

DIFFERENTIAL OR MATRIX: THE ACTIVATED SLUDGE MODELLING DILLEMA

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ABSTRACT: Activated sludge models are present in the theory and practice of wastewater treatment for over 50 years in consistent numbers, and none seems to be the perfect solution for plant operators. The existing models can be divided into two large categories, named differential and matrix models, based on their particular structure, a new terminology that we hope will prove useful. The two categories are compared from several points of view (complexity, limitations and restrictions, practical use, connectivity with complementary systems), in order to emphasize the strong points and the weak points of each category, providing information for the practical use in wastewater treatment plants.

1. INTRODUCTION

Since McKinney's 1962 model, over 15 different mathematical approaches trying to describe the functions and functionality of the activated sludge system are documented (Ognean and Vaicum, 1987, Henze et al., 2000).

The first attempts were made by individual researchers (mostly engineers), and the results are simple differential equations describing the mass fluxes of the system. The large majority of the models constructed in the 60's and 70's were based on a few theoretical assumptions, which we called "conceptual equations": the most important are the organic matter balance (*substrate accumulation = material entering the system – material removed from the system – material consumed in reaction*) and the bacterial – or, more correct, the activated sludge – balance (*bacterial mass accumulation = synthesized bacterial mass – endogenous consumption of bacterial mass – bacterial mass removed from the system*). The way researchers defined mathematically the terms of these conceptual equations assured the originality of the model. Some of those models were developed fractionally over several years, and the model was never published as a whole.

Because of technical difficulties encountered by plant operators, The International Association on Water Pollution Research and Control (IAWPRC) formed in 1982 a scientific structure called Task Group on Mathematical Modeling for Design and Operation of Activated Sludge Processes (referred as Task Group in this paper), which was gathering engineers, biochemists, biomathematicians from around the world, with the purpose of generating a coherent model for activated sludge systems. Their work resulted in a series of model surnamed "state-of-art", thought to resolve the problems in the field.

2. THE MODELS

We can divide existing activated sludge models into two separate categories: a) models prior to the formation of IAWPRC's Task Group, and b) the "state-of-art" models, developed by the Task Group.

Early models are usually formed of two or three mass balance differential equations, along with derivations based on stationary states, providing formulas for volumes of the aeration tank, hydraulic retention times, activated sludge fractions used for recirculation, etc. The equations are based on

conceptual equations identical or very similar to the ones described before. Such models were developed, among others, by McKinney (1962), Lawrence and McCarty (1970), Eckenfelder (1971), Goodman and Engle (1974), Grau et al. (1975), Gaudy (Ramanathan and Gaudy, 1971; Gaudy and Srinivasaraghavan, 1974; Srinivasaraghavan and Gaudy, 1975; Gaudy and Kincannon, 1977), Christoulas and Tebbut (1976) or Jones (1978).

The "state-of-art" models or ASMs (Activated Sludge Models, as named by the Task Group) are much more complex mathematical structures, represented as a matrix with components on columns and processes on rows. As components, the Task Group defined metabolic fractions of the community and substances from the influent, and as processes, biochemical reactions and results of the temporary evolution of the community. Four such models were created, chronologically encoded ASM No.1 (Henze et al., 1986; 1987), No.2 (Gujer et al., 1995), No. 2d (Henze et al., 1999) and No. 3 (Gujer et al., 1999).

3. DISCUSSIONS

3.1. A simple terminology

The two groups of models are relatively homogenous and can be treated as two separate entities. The problem comes from the lack of a coherent terminology when referring to the two categories: if "state-of-art" is used to define Task Group's models, the early models are usually treated separately; even more, the term "state-of-art" does not refer to a mathematical platform, but more to a scientific brand of the Task Group.

Since the early models are based solely on data from differential equations, they are, in fact, differential models of the wastewater treatment process and will be referred as *differential models* in this paper.

"State-of-art" models are based on a matrix of components versus processes, so they can be called *matrix models*, in order to maintain the structural approach used before.

Once divided and given names, the two categories will be evaluated in order to point out strengths and weaknesses, possibilities of improvement and practical applicability.

3.2. Number of components and structural complexity

Differential models were mostly constructed from separate equations, and the decomposition in separate elements is a little difficult. However, each model contains, mainly, two important equations: organic substance and activated sludge mass balances, each with three, respectively four main components (Ognean and Vaicum, 1987). We have, consequently, seven components for each linear model.

