A Brief History of Activated Sludge Process Models and Simulators

Background

Computer modeling of system behavior has had a significant impact on the development of design procedures for activated sludge systems in recent years. For full-scale plant operation it has also found application as an optimization tool in assessing the effects of changes in waste flows and loads, operational modifications (e.g. changes in recycles), and proposed modifications to plant configuration. Modeling has also proved valuable in operator training; through simulation exercises using the model, the operator acquires "instant" experience in the behavior to be expected with changes in inputs, system configuration and operational strategies.

The utility of simulation models becomes almost essential for nutrient removal systems incorporating nitrification, denitrification and excess biological phosphorus removal (NDEBPR), in addition to carbonaceous removal. In these systems the behavior involves a large number of compounds and biological reactions, many of which interact. An NDEBPR system involves at least three separate groups of microorganism (polyP or phosphorus-accumulating heterotrophs, non-polyP heterotrophs, nitrifying autotrophs) operating on a large number of chemical components in three distinct environmental regimes (aerobic zones, anoxic zones where nitrate but not oxygen is present, and anaerobic zones where both nitrate and oxygen are excluded as far as possible). These features make for complex behavior that has increased the level of difficulty in design, operation and control.

Activated Sludge Models

A full appreciation of the models can only be obtained through a detailed study of the literature.

Currently the approach to modeling activated sludge systems is to use mechanistic models. These mechanistic models incorporate mathematical expressions that represent the biological interactions, based on hypotheses proposed for the biological processes occurring within the system (Dold *et al.*, 1980; Grady *et al.*, 1986; Dold and Marais, 1986; Henze *et al.*, 1987a, b; Dold, 1990; Wentzel *et al.*, 1992; Henze *et al.*, 1994, 1995; Barker and Dold, 1997a,b; Henze *et al.*, 1999). It is useful to briefly review the historical development of the current generation of models.

In 1982 the International Association on Water Pollution Research and Control (IAWPRC, then IAWQ, and now IWA) appointed a task group to review modeling of activated sludge systems incorporating *carbonaceous energy removal, nitrification and denitrification*. The initial deliberations of the group resulted in a preliminary version of the "IAWPRC model" (Grady *et al.*, 1986). Dold and Marais (1986) conducted a comprehensive evaluation of the preliminary model. It was proposed that certain changes should be made, in particular with respect to the way in which the fate of organic nitrogen was modeled. These changes were subsequently adopted in the final version of the IAWPRC Activated Sludge Model No. 1 [ASM1] (Henze *et al.*, 1987a, 1987b).

The task group drew on a wide range of information in formulating the ASM1 model. One research initiative that had a major influence on the model was the dynamic activated sludge model developed by Marais and co-workers at the University of Cape Town (Dold *et al.*, 1980; van Haandel *et al.*, 1981). This dynamic model evolved out of the steady state model of Marais and Ekama (1976). The steady state model, in turn, constituted a development from a number of previous models for carbonaceous and nitrogenous material conversion and removal (McKinney, 1962; McKinney and Ooten, 1969; Lawrence and McCarty, 1970; Downing *et al.,* 1964).

The ASM1 model did not include the phenomenon of excess biological phosphorus removal (EBPR). Excess biological phosphorus removal (EBPR) is a microbial process which involves the cultivation, within the mixed community, of microorganisms that have the ability to take up phosphorus in excess of that required for growth. The net effect of this uptake is a reduced effluent phosphorus concentration that can be less than 1mg/L in a well-operated system. The removal of phosphorus is achieved through the microbially mediated storage of polyphosphate granules which can occupy up to 60% of the cell volume with a phosphorus mass as much as 38% of the volatile suspended solids (Lotter *et al.*, 1986; Wentzel *et al.*, 1989). Polyphosphate storage is encouraged in these systems by exposing the biomass to anaerobic and aerobic stages sequentially, favoring the growth of polyphosphate-accumulating facultative anaerobes.

Within an EBPR system, characteristic behavior is observed in each stage of the process (Figure 1). During the anaerobic stage, substrate is sequestered by the biomass and converted internally to polyhydroxyalkanoates (PHAs) while phosphorus is released from the biomass causing an increase in soluble phosphate. During the aerobic stage, PHA degradation occurs and soluble phosphate is accumulated as polyphosphate within the biomass, leaving a reduced level of phosphorus in the effluent.

