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ABSTRACT

A model is a representation of a system that is used to predict the behaviour of the system. The application of dynamic models of wastewater treatment processes depends on fundamental process knowledge, synthesis of this knowledge into a model, and implementation of the model in a simulator. These three have converged to provide tools that can be used for process design, analysis, and operation. By using models that encompass fundamental biological and chemical processes, a better understanding of the performance of a wastewater treatment facility is available.

Applications of the models presented in this paper show that better understanding and predictive capability can be used to improve plant performance or reduce the cost of plant operations or upgrades. At a municipal plant, a proposed upgrade based on modelling resulted in significant capital cost savings, in the order of $5 to 10 million, since plant expansion (e.g., building new aeration tanks) for nitrification could be avoided or significantly delayed. At an industrial facility, analysis with a dynamic model revealed that reducing the target F/M by 50% would decrease annual biological sludge disposal costs by 8% without adversely impacting effluent quality.

INTRODUCTION

A model is a representation of a system that is used to predict the behaviour of the system. Models can be physical, often reduced in scale, or conceptual, such as mathematical equations. Models are usually developed to "stand in" for a real system when the real system does not yet exist, or when it is not feasible for reasons such as cost or safety to subject the system to the conditions that need to be tested.

In wastewater treatment, systems that we want to represent include wastewater treatment processes (e.g., activated sludge process) or entire wastewater treatment facilities. Physical models include bench and pilot scale processes. Mathematical models used in the field of wastewater treatment range from a single explicit equation, to inter-related differential equations that require implicit numerical routines on powerful computers.

Mathematical models are usually classified as mechanistic or empirical. Mechanistic models are developed from a fundamental knowledge of the biological, physical, or chemical components of a process. Empirical models are derived from an analysis of experimental data. Models can also be classified as steady-state or dynamic. Steady-state models use constant values for input variables to predict constant values for output variables. Dynamic models predict the time-varying performance of a process [1].

An integrated approach to modelling is typified in the development and application of mathematical models for wastewater treatment described in *Activated Sludge Model No. 1* (ASM1) by the IAWPRC (now IAWQ) Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment [2]. These types of models integrate many of the key biological, physical, and chemical processes within the activated sludge process into a form that can predict dynamic behaviour of treatment plants.

This paper will describe the application of mathematical models to the design, analysis, and operation and control of activated sludge systems and complete wastewater treatment facilities. The focus of this paper will be on the breed of dynamic mechanistic models characterized by the ASM1 model.

STEADY-STATE DESIGN MODELS

The activated sludge process is the conversion of organic matter (substrate) and nutrients to gases and cell tissue (biomass), typically in the presence of oxygen. Figure 1 shows a typical schematic of the activated sludge process.

