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Review

A review of modeling approaches in activated sludge systems

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The feasibility of using models to understand processes, predict and/or simulate, control, monitor and optimize WasteWater Treatment Plants (WWTPs) has been explored by a number of researchers. Mathematical modeling provides a powerful tool for design, operational assistance, forecast future behavior and control. A good model not only elucidates a better understanding of the complicated biological and chemical fundamentals but is also essential for process design, process start-up, dynamics predictions, process control and process optimization. This paper reviews developments and the application of different modeling approaches to wastewater treatment plants, especially activated sludge systems and processes therein in the last decade. In addition, we present an opinion on the wider wastewater treatment related research issues that need to be addressed through modeling.

Key words: Mathematical modeling, water, wastewater, wastewater treatment plants, activated sludge systems.

INTRODUCTION

Activated sludge systems encompass biodegradation and sedimentation processes which take place in the aeration and sedimentation tanks, respectively. The performance of the activated sludge process is, however, to a large extent dictated by the ability of the sedimentation tank to separate and concentrate the biomass from the treated effluent. Since the effluent from the secondary clarifier is most often not treated any further, a good separation in the settler is critical for the whole plant to meet the effluent standards. Mathematical models are increasingly being deployed to understand complex interactions and dynamics in the activated sludge system. As such a mathematical model can be defined as the mathematical representation of a real-life phenomenon or process. It is built for a specific reason, with a specific aim in mind, which could be:

(i) To increase insight into physical processes;
(ii) To estimate non measurable quantities;
(iii) To predict future events, or
(iv) To control a process.

In industrial practice, most knowledge is available in the form of heuristic rules gained from experience with various production processes, while crisp mechanistic descriptions in the form of mathematical models are available only for some parts or aspects of the processes under consideration. A good model not only elucidates a better understanding of the complicated biological fundamentals but is also essential for process design (Oles and Wilderer, 1991; Daigger and Nalosco, 1995), process start-up (Finnson, 1993), dynamics predictions (Novotny et al., 1990; Capodaglio et al., 1991; Cote et al., 1995; Marsili-Libelli and Giovannini, 1997; Premier et al., 1999; El-Din and Smith, 2001), process control (Lukasse et al., 1998) and process optimization (Lesouef et al., 1992). This paper reviews developments and the application of different modeling approaches to wastewater treatment plants especially activated sludge systems and processes therein in the last decade. In addition, we present an opinion on the wider wastewater treatment related

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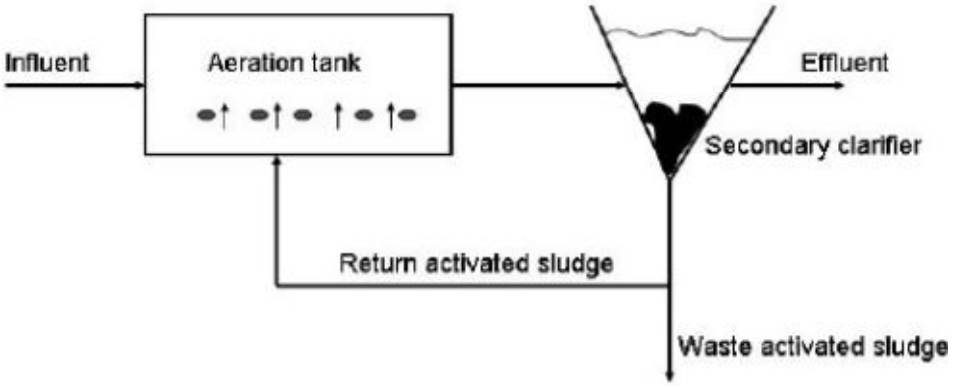


Figure 1. Archetypal flow scheme of a conventional activated sludge plant.

research issues that need to be addressed through modeling.

DEVELOPMENT OF THE ACTIVATED SLUDGE PROCESS

Although it is not the intention of this paper to present a chronology of the developments of activated sludge systems, some important 'milestones' on the subject will be highlighted. For more about the history and developments of activated sludge systems, readers are invited to consult reviews (Alleman, 1983; Albertson, 1987; Alleman and Prakasam, 1983; Casey et al., 1995). In order to understand the impact that the activated sludge process had on wastewater treatment technology, one must first appreciate the relative infancy of the 'sanitation engineering' which existed in the developed world during the mid-to late- 1800's. Lacking any means of collecting wastewaters, at that time, the convenient solution was either one of direct discharge from chamber pots to streets or, for those more affluent homes, to rely on fill-and-draw systems where the wastewater was aerated.

In England, the experiments with wastewater aeration did not provide expected results until May, 1914 when Ardern and Lockett introduced a re-use of the 'suspension' formed during the aeration period; hence paving a way for continuous-flow systems (Metcalf and Eddy, 1979; Alleman, 1983). The suspension, known as 'activated sludge' was in fact an active biomass responsible for improvement of treatment efficiency and process intensity. As it is known now, the activated sludge system is a unique biotechnological process which consists of an aerated suspension of mixed bacterial cultures which carries out the biological conversion of the contaminants in wastewater. At this point in time, the activated sludge process has proven itself to be a durable technology in an era where most engineering methods lapse into obsolescence only decades, if not years, after their original development. The process' supremacy to this day is supported by not only its flexibility and robustness but also its capability to fulfill the most stringent effluent criteria, if bad operating strategies or poorly designed clarifiers are avoided.