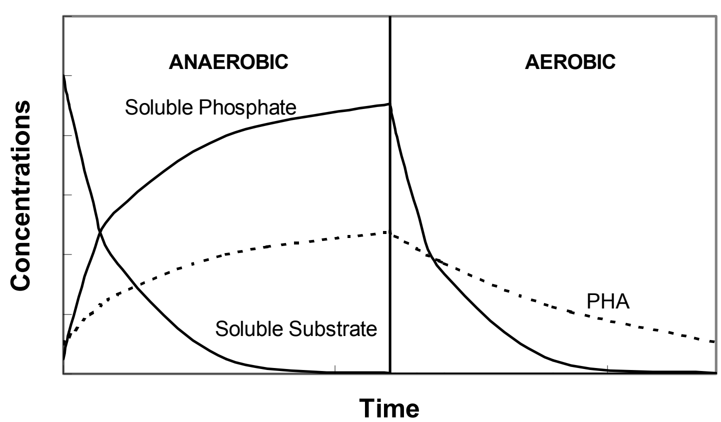

Figure 1. Schematic illustration of characteristic EBPR behaviour in an anaerobic/aerobic sequenced bioreactor.

Proposed explanations of the biochemical behavioral patterns associated with P release and uptake (and net P removal) have been presented in a number of models; for example, that of Comeau *et al.* (1986), extended and modified by Wentzel *et al.* (1986), and that of Mino *et al.* (1987). The biochemical models are largely in agreement regarding the biochemical control mechanisms and have provided an explanation for the essential requirements for attaining EBPR; namely, an alternating anaerobic/aerobic sequence with the provision of short-chain fatty acids (SCFA) during the anaerobic phase [also referred to as volatile fatty acids (VFA)]. These SCFA are taken up by the polyP organisms and stored as organic polymers, generally as either poly-β-hydroxybutyrate (PHB) or poly-β-hydroxyvalerate (PHV) [referred to collectively as poly-β-hydroxyalkanaotes (PHA).]

Since Comeau *et al.* (1986) and Wentzel *et al.* (1986) first introduced their biochemical models of excess biological phosphorus removal (EBPR), a substantial amount of research has resulted in variations to the original models (Mino *et al.*, 1987; Arun *et al.*, 1988; Wentzel *et al.*, 1991; Satoh *et al.*, 1994; Smolders *et al.*, 1994). However, the essence of the original models remains. More recently biochemical models have been proposed as extensions of these, but which include both glycogen-accumulating organisms (GAOs) and PAOs co-existing in these systems (Copp and Dold, 1999). It is proposed that observed behavior in EBPR systems is the net result of the combined behavior of both GAOs and PAOs and that the proportion of GAOs and PAOs in a single culture can significantly affect the behavior of the mixed microbial community. It is proposed that PAOs possess a selective advantage in the presence of sufficient phosphorus, but limiting PAO growth by limiting the available phosphorus allows for the proliferation of GAOs. Both PAOs and GAOs anaerobically sequester substrate that is stored internally as PHA. Under aerobic conditions, the breakdown of PHA provides the carbon and energy for growth utilizing oxygen as a terminal electron acceptor. In PAOs, excess energy generation is stored as polyphosphate whereas GAOs store excess energy as carbohydrate (glycogen).

For "normal" municipal wastewater the SCFA content usually is minimal. In EBPR systems the readily biodegradable COD component is transformed to SCFA by the non-polyP organism mass, thereby making SCFA available to the polyP organisms (Meganck *et al.*, 1985; Brodisch, 1985; Wentzel *et al.*, 1985). Aside from this linkage, the polyP and non-polyP organisms in EBPR systems have been shown to act essentially independently of one another. For this reason Wentzel *et al.* (1988) adopted the approach of developing "enhanced" cultures of polyP organisms as the basis for studying the kinetics and stoichiometry of EBPR without the behavior being masked by that of the non-polyP organisms.

Enhanced cultures of polyP organisms were developed by Wentzel *et al.* (1988) in continuous flow activated sludge systems (modified Bardenpho and UCT process configurations), with acetate as the only organic substrate. The sludge mass in these systems was shown to comprise the polyP organism *Acinetobacter* spp. in excess of 90 percent. Based on observations of the continuous flow systems and batch experiments using mixed liquor drawn from these systems, Wentzel *et al.* (1989a, 1989b) developed a kinetic mechanistic model for the enhanced culture EBPR system. The model provided a very reasonable description of the response observed in a number of continuous flow enhanced culture systems and the batch experiments with *a single set of kinetic and stoichiometric parameters*. The enhanced culture model constituted a most significant step towards the development of a general activated sludge model capable of modeling the biological processes of carbonaceous energy removal, nitrification, denitrification *and excess biological phosphorus removal*.