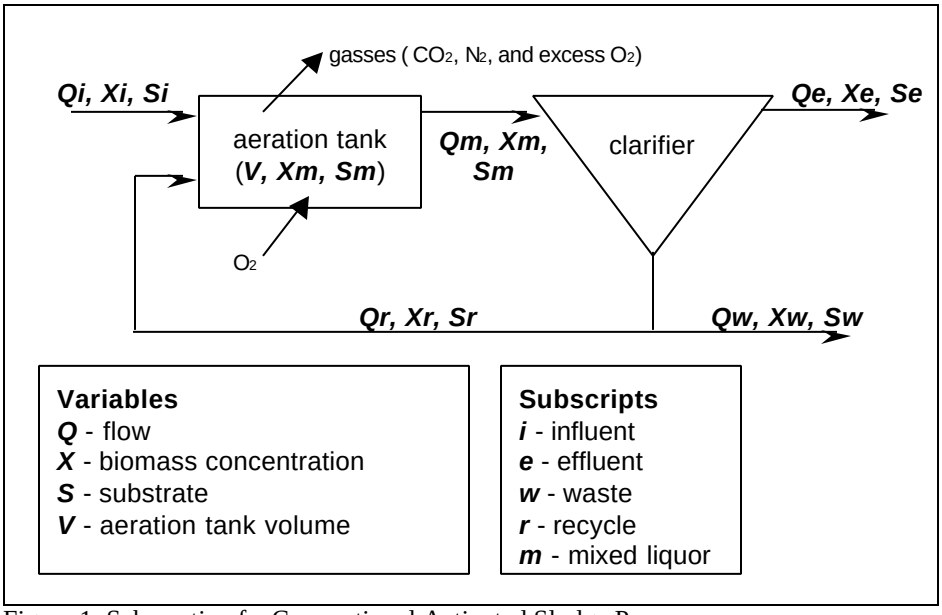

Figure 1. Schematic of a Conventional Activated Sludge Process

The basis of design is a mass balance around the reactor. Looking at the flows streams entering and exiting the system in Figure 1, the mass balance equation [3] for biomass is:

ACCUMULATION (Rate of accumulation of biomass within the system)	=	INPUT (Rate of flow of biomass into the system)	-	OUTPUT (Rate of flow of biomass out of the system)	+	REACTION (Net growth of biomass in the system)

Assuming that the aeration basin is a well-mixed reactor, and that all reactions occur within the aeration basin (assuming the clarifier is just used for solids separation), then the mass balance word statement for biomass growth using a single substrate can be represented symbolically as [3]:

$$\frac{dX_m}{dt}V = Q_i X_i - \left[Q_w X_w + Q_e X_e\right] + r_x V \tag{1}$$

The term for net growth rate "r_x" is often represented as a combination of biomass growth and biomass decay:

$$r_x = r_{xg} - r_{xd} \tag{2}$$

Biomass growth is typically represented by the Monod equation:

$$r_{xg} = \frac{m_m S}{K_s + S} X \tag{3}$$

where:

m_m = maximum specific growth rate

K_s = half saturation coefficient

And decay by a first order rate equation:

$$r_{xd} = k_d X \tag{4}$$

where:

k_d = the decay coefficient.

The growth and decay coefficients can differ significantly depending on the nature of the substrate and environmental conditions. For specific applications, these coefficients are often best determined through the use of pilot or lab scale experiments.

Combining equations (1), (3) and (4) produces:

$$\frac{dX_m}{dt}V = Q_i X_i - \left[Q_w X_w + Q_e X_e\right] + V\left(\frac{\mu_m S_m}{K_s + S_m} X_m - k_d X_m\right) \tag{5}$$

A similar mass balance can be written for the substrate using a reaction rate for substrate utilization:

$$r_s = -\frac{1}{Y}\frac{\mu_m S}{K_s + S} X_m \tag{6}$$

$$\frac{dS_m}{dt}V = Q_i S_i - \left[Q_w S_w + Q_e S_e\right] - \frac{V}{Y}\left(\frac{\mu_m S_m}{K_s + S_m} X_m\right) \tag{7}$$

where:

Y = Yield, the ratio of substrate consumed to biomass produced

To make these equations tractable from a design perspective (i.e., closed form explicit solutions), several assumptions are made:

- all flow rates are assumed constant
- influent substrate concentration is constant
- no change in solids storage in the clarifier
- influent biomass concentration (X_i) is zero
- no change in mixed liquor and substrate concentrations in the reactor (i.e., steady-state conditions):

$$\frac{dX_m}{dt} = 0 \quad \text{and} \quad \frac{dS_m}{dt} = 0$$

Using these assumptions, equations (5) and (7) can be simplified and used to determine the relationships between substrate utilization, tank volume, influent flow, biomass concentration and others [3]. Further manipulation of the mass balance equations can be used to account for plug flow reactions. If substrate is expressed in terms of oxygen demand (e.g., BOD) then oxygen requirements can be determined, which can be used in the design of the air distribution system.