Some of those components, especially the ones related to the masses extracted from the systems, may contain up to four mathematical elements. The longest organic mass balance expression (Eckenfelder, 1971) consists of seven such elements, while the longest activated sludge mass balance expression (Gaudy, 1971-1975) consists of six elements. In other words, considering the two main equations, the most complex differential model – the one developed by Gaudy – may be extended to 11 mathematical components.

Matrix models are by far more complex. ASM no.1 has eight different process equations and 13 components, some of them containing two mathematical expressions, while in ASM no. 2 and ASM no. 2d the numbers increased to 21 processes and 20 components (Henze, 2000). Process rates containing switching functions add to the complexity of the model. Although a process does not contain all the system components in its equation, the process rate can largely increase the complexity of this equation: ten such equations were extracted from the ASM no. 1 model by Jeppsson (1996), the most convincing one being the one of ammonia concentration variation, with 13 components involved and a very large amount of mathematical elements if expanded:

$$\frac{dS_{NH}}{dt} = [-i_{XB} * \mu_H * \frac{S_s}{K_s + S_s} * (\frac{S_O}{K_{O,H} + S_O} + \eta_s * \frac{K_{O,H}}{K_{O,H} + S_O} * \frac{S_{NO}}{K_{NO} + S_{NO}}) + k_s * S_{ND}] * X_{B,H} - \mu_A * (i_{XB} + \frac{1}{Y_a}) * \frac{S_{NH}}{K_{NH} + S_{NH}} * \frac{S_O}{K_{O,A} + S_O} * X_{BA} \quad [1]$$

Considering that ASM no. 2 has process rates with six or seven switching functions (unlike the maximum four of ASM no. 1) and almost twice as many components, the differential equations resulting from its decomposition will probably have close to one hundred mathematical elements. Such equations are difficult to manage and are the main reason of the matrix structure of the ASMs, creating the illusion of a much simpler model (Jeppsson, 1996). However, the comparison between Jeppsson's view on ASM equations and the two much more simple ones from Gaudy's Model (the one with the highest structural complexity from linear models) gives us an idea about the much higher structural complexity of "state-of-art" models.

Differential models can also be transcribed as matrices similar to ASMs (Table 1), but, obviously, with a lower structural complexity, proving that the matrix form is more a method of comprising large amounts of data in a small space than a revolutionary model and that the matrix models are more of an evolution of differential models, based on the increase of parameters included in the model.

Table 1. Gaudy's Model on a matrix structure.

Process	Component	I	E	C	B	Process rate
1	Organic substrate growth	$-Q*(C_0 + r*C)$	$-Q*(1+r)*C$	$-\frac{1}{Y} * \mu_m * \frac{C*X}{K_s + C} * V$		$\frac{1}{V}$
2	Activated sludge growth	$Q*X_0$	$-Q*(1+r)*X$	$-b*V*X$	$r*Q*X_r + \mu_m * \frac{C*X}{K_s + C} * V$	$\frac{1}{V}$
<i>Q</i> – influent discharge <i>q</i> – recycled sludge volume <i>C₀</i> – influent organic matter <i>C</i> – aeration tank organic matter <i>Y</i> – activated sludge production rate <i>X₀</i> – influent microorganisms density <i>X</i> – aeration tank microorganisms density <i>V</i> – aeration tank volume <i>r</i> – sludge recycle ratio <i>μ_m</i> – activated sludge growth rate <i>K_s</i> – substrate saturation constant		Influent contribution M^*T^{-1}	Effluent loss M^*T^{-1}	Consumption M^*T^{-1}	Biochemical reactions M^*T^{-1}	L^3

3.3. Mathematical flexibility and restrictions

Differential models are, in the larger part, independent activities of researchers or research groups. Therefore, each model has its unique or at least original approach of the original conceptual equations, the only stable term of the modelling effort of the 60's and the 70's. Those unique approaches provided sufficient information for the latter modelling developments, such as ASMs, now the main conceptual current in the field. In other words, the ASMs are using a large amount of information selected and filtered from the differential models. Those models are different conceptually, even if some equation terms or conceptual equations are similar. Some are describing only first order kinetics, other are comprising 0 order kinetics, some are based on first order delayed kinetics (Ognean and Vaicum, 1987), each one producing important information for future modelers and for plant operators.