Dold (1990, 1991) merged the ASM1 model for non-polyP heterotrophic organisms and autotrophic organisms (Henze *et al.*, 1987a, 1987b) and the Wentzel *et al.* (1989b) model for polyP organisms. In combining the models, certain extensions and modifications were incorporated in both the ASM1 and the Wentzel model components. Since the initial development this NDEBPR model has been evaluated extensively against experimental data from laboratory-scale and full-scale treatment plants. This has lead to further model refinement (Barker and Dold, 1997a, 1997b).

The IAWQ task group also extended ASM1 to include simulation of combined NDEBPR processes. The initial ASM2 model was proposed as "a compromise between complexity and simplicity, and between the many viewpoints on how the correct model should look like. It should be used as a conceptual platform for further model development." (Henze *et al.*, 1994a). Since the initial presentation of ASM2 the model has undergone refinements, and the current version is denoted as ASM2d (Henze *et al.*, 1999).

Different simulators may incorporate slightly different activated sludge models.

Most municipal wastewater treatment plant simulators incorporate the ASM2d activated sludge model (e.g. GPS-X, Stoat, EFOR). One exception is the BioWin simulator, which is based on the Barker and Dold (1997a) model. In many respects the models are very similar. However, a number of differences should be recognized; for example:

- In anoxic growth the heterotroph biomass yield is less than for aerobic growth (Copp and Dold, 1998). This is incorporated in the BioWin model, but not in ASM2d.
- A number of studies have identified COD mass balance problems in nutrient removal sludge systems (Power *et al.*, 1992; Randall *et al.*, 1992; Wable *et al.*, 1992; Smyth, 1994; Wable *et al.*, 1994; Barker and Dold, 1995, 1996). This manifests itself as a reduction in both sludge production and oxygen demand in NDEBPR systems (with anaerobic zones) compared to aerobic-only or anoxic-aerobic systems. This apparent COD "disappearance" is incorporated empirically in the BioWin model, but not in ASM2d.

The mechanistic activated sludge NDEBPR models incorporate a large number of stoichiometric and kinetic parameters relating to the different organism masses. It should be recognized that the different variations of the IAWQ-type models imply differences in model structure. Therefore, it is important to recognize that parameters in one model cannot necessarily be transferred directly to other models *(even where the parameters sometimes have the same name)*. Nevertheless, the true test (and utility) of any particular model should be whether or not the model can:

- satisfactorily track the changes in a range of key parameters (e.g. soluble phosphorus, ammonia, nitrate concentrations; volatile suspended solids concentration; oxygen demand; etc.).
- in different types of systems [e.g. aerobic systems (with and without nitrification), ND systems, EBPR systems, NDEBPR systems (under steady state and dynamic conditions)]
- operated over a range of conditions (sludge age, recycle rates, etc.)

using a single set of model kinetic and stoichiometric parameters.

Models *versus* Simulators

The biological models should not be confused with simulation models. A simulator incorporates the biological model (and also models for other unit operations), and must link the units of a specific system according to the particular flow scheme. Figure 2 highlights the requirements for setting up a simulation of a typical wastewater treatment facility that incorporates the activated sludge process. Depending upon the intended use of the simulator, information is needed on the inputs to the process, its configuration, and its operating conditions (Wilson and Dold, 1998).