The assumptions used to develop and solve these equations, while useful during a conceptual design process, do not account for many conditions encountered in real activated sludge plants. These include:

- time varying influent flows and concentrations
- time varying waste flows and recycle flows as dictated by process control needs

- changes in mass stored in the clarifier as sludge blankets rise and fall and settleability changes
- non-zero influent biomass concentrations
- complex flow streams (e.g., step feed, internal recycles)
- complex substrates that cannot be reasonably modelled as one composite substrate
- simultaneous nutrient removal with multiple biomass populations (e.g., nitrifiers)
- kinetic coefficients that are affected by variables not included in the equations (e.g., toxicity, temperature)

These conditions have three effects on the utility of steady-state design flow equations:

- they produce transient behaviours that are not predicted by steady-state equations
- they complicate the mass balance equations to the extent that explicit solutions are not possible
- they do not account for biological and chemical processes that can confound the reactions expressed in equations (5) and (7)

To resolve these problems, more comprehensive models have been developed. These models can be implicitly solved on personal computers using numerical methods. While these newer models often require more effort to implement, calibrate and apply, they improve process understanding which helps to reduce the uncertainty of model predictions. Reducing uncertainty ultimately reduces the risk of treatment process failure. Wastewater treatment process failure can result in lost production, fines, loss of public confidence, and environmental degradation. A better understanding of the processes can also lead to improved plant effluent concentration, or reduce the cost of capital works.

DYNAMIC MODELS

The current breed of dynamic activated sludge models represents a convergence of

- Fundamental knowledge – basic biology, chemistry, and physics of wastewater treatment processes
- Model development – synthesis of fundamental knowledge into mathematical form
- Simulation – solution of models using numerical methods and computer hardware

The IAWQ family of models represents the convergence of fundamental knowledge with model development. Simulation can be performed on moderately powerful personal computers and Unix workstations. Commercially available software for simulation can range from computer languages (e.g., variants of C, FORTAN, or specialized simulation languages) to treatment plant simulators that provide graphical model development tools and simulation interfaces.

Activated sludge models are based on biological and chemical processes acting upon state variables. State variables are the set of measurements or variables that are used to describe the internal status, or state, of a system [1]. A useful method of representing the interaction between state variables and internal processes is the Peterson Matrix. An example of a Peterson Matrix is shown in Table I. The model represented in Table 1 is essentially the model described by equations (1) through (7), with an additional state variable for dissolved oxygen. The Peterson Matrix is used to represent the reaction rate term (net growth or utilization) which is then added on to the input and output mass flow terms [2].

The reaction rate terms for a given state variable are based on the summation of the products of the stoichiometric coefficients and the process rate equations. For dissolved oxygen, this results in [2]:

$$r_{O2} = -\left(\frac{1-Y}{Y}\right)\frac{\mu_m S}{K_s + S} X - k_d X \qquad (8)$$

The biomass reaction is shown in Equations (2) (including Equations (3) and (4)), while the substrate reaction term is shown in Equation (6).

Table I – Peterson Matrix of a Simple Activated Sludge Model

State Variable i → / j Process ↓	1 X	2 S	3 O_2	Process Rate ρ_j $[ML^{-3}T^{-1}]$
1 Growth	1	$-\frac{1}{Y}$	$-\frac{1-Y}{Y}$	$\frac{m_m S}{K_s + S} X$
2 Decay	-1		-1	$k_d X$
Observed Conversation Rates $ML^{-3}T^{-1}$	$r_i = \sum_j r_{ij} = \sum_j v_{ij} r_j$			Kinetic Parameters:
Stoichiometric Parameters: Y = true growth yield	Biomass $[M(COD)L^{-3}]$	Substrate $[M(COD)L^{-3}]$	Dissolved Oxygen (negative COD) $[M(-COD)L^{-3}]$	m_m = maximum specific growth rate K_s = half saturation coefficient K_d = Decay rate

IAWQ Models

The first Activated Sludge Model (ASM1) by the IAWQ Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment was published in 1986 [2]. The ASM1 model has 13 state variables:

1. Soluble inert organics
2. Readily biodegradable (soluble) substrate
3. Particulate inert organic matter
4. Slowly biodegradable (particulate) substrate
5. Active heterotrophic biomass
6. Active autotrophic biomass (nitrifying bacteria)
7. Particulate products arising from biomass decay
8. Oxygen
9. Nitrate and nitrite nitrogen
10. NH_4^+ and NH_3 nitrogen
11. Soluble biodegradable organic nitrogen
12. Particulate biodegradable organic nitrogen
13. Alkalinity

For modelling purposes, the carbonaceous state variables (1 through 7) are presented in terms of chemical oxygen demand (COD) which, for modelling purposes, is preferred over others common measures of organic material in wastewater (e.g., TOC, BOD) [2]. Although these variables are not a direct reflection of typical plant measurements, it is possible to use typical plant measurements (e.g., BOD, suspended solids, TKN, etc.) to estimate state variable concentrations.

Eight processes in the ASM1 model act on these 13 state variables:

1. Aerobic growth of heterotrophic bacteria
2. Anoxic growth of heterotrophic bacteria
3. Aerobic growth of autotrophic bacteria
4. Decay of heterotrophic bacteria
5. Decay of autotrophic bacteria
6. Ammonification of soluble organic nitrogen
7. Hydrolysis of entrapped organics
8. Hydrolysis of entrapped organic nitrogen

This results in 13 inter-related mass balance equations, one for each state variable, in each well-mixed reactor. The model also uses 5 stoichiometric parameters and 14 kinetic parameters. The central process is still the aerobic growth of heterotrophic biomass based on the Monod equations shown in Equation (3). The Peterson Matrix for this model is available from several sources [1, 2, 4].

Model development and refinement is an ongoing activity and new models are continuously being developed or modified by researchers as fundamental knowledge improves or applications are better understood. Modifications to the original model by the Task Group have been published as the ASM2 [5], ASM2d [6], and ASM3 [7] models. These models include additional states and processes. For example, the ASM2 model, which includes biological phosphorus removal, has 19 processes and 20 state variables. All models are applicable in certain cases, and model selection is dependent on the particular application

These models can also be modified for particular applications. For example, the central reaction in the models is the aerobic growth of heterotrophs on soluble substrate. The state variable "soluble substrate" is really a composite of an array of organic material. In industrial applications, a single soluble substrate state variable with one heterotrophic biomass may not be suitable for modelling two or three complex organic wastes being treated in the same activated sludge reactor. In this case, the models can be modified to include multiple soluble substrates and multiple heterotroph types that focus on each substrate

All published models are based on suspended growth in a single complete mix reactor. Applying the model, say for a multiple reactors-in-series case with multiple raw influent inputs and recycle streams, requires that the mass balance equations be customized to include all input and output streams. Simulators usually provide the flexibility of applying the basic model to a variety of treatment process schematics. This has been extended to reactions in clarifiers and in fixed film systems [4]. In fixed film applications, the addition of diffusion terms to the mass balance is required.

Other Models

The activated sludge process is only one process in a wastewater treatment facility. A process simulation of a wastewater treatment facility may require models to simulate flow control, solids handling, and other biological processes. The most important model to work in conjunction with the biological model for activated sludge is a clarifier model. A suitable clarifier model should simulate both thickening and clarification in the clarifier, such as the model by Takács et al. [8]. A significant gap in current process models is the missing link between biological activity in the aerated reactor and biomass settleability in the final clarifier.

APPLICATION OF DYNAMIC MODELS

Dynamic process models have applications in the design, analysis, and control of wastewater treatment facilities. An important rule when using any model is that model limitations must be understood with respect to the conclusions that are drawn from model predictions.

A significant part of the effort of applying these models involves model calibration. As discussed earlier, the ASM1 model has 14 kinetic and 5 stoichiometric parameters. Any attached models (e.g., clarifiers) will also have parameters that will require calibration. Table II shows a general comparison between a low-effort versus a high-effort project using a commercially available wastewater treatment simulator.