A typical activated sludge process configuration as depicted in Figure 1, encompasses biodegradation and sedimentation processes which take place in the aeration and sedimentation tanks, respectively. The aeration tank, while having many possible configurations, basically retains well mixed aerated wastewater for a number of hours (or days) thereby providing an environment for biological conversion of dissolved and colloidal organic compounds into stabilized, low-energy compounds and new cells of biomass. This biodegradation is performed by a much diversified group of microorganisms in the presence of oxygen. The influent wastewater provides the basic food source for the microorganisms in the aeration tank. If the removal of nutrients that is nitrogen and phosphorus components is contemplated, anoxic and anaerobic zones must be provided in addition to the aerated zones.

APPLICATION OF MODELING TECHNIQUES IN UNDERSTANDING COMPLEX WASTEWATER TREATMENT SYSTEMS

Process control modeling

Three decades ago, it was shown that coexistence of two species, competing for one substrate, is generically not possible for Monod- and Haldane-type kinetics (Aris and Humphrey, 1977). Monod-type kinetics is defined by Equation (1).

$$\mu = \mu_{max} \frac{Cs}{Cs + Ks} \qquad (1)$$

with μ equal to the specific growth rate, μ_{max} equal to the

maximum specific growth rate, C_s the substrate concentration and K_s the affinity constant.

Essentially, filamentous microorganisms are slow growing microorganisms that can be characterized as having maximum growth rates (μ_{max}) and affinity constants (K_s) lower than the floc-forming bacteria. The μ_{max} is directly proportional to the maximum substrate uptake rate (q_s^{max}) times the yield of biomass on substrate ($Y_{X/S}^{max}$). Since substrate uptake rate (q_s) can be directly assessed from the experiments, this characteristic is preferred. The actual substrate uptake rate depends on the substrate concentration as shown in Equation (2).

$$q_s = q_s^{max} \cdot \frac{C_s}{C_s + K_s} \quad (2)$$

By performing an extensive stability analysis, the authors proved that the dilution rate and the substrate feed concentration determine which species will wash out. Models for the growth of one, two and multiple species were analyzed on one or multiple substrates (Smouse, 1980). He showed with a rigorous stability analysis that, the coexistence of multiple species is only possible if there are as much growth-limiting substrates as there are different species. This confirms the earlier work of Taylor and Williams (1975). The first bulking sludge mathematical model incorporating simultaneous diffusion of soluble organic substrate and Dissolved Oxygen (DO) through flocs with predetermined shape was developed by Lau et al. (1984). Parameters such as bulk liquid soluble organic substrate and DO concentration and floc shapes and sizes were used to predict the volume-averaged growth rate of filamentous bacteria (*Sphaerotilus natans*) and non-filamentous bacteria (*Citrobacter sp.*). The kinetic parameters, which were experimentally measured, had values according to the kinetic selection theory. The results of this model cannot be extrapolated because either the kinetic parameters do not apply to other filamentous or non-filamentous bacteria (Seviour and Blackall, 1999), or the representativeness of the model microorganisms in activated sludge systems can be questioned. In spite of these limitations, the model illustrates some aspects that may match reality.

Furthermore, the study warned that the one-dimensional (unidirectional) growth of filamentous bacteria might lead to a floc geometry that is better for substrate diffusion. The Activated Sludge model No.1 (ASM1: [Henze et al., 1987]) can be considered as the reference model, since this model triggered the general acceptance of Wastewater Treatment Plant (WWTP) modeling, first in the research community and later in industry (Gernaey et al., 2004). The model also aims at yielding a good description of the sludge production. Chemical Oxygen Demand (COD) was adopted as the measure of the concentration of organic matter. Many of the basic concepts of ASM1 are adapted from the activated sludge model defined by Dold and colleagues (Dold et al., 1980). Even today, the ASM1 model is in many cases still the state of the art for modeling activated sludge systems (Dircks et al., 2001; Roeleveld and van Loosdrecht, 2002). An alternative modeling strategy for the simplification of the ASM1 that yields computationally efficient models with reasonable prediction capabilities have been described (Anderson et al., 2000). Copp (Copp, 2002) reports on experiences with ASM1 implementations on different software platforms. For a full description of the ASM1 model, as well as a detailed explanation on the matrix format used to represent activated sludge models, the original publication (Henze et al., 1987) should be consulted.