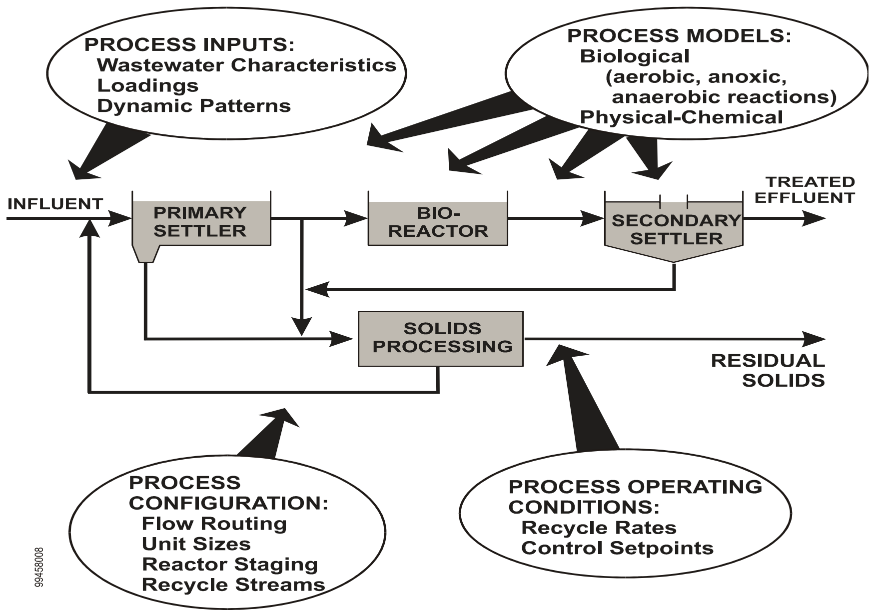

Figure 2. Essential Requirements for Wastewater Treatment Process Simulation (Wilson and Dold, 1998).

The *BioWin* Simulator

BioWin is a Microsoft Windows-based simulator used world-wide in the analysis and design of wastewater treatment plants. Figure 3 shows an example of a nutrient removal system configuration set up in BioWin. Many different process units can be included to “build” a specific treatment plant configuration; for example:

- Various influent elements for setting up wastewater inputs, storm flow inputs, or methanol addition streams.
- Equalization tanks.
- Continuous flow bioreactors incorporating sophisticated means for simulating the performance of diffused aeration systems.
- Variable volume / batch reactors.
- Various sequencing batch reactor (SBR) modules: single tank units, or SBRs with one or two hydraulically-linked prezones that are either continuously mixed or that allow settling of solids when the decant zone is in a settling phase.

- Aerobic digesters.
- Grit removal tanks.
- Primary settling tanks.
- Secondary settling tanks, where solids removal performance is either specified by the user, or where sludge settling behavior is based on flux theory using a one-dimensional model.
- A generic dewatering unit where the user specifies both solids capture and flow split between the thickened and un-thickened streams. This unit can be applied to simulating a range of dewatering processes such as centrifuges, belt presses, dissolved air flotation units, etc.
- Mixers and splitters for directing flow between units in the configuration. The user has full flexibility for specifying details of splits in streams (by actual rate, fraction, ratio, flow pacing, according to a timed schedule, etc.).

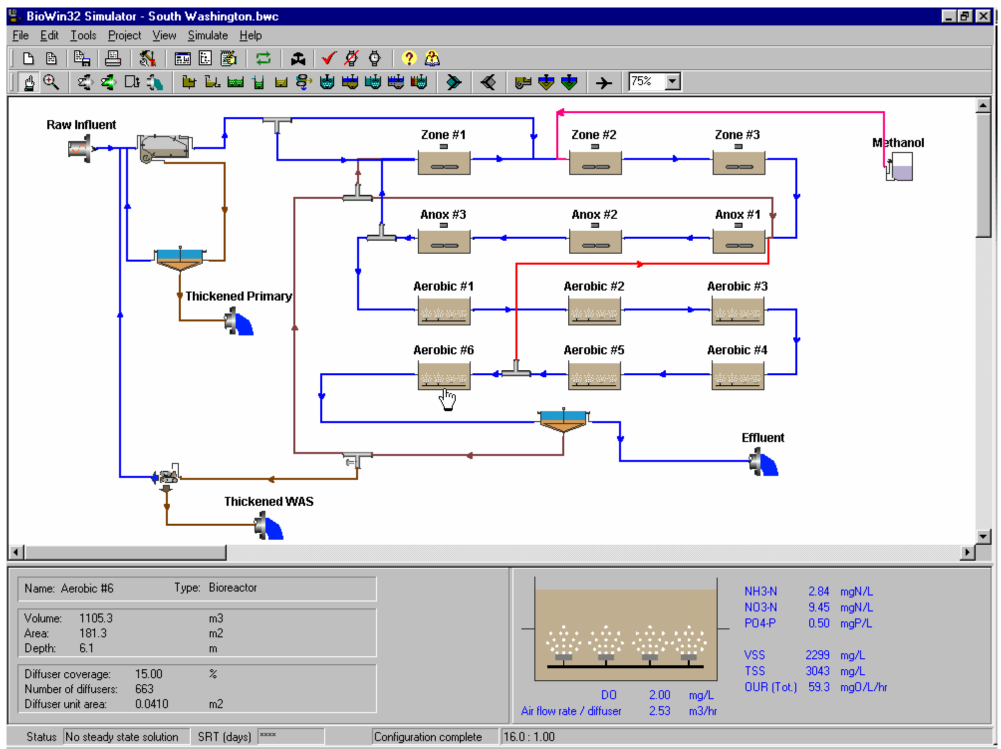

Figure 3. Example of a process configuration set up in BioWin.

