them support to simulate the effects of changing...
environmental conditions on complex biological treatment systems [9]. Anaerobic Digestion Model No. 1 (ADM1), developed by the IWA Task Group for Mathematical Modeling on Anaerobic Digestion, is one of the most sophisticated and complex model involving 19 biochemical processes and two types of physiochemical processes [2]. Whereas earlier models like Activated Sludge Model require very little wastewater characterization but the ADM1 demands a vast input characterization including the concentrations of soluble and particulate carbohydrates, protein, lipids, as well as individual volatile fatty acids (VFAs). It is impossible to have all these parameters on a regular basis. The main limitations usually are the laboratory facilities required for the measurement of these parameters which are not often available. Still, ADM1 is developed in such a way that the output quality strongly depends on the influent characteristics. So development of characterization procedures was a prerequisite of the situation. Since ADM1 was published, many methods have been developed to this end. One of them is Elemental analysis, developed by Kleerebezem and Van Loosdrecht in 2006 is based on biochemical fractionation of influent into proteins, lipids, carbohydrates and Volatile Fatty Acid. This kind of method uses quite simple concepts of mass balances and charge balances to split COD into fractions [3]. Another method is based on conversion of another model output into ADM1 input state variables developed by Copp et al. in 2003 [4]. In this case, the characterization data come from the output of ASM-type models. Model interfaces have been developed to convert ASM-type outputs into ADM1 inputs. This paper assesses the adequacy and accuracy of above two methods to be used as a characterization procedure for the implementation of ADM1. The two methods were applied to experimental data of wastewater from different locations and the resultant chemical oxygen demand (COD) after fractionation was compared with the experimental results. This gives us an idea of choosing the best one among the two and hence decreases the deviation from actual ADM1 hypothesis. The methods are discussed in detail with their limitations.

2. Material and Methods

2.1. Sample Analysis

Samples of water used for the above purpose are collected at various locations. Twelve samples were analyzed. Samples are analyzed according to standard procedures [5]. Fatty acids were determined according to the procedure discussed by Ripley et.al [6]. The results were represented by units as required by the elemental analysis method and the interface of ASM to ADM1[9].

2.2. Elemental Analysis

In this method the waste characterization of Chemical Oxygen Demand (COD), Total Organic Carbon (TOC), Organic Nitrogen (Norg) and Alkalinity (Alk), which contain bicarbonate Alkalinity (AlkIC) and fatty acids (AlkVFA) can be derived after collecting field data. The complete composition of the substrate can be obtained from the limited set of measurements required for the use of ADM1. This is done using the oxidation state of the organic carbon expressed in the COD-TOC-ratio, the formation of amino acids made by proteins in wastewater and the initial concentration of inorganic carbon, fatty acids and cations as obtained from the alkalinity measurement. First of all the elemental composition of influent is calculated by obtaining a standard chemical formula in the form of CxHyOzN-III u v. The stoichiometric coefficients calculated for one C-mole substrate or x are equal to one. The N coefficient is calculated from the Norg and TOC measurement ratio. The protein fraction is obtained from the assumption that it is the only product which contains nitrogen. The fraction of LIP can be calculated by comparing their oxidation state with other organic substrates. The total oxidation state of the wastewater sample can be based on the COD / TOC ratio, and then measured with the oxidation effect of the individual chemicals that give the following components. Equations calculating the coefficients and
fractions are presented below. [3] The MATLAB code of the above method was developed to ease the calculation of the fractions [9].

2.3 ASM2ADM Interface

In both ASM1 and ADM1 models the organic state variables are represented by total COD (COD_T) and the total Kjeldhal Nitrogen (TKN) represents organic nitrogen compounds including ammonia. Increasing Xc (composites) Sa (amino acids), Si (soluble inert COD) and Xi (particulate inert COD) with respect to the available incoming nitrogen and COD is basic idea supporting the interface. The state variables that are merely carbon (without nitrogenous fraction) and solely nitrogen (without carbon) are used to close the balances when necessary. This interface assumes Sus (monosaccharides), Xch (carbohydrates) and Xli (lipids) are used as the carbonaceous degrees of freedom and similarly, Sin (inorganic nitrogen) is used as the nitrogenous degree of freedom as it has no associated carbon. Mass and charge balances guide the interfacing from ASM1 variables to ADM1 [4]. The Matlab program used for this interface was provided by Industrial Electrical Engineering and Automation department, Lund University Sweden. Results and Discussion:

3. Results

The analyzed results were changed into the required units. Details used as input into the MATLAB program for the elemental analysis method [9]. The output include the stoichiometric coefficients for empirical formula and fractions of carbohydrates, lipids, proteins and volatile fatty acids (VFA). The equations for deriving the substrate composition are in the form of C-molar fractions of the substrates, but the standard ADM1 model requires COD-based substrate concentration definition. So the conversion from fractions to COD-equivalent concentration was done. As an example of carbohydrates is given here [3]: CODCHO \[ \text{gO}_2 \text{dm}^{-3} \] = TOC \cdot \eta_{\text{CHO}} \cdot Y_{\text{CHO}} \cdot 4 \cdot M_{\text{WO}_2} Where 4 represents the number of electrons that are accepted per mole oxygen, and MWO2 is the molecular weight of oxygen. Experimental COD of all samples was plotted against respective total COD after fractionation shown in Figure 1. The coefficient of determination R^2 was very low (0.75) as shown in figure 2. The variation with the experimental results may be due to the diverse wastewater composition and the assumptions which are very rarely true in actual conditions. The method assumes model lipid composed of one glycol molecule and three n-palmitic acid side chains, which may not be true in every case. Also overall oxidation state is derived from the VFA concentration assuming acetate as main VFA and hence other fatty acids like palmitic acid and butyric acid is ignored. And overall there may be error in experimental results which can be corrected by increasing number of trials on same sample. Same experimental results were converted to ASM1 input variables described by Henze et.al. [7]. The resultant COD after fractionation is plotted against experimental COD in figure 3. There was a variation between experimental and interface COD values. Coefficient of determination for this also comes out to be quite high (R^2=0.965) as shown in figure 4.
4. Conclusion

From the point of view of the complex state of ADM1, a characterization process is needed [9]. Among these two procedures, ASM2ADM interface is best option for its equivalency with experimental results. Moreover it provides all input variables for ADM1 which one has to assume many of them, if elemental analysis is opted. The interface can also be used for benchmarking of activated sludge wastewater treatment plants where it can be used before anaerobic digester [7].

![Fig. 1. Variation of COD values from Elemental Analysis Method and Experimental Data.](image-url)
Fig. 2. Validation of COD values from Elemental Analysis Method and Experimental Data

Fig. 3. Variation of COD values from Experiments and ASM2ADM Interface
Fig. 4. Validation of COD values from Experiments and ASM2ADM Interface

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