As for the ASMs, there are four in use at this moment, as described above, but there are no basic differences between the models: we have a different number of components, we have different formulas describing the relations between the components, but the model is based on the same experimental design and has the same basic rules. We can detect a structure that is different and more complex than the one from differential models, but common to all the ASMs, which are, from this angle, different variations of the same model, and not different models.

Even for such complex and attentively tested models as ASMs are, limitations are occurring. Some were eliminated gradually as the models evolved for No. 1 to No. 3 (e.g. the need for correction factors or the necessity of certain quantities of organic nutrients), but, even so, the latest model has its own limitations, the most important ones being related to the need of a neutral pH and an eight to 23°C temperature range, or its errors when confronted with a very high organic load (Henze et al., 2000).

In this area, the limitations of the differential models are far more complex. For example, even the simplicity of the models can be a problem, because they cannot reveal some functioning aspects of the system, increasing the probability of errors. Even more, the models treat organic matter as a homogenous component, ignoring wastewater characterization, situation to be detailed further on. For that reason, the models do not take into consideration variables like toxic or inhibitory loads or high non biodegradable concentrations of the organic load. Designed to help constructing or improving existing wastewater plants, they provide information about volumes, therefore forcing the plant operator to restrict the size and quality of the influent inside the calculated data, or needing supplementary installations to deal with the increase of the medium organic load or of the medium wastewater volume.

3.4. Degree and possibility of error

Differential models are often the result of several years of tryouts from a researcher or even a group of researchers, and the final result may consist of fragments from different papers put together. From that reason, some parts of the models are not described in detail, some terms of different equations, although referring to the same element, are constructed differently (Oprean and Olosutean, 2011), or some formulas are not completely derived: for example, the formula provided by Gaudy for volume calculation can be reduced significantly with the use of simple mathematical operations:

$$V = \frac{Y * Q * [C_0 - (1+r) * C] + r * X_r * Q}{b * X} - \frac{(1+r) * Q}{b} \quad [2]$$

$$V = \frac{Y * Q * [C_0 - (1+r) * C] + r * X_r * Q - (1+r) * X * Q}{b * X} \quad [3]$$

$$V = \frac{Q * [Y * C_0 - (1+r) * Y * C + r * X_r - (1+r) * X]}{b * X} \quad [4]$$

$$V = \frac{Q * [Y * C_0 + r * X_r - (1+r) * (Y * C + X)]}{b * X} \quad [5]$$

Although several scientists were working at the ASMs and the Task Group's composition changed throughout its activity, the effort was much more coherent, and each model was presented as a final product, not as smaller pieces. From that point of view, matrix models are free of conceptual errors, but their high complexity makes them a good candidate for calibration errors, easily avoidable when working with the much simpler differential models.

3.5. Calibration

The first models were designed to explain the mass balances from the activated sludge systems, in order to construct a proper volume aeration tank and to maintain inputs and outputs inside certain limits; therefore no specific calibration was necessary. The system was created with data from the model and was controlled from the inputs (mainly from the influent's volume and organic matter concentration). Neither of the modelers considered particular environmental conditions of a certain area and all systems were treated as uniform. The parameters of the models were mostly obtained empirically and only few of them (such as activated sludge growth rate or substrate saturation constant) were experimentally calculated or estimated as average values from existing data. The big picture looks a little unorganized and all additional data that will be necessary is to be obtained empirically.

The ASMs, on the other hand, are highly organized models. The system is not created starting from the model, therefore the model is the same for all wastewater treatment plants. Aeration tank volume is a variable of the model, not a solution, and it can be easily changed throughout the station's evolution, with a simple recalibration. The model is clearly establishing which parameters are to be assumed from existing data (those with constant or near constant values for any given conditions) and which ones are to be evaluated (calculated, obtained empirically or experimentally). Since we are talking of a much larger number of parameters, the ASMs need a larger number of experimental and numerical analysis to be made in order to be calibrated (Fig. 1), requesting a proportional quantity of equipment, personnel and time, in order to do that.

3.6. Relations with Artificial Intelligence

Expert systems (Paraskevas, 1999; Baeza, 2000), fuzzy systems (Huong et al., 1994; Puñal et al., 2001; Cakmakci, 2007) and artificial neural networks (Choi et al., 2000; Lee, 2000; Popa et al., 2000; Gadkar et al., 2003, 2005) are some of the Artificial Intelligence (AI) environments used for operation and control of wastewater treatment plants. They can use empirical information, specific to the conditions they control, or information calculated from mathematical models (even though they might not need all the information stored in the model).