The facility to view simulation results rapidly, and in detail, is of paramount importance in the design and analysis of systems. BioWin incorporates an Album for this purpose. The Album consists of a series of tabbed pages (somewhat like spreadsheet programs) showing simulation results in tabular and/or graphical format. Figure 4 shows example views of Album pages.

BioWin offers a number of features to aid in creating attractive, professional reports, and includes its own internal Notes editor to help keep track of project details. It is very easy to get results from BioWin into a word processor or spreadsheet. Charts, tables, system configuration layouts, etc. can be copied and pasted from BioWin to reports. Tables can be exported as tabbed text and then quickly converted to tables.

BioWin's on-line Help and Tutorials provide comprehensive user support. Further resources, such as downloadable configuration files and a Discussion Forum, are available from the EnviroSim Web site http://www.envirosim.com.

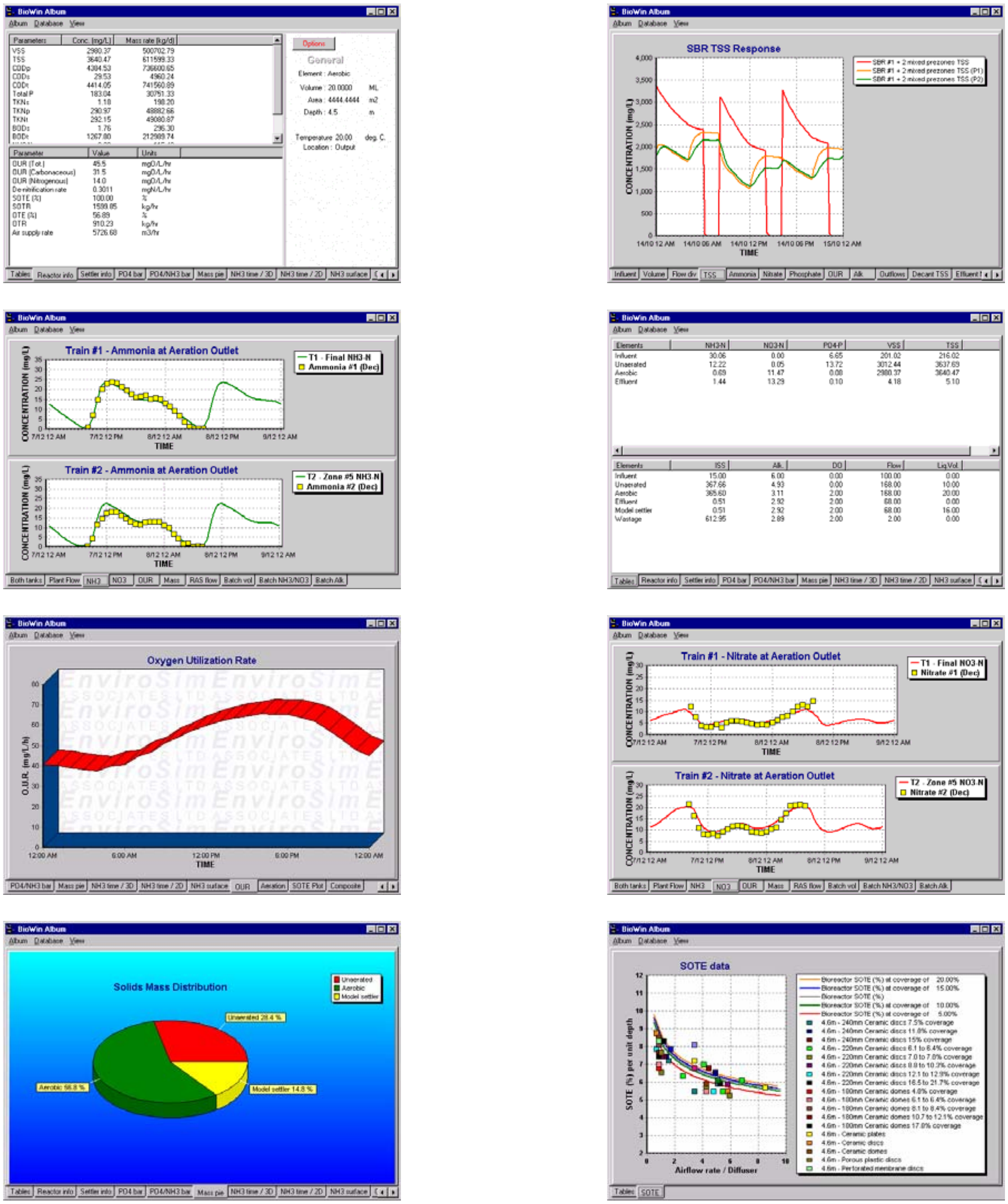

Figure 4. Examples of Album pages in BioWin.

