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Computer Simulation of Activated Sludge Clarifiers in the Pulp and Paper Sector

SFM Network Project: Development of Simulators for Ex-plant Biological Treatment Systems

by

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ABSTRACT

To ensure compliance with water quality regulations, pulp and paper mills have been trying to optimize their wastewater treatment facilities, and, if necessary, to extend their treatment systems with new components. Optimization and design of the systems can be significantly improved with a better understanding of treatment process behaviour and the influence of various operating conditions on the process. The development of a mathematical model is a widely used approach for attaining a better understanding of a process. A comprehensive mathematical model could be a valuable tool in simulating variations in treatment system response caused by changes in plant operational conditions or changing loadings from the pulp and paper mill. A model, capable of coping with the processes and components of substrate and biomass occurring in the system, makes it possible to develop a simulator that is able to predict the behaviour of the activated sludge system under dynamic conditions. The simulator could serve as a technical aid for design, control, optimization, training, performance analysis, research, and education.

This report summarizes the results from the first stage of a larger project to develop a dynamic simulator of a pulp and paper activated sludge process. A one-dimensional clarifier model for a primary clarifier treating pulp and paper wastewaters was calibrated and verified against a long term dynamic, full scale data set using a sophisticated calibration technique. The mechanistic model exhibited good accuracy for predicting both the underflow and overflow suspended solids concentrations in a pulp and paper wastewater treatment plant primary clarifier. The relative error over the whole data set was 0.25 for the overflow SS concentration and 0.20 for the underflow suspended solids concentration. The major sources of the mechanistic model error for the overflow suspended solids of differing nature. A hybrid model (mechanistic model plus artificial neural network) did not improve the mechanistic model response. The major reason was thought to be that the mechanistic model residuals contained insufficient information to train the neural network. In addition to determining the behaviour and parameter values of a one-dimensional mechanistic model, the primary clarifier model calibration was useful, as it indicated that the model behaviour depended on the nature of the influent suspended solids.

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INTRODUCTION

Wastewater treatment facilities have received increased attention in the last decade with the introduction of new water quality criteria regulating the quality of effluent discharged from municipal and industrial wastewater treatment plants. Similar to other industries, the pulp and paper industry, a world scale industry, is faced with stringent effluent standards and requirements to reduce contaminants discharged to the environment. The first Canadian regulations were introduced at the beginning of the seventies (Environment Canada, 1972) and they set discharge limits for effluent suspended solids (SS), biochemical oxygen demand (BOD) and toxicity. New federal regulations were introduced in 1992 which set more stringent limits on effluent BOD, total suspended solids and toxicity (Fisheries Act, 1992).

To ensure compliance with water quality regulations, pulp and paper mills have been trying to optimize their wastewater treatment facilities, and, if necessary, to extend their treatment systems with new components. Optimization and design of the systems can be significantly improved with a better understanding of the treatment process behaviour and the influence of various operating conditions on the process. Even though each treatment step is important, the secondary treatment process is critical to successful wastewater treatment, because it has the greatest impact on the reduction of contaminants. It is the most complex process and the most difficult to operate and control. Understanding the behaviour of this process is the most important element in optimizing the performance of a wastewater treatment system and achieving the treatment objectives.

The development of a mathematical model is a widely used approach for attaining a better understanding of a process. A good example is the Activated Sludge Model No.1 (ASM1) (Henze et al., 1987), a mechanistic model that demonstrates that a dynamic model for predicting the behaviour of the activated sludge process in municipal wastewater treatment is a powerful tool. This model has been successfully used in the design, control and optimization of municipal activated sludge systems. A comprehensive mathematical model, such as the ASM1, but specific to the behaviour of an activated sludge system treating pulp and paper process wastewater, could be a valuable tool in simulating variations in the system caused by changes in treatment plant operational conditions and the pulp and paper process. A model, capable of coping with the processes and components of substrate and biomass occurring in the system, makes it possible to develop a simulator that is able to predict the behaviour of the activated sludge system under dynamic conditions. The simulator could serve as a technical aid for design, control, optimization, training, performance analysis, research, and education.

- 1. The simulator can be used to improve *design* of an activated sludge system, given information on influent wastewater characteristics. A range of process configurations and operational strategies can be evaluated.
- 2. The simulator can be used as an aid in the *control* of activated sludge systems to produce high quality effluent. By running the model under time-varying influent conditions, the appropriate operating conditions and control strategies can be identified and corrective measures

suggested. The ability to assess operating strategies for changing wastewater characteristics is important for industrial sites at which the wastewater can originate from a number of unit processes with widely varying wastewater characteristics, in addition to fluctuations in hydraulic loading. Without the ability to verify the outcome of process changes, optimal biological treatment conditions would be difficult to achieve.

- 3. Being able to control system behaviour, the simulator would make it possible to *optimize* the system in terms of costs and/or performance.
- 4. The simulator can be used as a tool for *training* plant operators. The model is able to simulate system behaviour under different conditions, to illustrate how changes in process parameters impact plant performance. Using the simulator, an operator can understand which parameters to change and what magnitude of change is required to correct problems in process operations. Where there is both limited design and operating experience available for a particular wastewater treatment facility, a simulator can be used to prepare contingency plans for emergency conditions and to train operations staff prior to commissioning the plant.
- 5. The simulator can allow analysis of total plant *performance* over time when compared to laws and regulations and to determine the impacts of new effluent requirements on plant design and operational cost.
- 6. The simulator could serve as a *research* tool to build and test hypotheses and gain new knowledge about processes.
- 7. The simulator may provide students with an *educational* tool to explore new ideas and improve the learning process.