Table II – Comparison of Low and High Effort Modelling Projects

	Low-Effort	High-Effort
Person-hours (order of magnitude)	Tens to Hundreds of hours	Thousands of hours
Modeled Layout	Simplified representation of the plant focusing on liquid line processes.	Complete representation of the plant including liquid and solids processes and parallel process lines.
Data	Existing data only, focus on average plant performance.	Sampling and monitoring program designed specifically for model calibration and evaluation – including stress testing and dynamic event monitoring.
Calibration	Based on one or two pseudo-steady-state events (average performance over a period of time with relatively consistent influent and stable operation).	Numerous steady-state and dynamic calibrations over a wide range of plant operating conditions. Kinetic and stoichiometric parameters identified using, for example, respirometry.
Evaluation	Limited (if any) formal evaluation of model calibration using independent data sets.	Formal evaluation using multiple independent data sets that represent a wide range of plant operating conditions.
Plant Analysis	Steady-state analysis of a few key scenarios.	A wide-ranging analysis of plant layout and operations under existing and future loading conditions. Optimization of planned upgrades and operation.

The low-effort project requires more faith in the applicability of the model to the plant in question compared to the high-effort project. The high-effort project provides sufficient calibration and model evaluation to quantify and minimize the uncertainty of predictions made with the model.

Design Applications

Models have always been part of the design process. And while simplified mass balance models are still used as an initial step in designing an activated sludge facility, the dynamic models described in this paper also have a role to play in the design process. They can be used to simulate the performance of the designed facility under a variety of conditions that are not considered in the initial design process. These may include:

- Use dynamic models to check plant performance under dynamic conditions (e.g., storm flow, batch influents)
- Test various process control options (e.g., influent management, waste and recycle control)
- Examine the effects of unusual influents (e.g., toxic inputs)
- Effects of equipment going out of service (e.g., tanks and pumps) for discrete periods of time
- Sensitivity of design to changes in fundamental assumptions (e.g., growth rates) to get some understanding of uncertainty and risk
- Test the interaction between different processes (e.g., side streams from solids handling facilities entering the activated sludge process)

An example of using dynamic models in the design process for integrated plant wide analysis occurred for a large municipal plant [9]. The construction of Stage 1, the first of three 1000 ML/d treatment modules, was near completion and Stage II was in the preliminary design stages. The owner required an evaluation of the current design to assist with the operation of Stage I and to provide new alternatives for Stage II. Since the Stage I facility was not operational, a simulation approach using dynamic modelling was used to address analysis objectives.

Modelling of the entire wastewater facility's liquid and solids trains provided the ability to evaluate the impact of operational changes on the whole plant. Unique conditions including strong wastewater conditions and high temperatures resulted in simulation results that were not contemplated during the plant's initial design. The plant was designed to provide only organic carbon removal, but given the warm wastewater conditions and the size of the aeration system, nitrification is expected to be difficult to inhibit, especially during warm wastewater periods.

Overall, the capacity of the Stage I liquid train is expected to be between 1400 and 1500 ML/d. The solids handling system appears to be limiting around the 1100 to 1200 ML/d range. The complex pre-thickening process (including gravity thickening, and coil filters) limits throughput of solids at elevated flows. Recommendations for the Stage I facility included changing the operating strategy to minimize nitrification.

Stage II considerations included evaluating fine bubble diffusers for aeration (energy savings and control), and providing a one-step thickening process prior to digestion (e.g. gravity belt thickening).

Analysis Applications

Dynamic models can also be used to analyze existing plants. Analysis of existing plants may be warranted based on expected capacity problems, changing effluent guidelines, or to find ways to improve effluent loads or reduce operating costs. In this application, the model may be used as a tool during a plant audit process. During a plant audit, historical data is usually reviewed, and new data is often collection. The model provides a useful platform to synthesize data analysis, and for predicting the impacts of proposed changes to plant layout or operation. Since the model looks at the process or plant as whole, proposed changes simulated with the model will help to identify unintended side effects.