Simulator Calibration

Some degree of calibration usually is required for a simulator to accurately predict effluent characteristics, sludge production, oxygen requirements, etc. The importance of this step in the simulation process cannot be over-emphasized since inappropriate calibration can lead to erroneous interpretation of simulator output as well as incorrect or non-optimal designs.

Different terminology is sometimes used to describe "sludge age". For example, solids retention time (SRT) or mean cell residence time (MCRT).

In terms of Figure 2, to simulate an activated sludge system, it is necessary to obtain details of the physical configuration (reactor volumes, clarifier dimensions, etc.), operating conditions (wastage rate, recycle rates, DO concentrations, etc.) and the influent loading pattern (flow rate, COD, TKN, etc.). All of this information essentially is "measurable", and it should be possible to establish this data without difficulty. [In practice, problems often are encountered with determining the sludge wastage. This is crucial as it determines the system sludge age / solids retention time (SRT). Also, influent concentration measurements often are unreliable as a result of sampling problems].

In addition to the "measurable" parameters, the current generation of biological models require information on:

- Influent wastewater composition
- Model kinetic and stoichiometric parameters

Influent Wastewater Characteristics

Even though model structures may differ, the division of influent COD and TKN is common to the different models.

The term "wastewater characteristics" refers to the partitioning of influent organic material into biodegradable and inert portions, the ammonia portion of the total nitrogen, and so on. The influent wastewater characteristics may vary, often appreciably, from one municipal waste to another. Wastewater characteristics have a very significant impact on system performance, particularly for nutrient removal systems. A single characteristic such as the readily biodegradable COD fraction can determine whether or not a system designed for excess phosphorus removal will in fact remove phosphorus. Therefore, if the model is to provide reasonable predictions of system behavior, adequate knowledge of wastewater characteristics is extremely important.

Activated Sludge Model Kinetic and Stoichiometric Parameters

The biological models contain many *stoichiometric and kinetic parameters*; for example, yields and growth rates. Several studies have shown that the stoichiometric and kinetic parameters (with one notable exception discussed below) do not change appreciably for different systems *treating municipal wastewaters*. For example, the decay rate estimated from the decline in oxygen utilization rate in a batch aerobic sludge digestion test is very similar for activated sludge drawn from aerobic systems in different parts of the world (at least at 20°C). The uniformity of parameters likely reflects uniformity in the composition of municipal wastewaters, and a resultant similarity in the diversity of the microorganism populations in different systems.

If large changes in default kinetic and stoichiometric parameters are necessary to match simulated and measured results this usually indicates that the system or the wastewater was not properly characterized. The most common problem is poor information on sludge wastage.

Consult Peer Review Group: Is there agreement on this broad statement? Note that the statement applies only to municipal systems.

It is proposed that the values for the stoichiometric and kinetic model parameters tabulated for a particular model (presumably derived from calibration studies on a range of treatment systems) should be acceptable initial estimates, and should not require substantial adjustment in model calibration exercises.

The exception referred to above is the maximum specific growth rate of the nitrifiers, μ_A. This parameter shows marked variations between systems treating different wastewaters. In the models, nitrification usually is considered as a single step process mediated by one group of nitrifying autotrophic bacteria. The growth rate parameter for the nitrifiers (μ_A) defines the maximum specific growth rate of this surrogate organism mass. Values for μ_A (at 20^{o}C) ranging from 0.2 to 1.0 d^{-1} have been observed in activated sludge systems treating a number of different municipal wastewaters (WRC, 1984). It has been suggested that the variation appears to correlate with the extent of the industrial component in the wastewater; with increased industrial input there likely is an increased possibility of inhibition of nitrifying organisms. However, many other factors influence nitrification behavior; for example, pH, Alkalinity, etc. This parameter has a major impact on nutrient removal system design and performance, and obviously on model predictions as well. Therefore, special attention should be paid to measurement or estimation of μ_A. In a sense, μ_A can be regarded as a wastewater characteristic.

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