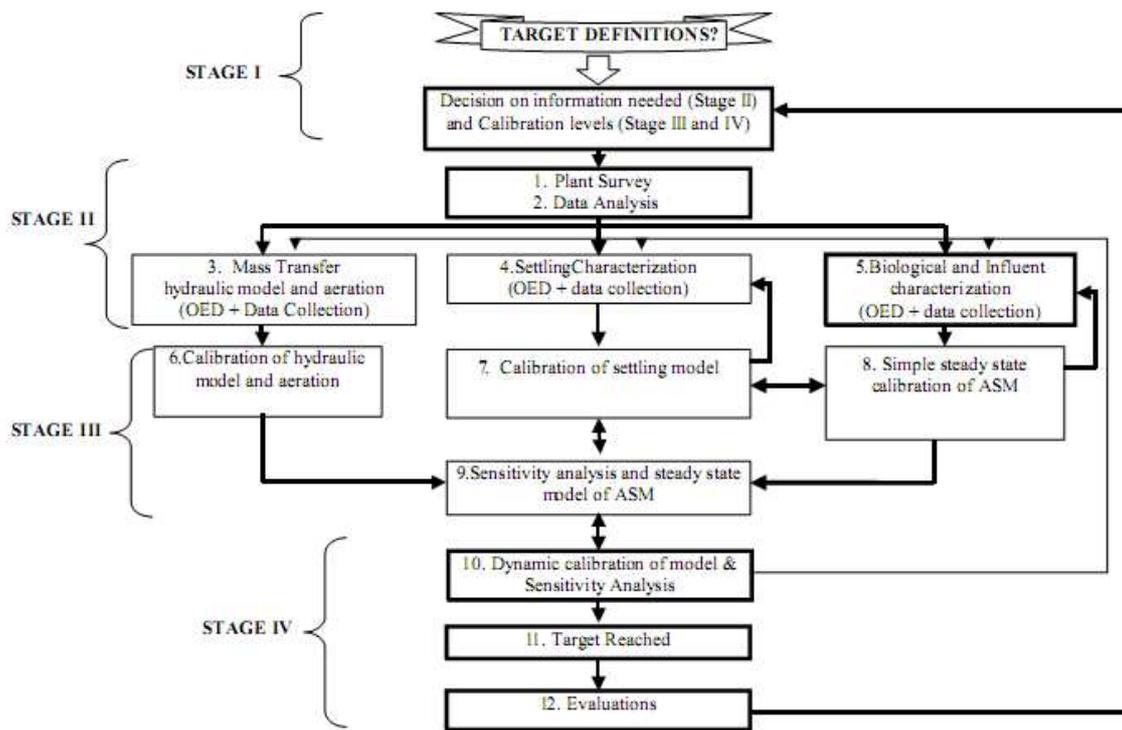


Figure 1. Calibration algorithm for ASM No. 2d (after Vanrolleghem et al., 2003).

For the last situation, data from the ASMs is definitely more suitable, not necessarily because of their complexity, but more because of their lower limitations (e.g. the system can react at the change of influent volume using data from both differential models and ASMs, but only the latter provide data regarding the biodegradability of the organic matter from the influent). The switching functions included in ASMs are easily adaptable to any AI system and are the most important feature that recommends those models as AI data suppliers.

3.7. Implementation in computer software and specialized personnel necessity

An important problem was related to the practical application of the models: their need for software assistance and for specialized personnel. Differential models were designed, as a primary goal, to provide dimensioning data for future installations, hence their final formulas referring to volumes, hydraulic retention times or sludge recirculation ratios.

Therefore, following the variation of some station parameters was everything the station's operators needed to do, in order to maintain the system between certain limits, usually by modifying oxygen input or the hydraulic retention time. No complicated software or specific training was required, and operation was a low qualification job with the differential models.

The development of "state-of-art" models completely changed the picture. The complexity of the models, starting with the first one, opened the discussion about their implementation, and the need for software assistance and specialized personnel. The first software environment used for ASM simulations was the widely used SSSP (Bistrup and Grady, 1988), shortly after ASM no. 1. Its main quality was free accessibility, hence its wide use for computer simulations. Alongside SSSP, other simulation environments, like ASIM, EFOR or GSP-X, were

used in station operation even before the development of ASM no. 2 (E.P.A., 1993).