In 1995, an updated version (ASM2) was introduced to incorporate biological phosphorous removal (Henze et al., 1995). The ASM2 publication points out that, this model allows description of bio-P processes, but does not yet include all observed phenomena. In 1999, further revisions were presented by building on the ASM2 model to introduce the ASM2d model (Henze et al., 1999). A model developed at Delft University of Technology, TUDP (van Veldhuizen et al., 1999; Brdjanovic et al., 2000) combines the metabolic model for denitrifying and non-denitrifying bio-P of (Murnleitner et al., 1997) with the ASM1 model (autotrophic and heterotrophic reactions). Contrary to ASM2/ASM2d, the TUDP model fully considers the metabolism of phosphorus accumulating organisms and models all organic storage components explicitly (Gernaey et al., 2004). The TUDP model was validated in enriched bio-P sequencing batch reactor (SBR) laboratory systems over a range of sludge retention time (SRT) values (Smolders et al., 1995), for different anaerobic and aerobic phase lengths (Kuba et al., 1997), and for oxygen and nitrate as electron acceptor (Murnleitner et al., 1997).

Another version of ASM1 called the ASM3 model (Gujer et al., 1999) has also been introduced which corrects a number of known defects present in the original model. A common trait among the versions of these models is that each is high-dimensional and possesses a large number of kinetic and stoichiometric parameters. For example, ASM3 comprises 12 process rate equations involving 7 dissolved and 6 particulate components, 21 kinetics parameters, and 13 stoichiometric and composition parameters. Though this level of model complexity is necessary to describe and relate dynamics over a wide range of operating conditions, it can present a significant computational burden for performing simulations and analysis and calibration is hard (Vanrolleghem et al., 1999).

Process dynamic modeling

Traditional time series analysis models have been applied to the wastewater treatment plants (Berthouex and Box, 1996; Geselbracht et al., 1988; Oles and Wilderer, 1991; Capodaglio et al., 1991; Banadda et al.,

2005). Beyond this, literature survey indicates that a number of authors (Beun et al., 2000; Pandit and Wu, 1983; Smets et al., 2006; Van Dongen and Geuens, 1998) have postulated that, in most cases time series analysis is an ideal tool to identify models of dynamic systems such as activated sludge. Actually, time series models can be developed from input and output monitoring data, in contrast to common deterministic dynamic mathematical models which require knowledge of a large number of coefficients.

Linear regression analysis, the statistical methodology for predicting values of model outputs from a collection of model inputs values is used to exemplify the static approach. Linear models have a simple structure, which makes them easily learnable, and also enables them to be easily extended and generalized. Linear models take weighted sums of known values to produce a value of an unknown quantity. In general, a linear regression model to vector u and vector y is a function p of the form (Equation 3).

$$p(u) = C_1 u^n + C_2 u^{n-1} + \cdots + C_n \quad (3)$$

with n the model order, d = n+1 the number of model parameters and C_1, C_2, ⋯ , C_n the model parameters determined by solving a system of simultaneous linear equations.

The persistence of the filamentous bulking problem coupled with the need for an easy to use predictive tool has led to a number of researchers (Banadda et al., 2004; Banadda et al., 2005; Novotny et al., 1990; Capodaglio et al., 1991; Sotomayor et al., 2001; Sotomayor and Garcia, 2002a; Sotomayor and Garcia, 2002b; Smets et al., 2006) to turn to time series models. Artificial Neural Networks ANNs have been applied in capturing the non-linear relationship that exists between variables in complex systems (Capodaglio et al., 1991; Pu and Hung, 1995; Zhao et al., 1999). Other modeling techniques such as hybrid modeling offer possible avenues for creating simplified representation of complicated systems such as activated sludge. Also modeling approach, individual-based modeling (IbM) was developed and implemented for biofilm systems (Kreft et al., 1998; Kreft et al., 2001; Picioreanu et al., 2003; Picioreanu et al., 2004). IbM allows individual variability and treats bacterial cells as single units.

Furthermore, the IbM approach can make a distinction between spreading mechanisms adopted by different bacteria (Picioreanu et al., 2003). Ward and colleagues (Ward et al., 1996) combined the Activated Sludge Model No.1 (Henze et al., 1987) with time series models to establish a hybrid model of the activated sludge process and to enable prediction of suspended solids in the effluent. Authors (Zhao et al., 1999) compared the Activated Sludge Model No.2 (Henze et al., 1995) with a simplified model and a neural net model, while researchers (Pu and Hung, 1995) established a neural network model for a trickling filter plant.

In (Grijspeerdt et al., 1995) both steady state and dynamic properties of the examined models are compared. It was found that the Tak'acs model (Tak´acs et al., 1991) is the most reliable. Statistical modeling methods form another framework in which the black-box approach is used for monitoring wastewater settleability as reported in (Capodaglio et al., 1991; da Motta et al., 2002). However, researchers (Naghdy and Helliwell, 1989) point out that, univariate statistical modeling can be used to characterize properties of time series data but only for short-term forecasting and control. One of the disadvantages of a univariate monitoring scheme is that for a single process, many variables may be monitored and even controlled. This disadvantage has been overcome by multivariate statistical modeling, where more variables are monitored simultaneously and later on incorporated to improve the applicability for forecasting and control (Marsili-Libelli and Giovannini, 1997; Van Dongen and Geuens, 1998; Eriksson et al., 2001).