An example of this approach was used during a facility plan for the 400 ML/d Woodward Avenue Treatment facility in Hamilton, Ontario [10]. Stringent new plant effluent goals for suspended solids, ammonia, and phosphorus were established based on receiving water needs. A dynamic simulation model was used to evaluate proposed upgrades during a Facility Planning Study. Upgrades evaluated included pre-treatment, primary clarifier basin expansion with

chemical addition, and aeration basin reconfiguration from complete mix to plug flow to improve nitrogen removal and wet weather flow capacity with step-feed. This application illustrates the usefulness of including separate states for nitrifying bacteria.

Modelling results showed that a proposed aeration basin reconfiguration with fine pore aeration, including selector zones, would significantly increase the maximum attainable degree of nitrification and wet weather capacity. Table III shows the results of an analysis of physical and operational changes on plant performance for different flow and seasonal conditions. This analysis showed that the planned upgrade significantly reduces effluent ammonia concentration.

Table III – Results of Scenario Analysis at the Woodward Avenue Plant

	Existing Plant	Reconfigured Plant			
	Summer Existing Flow	Summer Existing Flow	Winter Existing Flow	Summer High Flow	Summer High Flow
Case Definition					
Influent Flow (ML/d)	400	400	400	600	600
Influent BOD_5 (mg/L)	140	140	140	88	88
Influent Suspended Solids (mg/L)	260	260	260	160	160
Influent TKN (mg/L)	32.	32.	32.	20.	20.
Temperature (C)	20.	20.	12.	20.	12.
Primary Surface Area (m^3)	7,600	12,400	12,400	12,400	12,400
# of primary tanks	8	13	13	13	13
Convert aeration basins to plug flow	No	Yes	Yes	Yes	Yes
Final Effluent					
Alkalinity (mol)	0.33	0.46	0.84	1.8	2.1
Suspended Solids (mg/L)	45.	5.4	5.6	10.	10.
Volatile Suspended Solids (mg/L)	31.	3.9	4.1	5.2	5.6
BOD_5 (mg/L)	18.	3.7	4.6	4.4	5.9
COD (mg/L)	91.	40.	42.	43.	45.
TKN (mg-N/L)	13.	1.3	2.5	1.4	2.4
Soluble TKN (mg-N/L)	12.	1.2	2.5	1.2	2.2
Ammonia (mg-N/L)	12.	0.17	1.4	0.2	1.1
Nitrate/Nitrite (mg-N/L)	14.	9.8	9.7	6.8	6.6

The ammonia profile for the upgraded plant during the summer season with existing flow is shown in Figure 2. Figure 2 also shows the required oxygen transfer required to achieve the targeted level of nitrification along with the oxygen transfer capabilities of the existing mechanical surface aerators. This confirmed that the surface aerators that were in place could not deliver the oxygen transfer required for the proposed degree of nitrification.

This proposed upgrade results in significant capital cost savings, in the order of $5 to 10 million, since plant expansion (e.g., building new aeration tanks) for nitrification could be avoided or significantly delayed.

This model was also used to simulate the plant during storm flow conditions. Extensive sampling during a storm flow event was used to calibrate the model. The model was used to investigate the effect of various control options on plant effluent. The results showed that implementing influent step feed prior to a storm would result in a 10 to 35% decrease in effluent suspended solids concentration during the storm peak compared to not using step feed.