More recently, other software were especially designed as control environments for wastewater plants, based on different ASM versions, the most notorious being WEST++ (Vangheluwe et al., 1998) and the WATER series, designed by the U.S. E.P.A. (2001) – the program reaches the third version of its ninth edition (WATER9 v. 3.0), proving the wide use and application success. Other software, designed for different applications or for a wider scientific use, are transformed or adapted for the use in wastewater treatment, such as G.U.I. (Graphical User Interface) (Sorour, 2003) or BIOWIN (Envirosim Associates, 2003), confirming the necessity for a software assisted operation if based on "state-of-art" models.

Specific software requires trained operators, capable of understanding and operating the systems. Even more, the complicated calibration of ASM based plants pose the need for special laboratory personnel and for qualified technicians. In other words, the ASM based station represented the transition from the low qualification operation to a highly specialized, advanced operation, where the system variation is controlled and maintained between standardized limits.

3.8. Wastewater characterization

The concept of wastewater characterization was introduced by Sollfrank and Gujer (1991), thus being completely ignored by the differential models, all constructed prior to that date. It is a major drawback for those models, which considered the entire mass of organic matter (expressed as COD, the most common method of estimation) as uniform and decomposable at the same rate. Sollfrank and Gujer's ideas are standing at the base of the state-of-art models: splitting the organic compounds into soluble and insoluble (the latter having a completely different evolution inside the treatment system) and, even more, splitting

each of the mentioned categories into biodegradable and inert (or almost inert, in the case of slowly biodegradable material). It is a different approach, because we are now having at least four categories, and their proportion from the estimated organic mass will determine the values of some of the model's most important parameters, like the biomass growth or the organic load of the effluent.

3.9. Practical applications and applicability

At first glance, ASMs look like the proper tool for the wastewater plant operator: they provide information about the entire system, they were sufficiently tested in both theory and practice (Gernaey et al., 2004), they definitely have fewer limitations than the competitors and they are the result of a common effort of the best specialists in the field. However, small wastewater plants, operating in rural areas or near small towns and receiving almost constantly small organic loads don't need the conceptual complexity of such models from at least two reasons: most of the existing treatment plants are designed to support much higher organic loads than received and are able to deal with periodic fluctuations, and they are not in the way of possible inhibitory influents, associated with the industrial development of big cities. Even more, construction and calibration of an ASM based plant implies supplementary costs, difficult to sustain by such small plants.

If the station is treating wastewaters from a larger urban structure, the variables implied by this situation are suitable for an ASM approach. Organic loads are much more fluctuant, local industry is associated with influent quality modifications and financial resources are available for implementation. Even if the model is partially applied for the design of an AI controlled environment, differential models data are not offering enough data quality, necessary if a conform effluent is wanted.

3.10. Biology vs. Biochemistry vs. System Engineering

Activated sludge is a living system formed by several groups of microorganisms. Although this affirmation is accepted by the entire scientific community, models of the system are not inspired from ecosystems or populations methods of modelling, and the community is treated as a mechanical structure or as a provider of substances for biochemical reactions. The differential models are created by engineers and their results are equations describing volumes, masses, retention times, and the community is simply referred to as activated sludge.

ASMs are dividing the community into several components, but species composition, relations between species or higher taxa are not on discussion. Even more, the biological community is split according to its trophic preference into autotrophs and heterotrophs and expressed as growth or decay of masses, in a similar way to differential models. In fact, the only important difference between the two categories of models is the complexity of the description, and no fundamental distinction is observable.

From this point of view, all models are losing the essence of the system, and are subject to future errors, or need to operate inside large limits. A more biological approach can be very useful, if not for complete plant operation, maybe for improvement of biochemical/engineering models, providing important information about variables not considered before, such as e.g. growth inhibition of some crucial species because of components released by other species. Small steps in this

field are made by researchers using individuals based models (Prats et al., 2006; Ferrer et al., 2007, 2008) or superindividuals based models (Grimm, 1999; Grimm and Railsback, 2005; Grimm et al., 2006) in microbiology as a general concept, with results applicable for the microorganism community present in the activated sludge, but it is obvious that the problem is far from a solution and the field is opened for further research.

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