In another development, multivariate statistical modeling tools such as Principal Component Analysis (PCA) has been exploited in monitoring settleability in lab-scale set-ups (Amaral and Ferreira, 2005) and in many industrial applications for process monitoring, fault detection and isolation (Gregersen and Jorgensen, 1999). Also, researchers (Miyanaga et al., 2000) adopted a multivariate statistical modeling tool, namely Partial Least Squares (PLS), to predict the deterioration of sludge sedimentation properties, and indicated that it was usually able to predict deterioration of sludge sedimentation properties 2 to 4 days in advance. Generally, multivariate statistical models are able to cope with the following:

(i) Noisy data sets;
(ii) Missing data in the data sets;
(iii) Correlated variables within the data sets;
(iv) Data sets with many variables and a small number of observations and
(v) Data sets with many observations and a small number of variables.

In brief, PCA utilizes directly the information from the data, compacted in the form of a covariance matrix, to extract more relevant information and to generate new variables known as principal components. Researchers (Pan et al., 2004) proposed to use a combination of PCA with a subspace identification method to obtain a model, that describes the period-to-period multivariate behavior of all the samples collected during each period of time in a WWTP. In their works, (Van Niekerk et al., 1988) developed a mathematical model to predict the behavior of floc-forming and filamentous bacteria under carbon-limited conditions in low F/M activated sludge. A biokinetic model which includes a floc-forming and three common filamentous microorganisms (*S. natans*, *Type 021N*, *Type 0961*) was proposed (Kappeler and Gujer,

1992). With this competitive model, which accords with a variety of experimental observations, different bulking phenomena were explained. Researchers (Gujer and Kappeler, 1992) introduced a similar model, a biokinetic model, which allows the prediction of the development of floc-forming, filamentous and Nocardia type microorganisms in aerobic activated sludge systems with a variety of different flow schemes and operating conditions.

Also, researchers (Kappeler and Gujer, 1994a) proposed a mathematical model which describes the behavior of facultative aerobic floc-forming, obligate aerobic filamentous and nitrifying microorganisms in the case of aerobic bulking. This model is verified by experiments in a full-scale and pilot-scale plant (Kappeler and Gujer, 1994b). Authors (Kappeler and Brodmann, 1995) formulated a mathematical simulation model for low Food to Microbe (F/M) bulking among other problems encountered in activated sludge systems. To date, most of the work in black-box modeling has been aimed at static model types. Researchers (Capodaglio et al., 1991) developed predictive models namely, time series analysis (as a function of F/M) and artificial neural networks (models inputs: Biological Oxygen Demand/Nitrogen (BOD/N), Nitrogen/Phosphorus (N/P), DO, Temperature (T), F/M) to model filamentous bulking sludge volume index.

The neural network models employed by researchers (Oles and Wilderer, 1991) analyzed the levels of sludge bulking organisms using the F/M, the BOD load, the N and P, BOD/P ratio, DO, temperature and sludge age as inputs. Authors (Mujunen et al., 1998) used Partial Least Squares (PLS) Regression models to predict deterioration of sludge sedimentation properties as a function of process parameters, namely, soluble N, soluble P, DO, BOD, pH, temperature, and indicated that the PLS model was usually able to predict deterioration of sludge sedimentation properties 2 to 4 days in advance. PCA/PLS analysis relies on static models, which assume that the activated sludge process operates at a predefined steady-state condition. This is often not the case as the process undergoes changes, which results in dynamic process variables (Treasure et al., 2004). However, researchers (Amaral and Ferreira, 2005) sought relationships between biomass parameters including filamentous bulking scenarios and operating parameters, such as the Total Suspended Solids (TSS) and SVI by exploiting another static multivariate statistical technique: PLS regression.

Biomass morphology based modeling

Later studies took into account both the micromorphology of the floc and the oriented growth characteristics of the filamentous bacteria (Tak´acs and Fleit, 1995). This study was the first attempt to combine the morphological characteristics with the physiology of filamentous and non-filamentous bacteria. However, similar to Lau and co-workers (Lau et al., 1984), researchers Tak´acs and Fleit (1995) attributed different kinetic parameters to the two different bacterial morphotypes (filaments and floc-formers). Some authors proposed a mathematical model based on the kinetic selection and filamentous backbone theory (Sezgin et al., 1978; Cenens et al., 2000a; Cenens et al., 2000b; Cenens et al., 2002a) that predicts the coexistence of both Food to Microbe ratio and floc-forming bacteria for a wide range of dilution rates; this model considers that FMs are incorporated to the flocs decreasing its concentration.