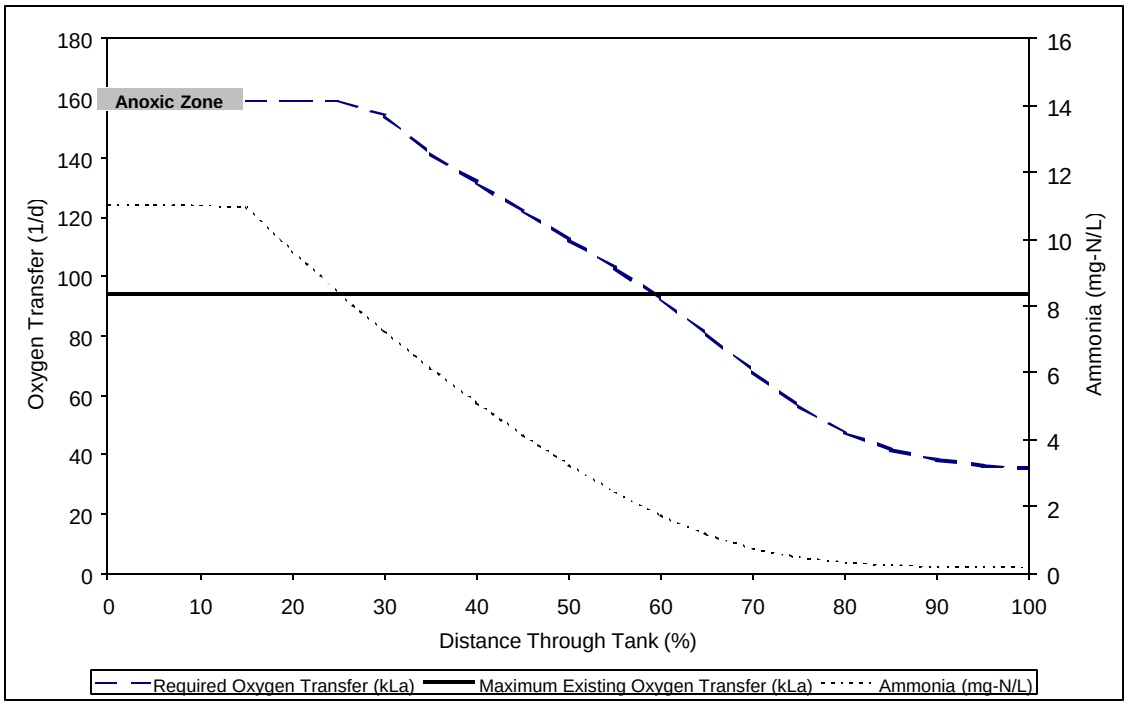

Figure 2. Oxygen Transfer and Ammonia Modelling at the Woodward Avenue Plant

Operation and Control Applications

Dynamic models can also be used to evaluate and design control and operating systems. This may range from developing and testing general operating strategies (e.g., target of manual control of sludge wasting from final clarifiers) to tuning on-line automatic control systems. Tools are also now available to link dynamic simulation models to treatment plant monitoring and control systems [11]. This link provides continuous on-line model calibration so that the model can be used for sensor fault detection, process fault detection, forecasting, and control.

A dynamic simulation model of the GE Plastics (GEP) manufacturing facility in Selkirk, NY was developed [12, 13]. Effluent from multiple process areas is treated through a combined physical/chemical and biological wastewater treatment system. Treatment unit operations include equalization, dissolved air flotation, activated sludge with addition of powdered activated carbon (PACT), secondary clarification, sand filtration, gravity thickening for waste activated sludge, and a filter press. Two large storm impoundments provide storage for management of storm flows. Effluent criteria are based on conventional measurements such as BOD_5 and suspended solids in addition to specific industrial chemicals.

The objective of preparing the model in this project were to:

- Provide a predictive analysis tool for plant operators to analyze impacts on plant operations from variances such as shut downs, excursions and storm events
- Assist GEP with maintaining consistent effluent quality compliance as mandated by regulatory agencies and the effluent discharge permit
- Assist GEP with optimization of the treatment process and increase operational efficiency
- Provide the operators with a customized training platform

The operators at Selkirk use the dynamic model to assist with management of daily operations including spill tank pumping, biomass inventory and wasting, hydraulic loading, tank bypass, and powdered activated carbon dosage. A particular example was an analysis by operators of the effect of lowering the target food to microorganism ratio (F/M) on annual sludge disposal costs. Analysis revealed that reducing the target F/M by 50% would decrease annual biological sludge disposal costs by 8% without adversely impacting effluent quality.