Similarly, authors (Cenens et al., 2002a) demonstrated that the coexistence of filamentous and floc forming bacteria for a single substrate growing in a continuous stirred tank reactor (CSTR) or in CSTR with an ideal settler and biomass recycling is generically not possible. Other factors (that is, storage and decay rates) were later added to model the competition (Liao et al., 2004). Over the past two decades, biosensor technology has evolved rapidly; however, the benefits of its application are still to be realized in preventing filamentous bulking episodes. Lack of biosensor reliability and more importantly the financial consequences of sensor failure in its widest sense have served to maintain the prevalence of off-line sample analysis for bioprocess monitoring and supervision (Spinosa, 2001). A potential solution to this problem is to develop model-based sensors exploiting Image Analysis Information (IAI) for on-line estimation rather than reliance on off-line and time-consuming measurements to provide fast inferences of variables during the off-line analysis intervals (Novotny et al., 1990; Capodaglio et al., 1991). IA has indeed received special attention from many researchers in all kind of applications due to the decrease in the price/quality ratio of the IA systems (Russ, 1990; Glasbey and Horgan, 1995). Figure 2 depicts the principle of image analysis in wastewater treatment process control. The commonly used shape parameters used in monitoring wastewater systems are:

1. The Form Factor (FF) is particularly sensitive to the roughness of the boundaries. It is defined by the ratio of the object area to the area of a circle with a perimeter equal to that of the object (Equation 4). A circle has an FF value equal to one, for irregular shapes the value becomes much smaller: $0 < FF \leq 1$.

$$FF = 4\pi \frac{area}{perimeter^2} \quad (4)$$

2. The Aspect Ratio (AR) is mainly influenced by the elongation of an object. It encompasses the ratio of the measured object length to its breadth (Equation 5). It varies between 1 and infinity. A circle has an AR value equal to one, the more extended an object is, the larger is the perimeter value implying: $1 \leq AR < \infty$.

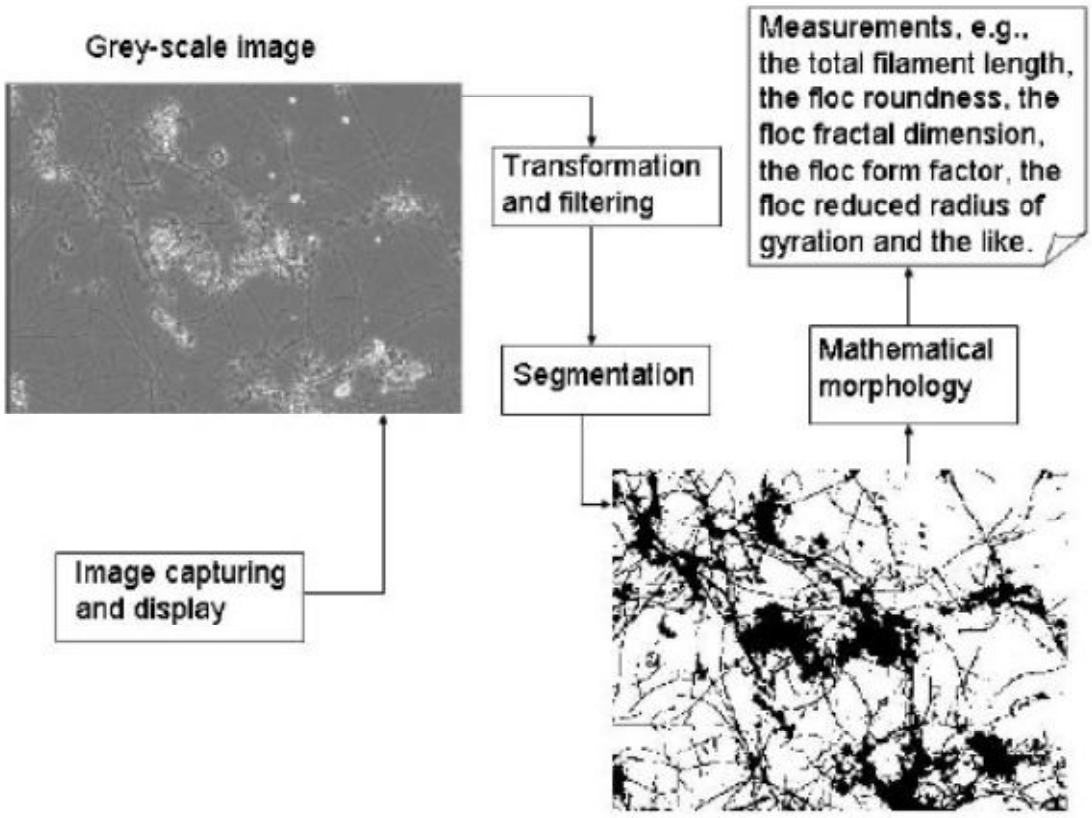


Figure 2. Principle of image analysis.

$$AR = 1 + \frac{4.(length - width)}{\Pi.width} \quad (5)$$

3. The Roundness (R) is also mainly influenced by the elongation of an object. It is a ratio of the object area to the area of a circle, with a diameter equal to the object length (Equation 6). It varies between 0 and 1. A circle has an R value equal to one, for irregular shapes the values become much smaller: 0 < R ≤1.

$$R = \frac{4.area}{\pi.length^2} \quad (6)$$

Besides the size based shape descriptors that measure the deviation from a circle, another set of shape parameters deals with how convex the object is. This can be described based on either the perimeter or the area.

4. The Convexity (C) is the ratio of the perimeter of the convex object to the net (exterior) perimeter of the object (Equation 7). This parameter is one for an object that has no concavities or indentations around its periphery, for all other objects it is smaller: 0 < C ≤1.

$$C = \frac{convex\ perimeter}{perimeter} \quad (7)$$

5. The Solidity (S) is the ratio of the (net) object area to the convex area (Equation 8), and again this descriptor is one if the object is fully convex, so that: 0 < S ≤ 1.

$$S = \frac{area}{convex\ area} \quad (8)$$

The Reduced radius of Gyration (RG) is also influenced by the elongation of an object. It is actually the average distance between the object pixels and its centroid. It is determined by dividing this average distance by half of the equivalent circle diameter (D_{eq}) (Equation 9). A more elongated floc will have a larger RG. A circle has an RG value equal to $\frac{\sqrt{8}}{2}$ as such: $\frac{\sqrt{8}}{2} \leq RG < \infty$.

$$RG = \frac{\sqrt{M_{2x} + M_{2y}}}{\frac{D_{eq}}{2}} \quad (9)$$

M_{2x} and M_{2y} are second order moments. Research contributions of interest on IA applications on filamentous bulking phenomena are due and promising, among others (Li and Ganczarczyk, 1990; Albertson, 1991; Pons et al., 1993; Drouin et al., 1997; Grijspeerdt and Verstraete, 1997; Mauss et al., 1997; Condron et al., 1999; Miyanaga et al., 2000; da Motta et al., 2000, 2001;

Cenens et al., 2002a; Heine et al., 2002; Jenn´e et al., 2002, 2003; Jin et al., 2003; Jenn´e et al., 2004; Banadda et al., 2004a, b, c; Smets et al., 2006; Jenn´e et al., 2006, 2007). Promising research contributions on IA applications in the context of filamentous bulking are discussed (Debelak and Sims, 1981; Grijspeerdt and Verstraete, 1997; Pons and Vivier, 2000; da Motta et al., 2000, 2001; Heine et al., 2002; Jenn´e et al., 2003; Contreras et al., 2004; Jenn´e et al., 2004a, b).

Interested readers are invited to read more about other IA applications, that span from quantifying different bacterial properties in both suspended and immobilized pure cultures (Pons et al., 1993; Drouin et al., 1997; Mauss et al., 1997; Condron et al., 1999), studying competition between filamentous and non-filamentous bacteria (Contreras et al., 2004), quantifying pigments in vegetal cells (Miyanaga et al., 2000) to enumerating marine viruses in various types of sample (Cheng et al., 1999) among others. There has been an attempt to utilize biomass parameters generated by IA techniques (input data) into various forms of models with an objective of predicting settling characteristics. da Motta and coworkers (da Motta et al., 2002) have proposed static models that exploit IA, in order to detect altered operation conditions or threatening or existing operation problems at an early phase. Available literature (Jenn´e, 2004; Gins et al., 2005), indicates the application of a static Multivariate Statistical (MVS) method, Principal Component Analysis (PCA), to monitor settleability in lab-scale setups.

Secondary clarifier modeling

Modeling of secondary clarifiers is treated by Ekama et al. (1997) which include a description of the Vesilind model (Vesilind, 1968) for hindered sludge settling velocity. Researchers (Hartel and Popel, 1992) re-parameterized the original Vesilind model to include the dependency of Sludge Volume Index on the settling velocity. Authors (Dupont and Dahl, 1995) suggested a model that is adequate for both free and hindered settling. Comparison of different one-dimensional sedimentation models is carried out by researchers (Grijspeerdt et al., 1995) and (Koehne et al., 1995).

MODELING APPROACHES

Many different classifications have been produced for the different model types which are available (Murthy et al., 1990). It is possible to distinguish mathematical models based on the philosophy of the approach and with regard to the mathematical form of the model (at times also depending on the application area of the model). The following sections deal with some of the common philosophies in the modeling of WWTPs.

Mechanistic models

Historically, mechanistic models describe the mechanisms behind the coupling of variables and may consequently, be used for almost any operating condition. The idea is that, a realistic description of the system can be obtained by identifying and describing all the physical, chemical and biological laws that govern the system concerned. Due to the large number of parameters, it is, however, often impossible to estimate the parameters uniquely from available measurements. Probably one of the most recognized mechanistic model is the Activated Sludge model No.1 (ASM1: Henze et al., 1987) as it triggered the general acceptance of WWTP modeling, first in the research community and later on also in industry (Gernaey et al., 2004). ASM1 was primarily developed for municipal activated sludge WWTPs to describe the removal of organic carbon compounds and nitrogen, with simultaneous consumption of oxygen and nitrate as electron acceptors. The model furthermore aims at providing a good description of the sludge production. Chemical Oxygen Demand (COD) is adopted as the measure of the concentration of organic matter. Many of the basic concepts of ASM1 are adapted from the activated sludge model defined by researchers (Dold et al., 1980).