Multiple chemicals from various process effluents enter the treatment system at any given time. Before initiating this project, the kinetics of the removal processes for these chemicals were unknown. GEP personnel conducted respirometric experiments. A simulation model of the respirometer was used with the respirometry data to extract the kinetic coefficients required to calibrate the model for the removal of specific chemical substrates. A typical respirogram is shown in Figure 2 for a specific organic chemical. The data points represent data from the respirometer, while the solid line is from simulations of the respirometer using a dynamic model.

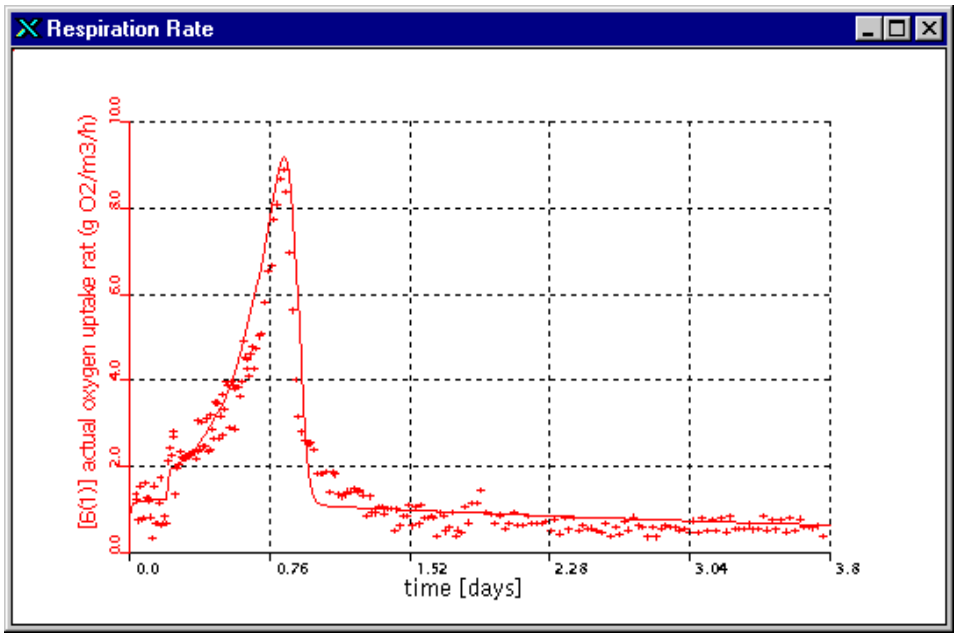

Figure 3. Simulated and Actual Respirometer Oxygen Uptake Rate

The simulated curve in Figure 2 was based on a Haldane equation for modelling reactor kinetics (growth and inhibition) in place of the Monod equations shown in Equation (3). The Haldane equation is:

$$r_{xg} = \frac{m_m S}{K_s + S + \frac{S^2}{K_i}} X \qquad (9)$$

where:

K_i = inhibition coefficient

This procedure was repeated for 5 different organic chemicals, at various concentrations, that are treated at the Selkirk plant. The models were modified to include separate heterotrophic bacteria for each chemical. When a known concentration of a chemical is in a holding tank, the operators can use the model to predict the dynamic effect of introducing the contents of the holding tank into the activated sludge process. An appropriate loading rate can then be found to maximize the loading rate while minimizing the risk of process upset.

SUMMARY AND RECOMMENDATIONS

The application of dynamic models of wastewater treatment processes depends on fundamental process knowledge, synthesis of this knowledge into a model, and implementation of the model in a simulator. These three have converged to provide tools that can be used for process design, analysis, and operation. By using models that encompass fundamental biological and chemical processes, a better understanding of the performance of a wastewater treatment facility is available. Applications of the models presented in this paper show that better understanding and predictive capability can be used to improve plant performance or reduce the cost of plant operations or upgrades.

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