Even today, the ASM1 model is in many cases still the state of the art for modeling activated sludge systems (Roeleveld and van Loosdrecht, 2002). Copp (2002) reported on experiences with ASM1 implementations on different software platforms. For a full description of the ASM1 model, as well as a detailed explanation of the matrix format used to represent activated sludge models, the original publication (Henze *et al.*, 1987) should be consulted. In 1995, an updated version (ASM2) was introduced to incorporate biological phosphorous removal (Henze et al., 1995). The ASM2 publication points out that, this model allows description of bio-P processes, but does not yet include all observed phenomena. In 1999, further revisions were presented by building on the ASM2 model to introduce the ASM2d model (Henze et al., 1999). A model developed at Delft University of Technology, (TUDP) (Vanrolleghem et al., 1999; Brdjanovic et al., 2000) combines the metabolic model for denitrifying and non-denitrifying bio-P (Muhirwa et al., 2010) with the ASM1 model (autotrophic and heterotrophic reactions). Contrary to ASM2/ASM2d, the TUDP model fully considers the metabolism of phosphorus accumulating organisms, modeling all organic storage components explicitly (Gernaey et al., 2004). The TUDP model was validated in enriched bio-P Sequencing Batch Reactor (SBR) laboratory systems over a range of Sludge Retention Time (SRT) values (Smolders et al., 1995), for different anaerobic and aerobic phase lengths (Kuba et al., 1997), and for oxygen and nitrate as electron acceptor (Murnleitner et al., 1997). Another version of ASM1 called the ASM3 model (Gujer et al., 1999) has also been

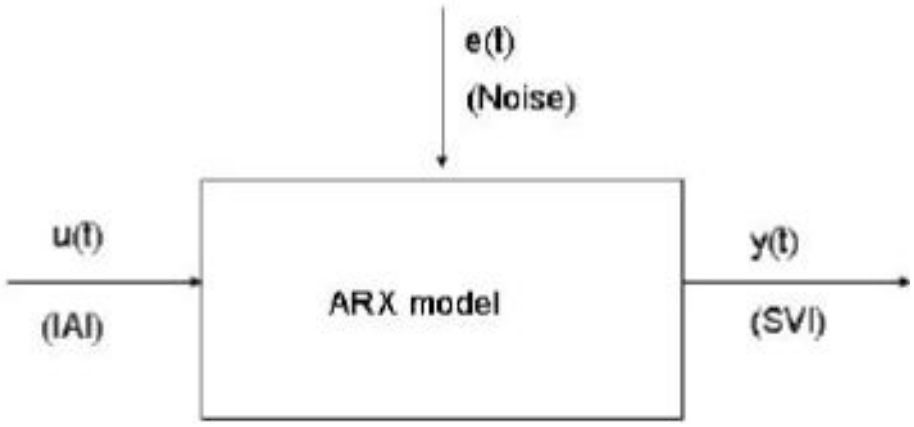


Figure 3. ARX model prototype for modeling settleability dynamics.

introduced which corrects a number of known defects present in the original model. A common trait among the versions of these models is that each is high-dimensional and possesses a large number of kinetic and stoichiometric parameters (Smets, 2002; Vanrolleghem et al., 1999). However, the complexity of the activated sludge processes casts doubt on a number of mechanistic modeling approaches.

Black-box models

On the other extreme, black-box models (Ljung, 1995; Sjoberg et al., 1995; Ljung 1999) have been proposed when analytical equations are unavailable or difficult to develop. These models are developed following a data-based approach. The objective is to describe the input-output relations by equations that do not reflect physical, chemical or biological considerations. Examples of black-box models are Auto Regressive (AR), Auto Regressive Moving Average (ARMA), AR with eXternal input (ARX), ARMA with eXternal input (ARMAX), Box-Jenkins and state space models (Box and Jenkins, 1976; Box et al., 1994; Ljung, 1995, 1999). The basic input-output configuration (ARX model structure) is shown in Figure 3. Basically, ARX models as shown in Equation (10) relate the current output y(t) to a finite number of past outputs y(t – k) and inputs u(t – k).

$$y(t) + a_1y(t-1) + (\cdots) + a_{na}y(t-na) = b_1u(t-nk) + b_2u(t-nk-1) + (\cdots) + b_{nb}u(t-nk-nb+1) + e(t) \quad (10)$$

with y(t) equal to the output response at discrete time t, u(t) the input at discrete time t, na the number of poles, nb the number of zeros, nk the pure time-delay (the dead-time) in the system and e(t) a white noise signal. ai and bj are model parameters, with i = 1 ... na and j = 1 ... nb. The model structure is entirely defined by the three integers na, nb, and nk.

These models are mostly formulated in discrete time, that is, the dynamics of the phenomena concerned are described by difference equations. As the models do not incorporate any prior knowledge, the parameters have to be estimated. Also, because of the high degree of nonlinearity of activated sludge processes and extending a basic linear modeling scheme to take all possibilities, it may not be a realistic proposition. A more realistic way of tackling this is to employ a black-box modeling framework that caters for these nonlinearities. Examples of nonlinear black-box type of models include Artificial Neural networks (ANNs), Nonlinear AR with eXternal input (NARX) and Nonlinear ARMA with eXternal input (NARMAX).

Standard MultiVariate Statistical (MVS) methods such as Principal Component Analysis (PCA) and Partial Least Squares (PLS) have been used in many industrial applications for process monitoring, fault detection and isolation (Gregersen and Jorgensen, 1999). A number of attempts have been made to implement MVS modeling methodologies on WWTPs. Several applications are focusing on predictions of quality parameters of the WWTP influent or effluent. Eriksson et al. (2001) applied MVS methods to predict the influent COD load to a newsprint mill WWTP. Advanced MVS tools, such as adaptive PCA and multi-scale PCA, have been used for WWTP monitoring by Rosen and Lennox, 2001; Russ, 1990.

On the other hand, motivated by the population dynamism characteristic of activated sludge, a number of researchers (Box and Jenkins, 1976; Pandit and Wu, 1983; Novotny et al., 1990; Capodaglio et al., 1992; Berthouex and Box, 1996; Sotomayor and Garcia, 2001, 2002a, b; Van Dongen and Geuens, 1998; Banadda, 2006; Nkurunziza et al., 2009; Banadda et al., 2009; Muhirwa et al., 2010) have proposed dynamic black-box models (such as ARX, ARMA, ARMAX, Box-Jenkins, discrete state space models) to describe a number of

process parameters including, Mixed Liquor Suspended Solids (MLSS), effluent flow rate, effluent total suspended solids (TSS), effluent BOD, effluent COD, carbon removal, Sludge Volume Index (SVI) just to name but a few. Researchers (Berthouex et al., 1976, 1978) modeled effluent BOD data of a full-scale plant using the influent BOD as explanatory variable.

They found the correlation between influent and effluent BOD to be insignificant. Debelak and Sims (1981) arrived at a similar conclusion for influent and effluent COD data from a full-scale plant. Novotny et al. (1990) developed both ARMA time series model and neural network models. The ARMA models proposed are for the MLSS concentration derived partly from causal relationships, with influent Biological Oxygen Demand (BOD) and suspended solids as explanatory variables. They can be made consistent and identical in concept with mechanistic mass balance models (avoid a pure black-box approach) but are restricted to linear(ized) processes. In addition, the model structure must be known beforehand. Capodaglio et al. (1992) presented and discussed both univariate and multivariate ARMAX applications to WWTP modeling, and the results are compared to those of conventional mechanistic models. The independent variables are rainfall, flow to the clarifiers, BOD load and F/M ratio. The observed variables are the influent flow, primary clarifiers' effluent suspended solids concentration, MLSS concentration, SVI and recycle suspended solids concentration. Belanche et al. (1999) availed black-box models characterizing the time variation of outgoing variables in WWTP via a soft computing technique, in particular, by experimenting with fuzzy heterogeneous time-delay neural networks. The models inputs considered are the influent flow rate, return sludge flow rate, waste sludge flow rate, influent COD and Total Suspended Solids, while the model outputs are effluent BOD and COD. Researchers (Sotomayor, 2001) identified a Linear Time-Invariant dynamical model (LTI) of activated sludge process based on simulation data obtained by combining the ASM1 model and the Tak'acs settler model.

Grey-box models

In practice, models are often a mixture of mechanistic and black box models, that is the so called grey-box modeling. Grey-box models are based on the most important physical, chemical and biological relations and with stochastic terms to count in uncertainties in model formulation as well as in observations. The objective is to have physically interpretable parameters that are possible to estimate by means of statistical methods.

In other words, the advantages of mechanistic and black-box modeling can be combined in such a modeling scheme. Alternative modeling strategies for the complexity reduction of ASM1 that yield computationally efficient models with reasonable prediction capabilities have been described (Anderson et al., 2000; Smets, 2002). Ward et al. (1996) combined the Activated Sludge Model No.1 (Henze et al., 1987) with time series models to establish a hybrid model of the activated sludge process and to enable prediction of suspended solids in the effluent. Zhao et al. (1999) compared the Activated Sludge Model No.2 (Henze et al., 1995) with a simplified model and a neural net model.

POTENTIAL APPLICATION OF MODELING TOOLS

The future of wastewater treatment modeling, especially activated sludge modeling is not limited to the following issues:

1. Maximum uptake capacities of different plant species in wetlands;
2. Maximum nutrient uptake capacities of wetlands;
3. Distribution of microbial cells and microbial activity in WWTPs;
4. Correlation of microbial dynamics in activated sludge modeling to socio-economic indicators;
5. Settleability and separation of microbial cells from effluents;
6. Understanding the chemical breakdown in industrial WWTPs especially activated sludge systems;
7. Pollutant reduction and attenuation in receiving waters after wastewater treatment effluent discharge.

CONCLUSION

In this paper, the general activated sludge process was introduced and discussed. A general overview of the mathematical approaches (ranging from white over grey to black-box) in the context of activated sludge modeling was presented and discussed. The distinct developments in modeling wastewater treatment process(es) were presented. It can be concluded that most of the previous modeling efforts have focused on municipal wastewater systems; although such models can be adapted to industrial wastewater systems.

On one hand, most of the modeling attempts that seek to use black box models have little practical relevance to process control practitioners. On the other hand, white box models require a good knowledge of system dynamics which are very difficult to predict in complex systems like activated sludge. Grey-box models seem to address the pitfalls of black and white box models.

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