Treatment Process

The treatment of effluent generated from pulp and paper mills involves several sequential steps. Each step is designed to remove one or more classes of contaminants. The first step involves primary treatment, where a fraction of the suspended solids is removed from the wastewater. Following primary treatment, the wastewater undergoes secondary treatment, which is a biological process, often involving an aerated lagoon or an activated sludge system. This part of the system is responsible for removing the bulk of the organics and reducing the influent toxicity. Although each treatment step is important, the secondary treatment stage is critical, since it has the greatest impact on the reduction of contaminants to low levels. It is the most complex unit process and the most difficult to operate and control. Understanding this stage of the treatment process is a key element in optimizing the performance of the treatment system.

In practice, aerated lagoons, as a form of biological treatment, have often been found inadequate for the new water quality criteria, so that a more sophisticated process is required. In the absence of specific process guidelines, secondary treatment facilities which have been constructed to meet the criteria are typically activated sludge processes. Settling of the biomass produced in the aeration basin during treatment is also considered a part of the secondary treatment process and it is achieved in the secondary clarifier.

Wastewater treatment plant design is usually based on steady state assumptions and for that reason has employed large safety factors. However, plant performance is sensitive to timevarying conditions that are sometimes beyond the control of the plant operators. The performance of wastewater treatment facilities depends on the experience of the operations staff, who develop a "feel" for the operation, allowing them to cope with changing influent conditions in operating conventional treatment technologies. Often, operations staff do not have the knowledge and experience base for complex wastewater treatment facilities, with the associated inter-dependence of process operations. This can result in poor effluent quality, high operating costs, and the inability of advanced treatment processes to achieve optimal levels of performance.

If properly operated under design steady state loading conditions, pulp and paper wastewater treatment plants can satisfy the discharge requirements. However, dynamic changes occurring in the pulp and paper process can disturb the wastewater treatment process and alter the discharged concentrations of the regulated parameters.

Research Objectives and Approach

The overall research aim was to establish a framework for a comprehensive dynamic model to predict the long term dynamic behaviour of an activated sludge plant treating pulp and paper wastewater. To date, comprehensive modelling of activated sludge systems has concentrated on the treatment of municipal wastewaters. The prime example is the Activated Sludge Model No.1. A review of the literature confirmed that an analogous model is not available for predicting dynamic behaviour of a system treating pulp and paper process wastewaters. Due to differences in the characteristics of municipal and pulp and paper process wastewaters, the Activated Sludge Model No. 1 cannot be used directly for predicting the behaviour of pulp and paper WWT systems. However, development of the municipal activated sludge treatment models provides guidance on developing equivalent models for the treatment of pulp and paper wastewaters.

This report summarizes the first step in the overall project – the construction and verification of a dynamic model for a pulp and paper primary clarifier. The model was calibrated and verified against multiple multi-annual and multi-monthly full scale facility data sets.

In order to further improve the model response, the mechanistic model was connected to a neural network to form a hybrid model. The mechanistic model error function was used to train the neural network. The neural network outputs were added to the mechanistic model outputs to make the final, hybrid model outputs. In this way, the hybrid model could be used to introduce variables not included in the mechanistic model, but affecting the process, to quantify the impact of additional variables, and to improve the accuracy of the mechanistic model.

RESULTS AND DISCUSSION

The Primary Clarifier Model

In an activated sludge (AS) process, the separation and concentration of solids is performed in a settling basin, often referred to as a clarifier. The force that makes the sedimentation of the particles in the liquid possible, originates from gravity and density differences between the particles and the liquid. Other factors that influence the settling behaviour are the hydraulic regime, temperature, basin design, flow and feed variations, sludge characteristics, predators consuming dispersed bacteria, etc.

The mechanistic model used in the present study was a 10-layer, one-dimensional model with two layers above the feed. The settling velocity function proposed by Takacs and Patry (1991) was incorporated. One-dimensional models are complex enough to describe some of the hydraulics occurring in the process of settling and mathematically simple enough to provide relatively short computational times. Furthermore, they are known to offer good settling results and thus, are commonly used for commercially available simulations in the field. Although the best one-dimensional models still do not provide first class clarification outputs, the use of neural networks as a black-box addition was proposed to compensate for this weakness.

The one-dimensional mechanistic clarifier model used in the present study incorporated six parameters: X_t , V_o , V'_o , r_h , r_p and f_{ns} , that must be estimated by model calibration if they are not available from experimental measurements. In the present case, these parameters were estimated by calibration against data sets from the activated sludge plant at a CTMP (chemi-thermomechanical pulp) mill in Port Alberni, B.C.

Mechanistic Model Calibration

Parameter ranges

Genetic algorithms (GA), the calibration technique used for calibration, require ranges for each model parameter as input data. The body of literature related to clarifier parameter values is not rich and does not report any long term dynamic full scale clarifier calibration attempt. The existing literature on the topic reports different ranges for the parameters (Takacs and Patry, 1991; Sorour and Horan, 1996). The parameter values reported in the literature are summarized in Table 1.

parameter	V_{o}	V _o '	r _p	$r_{\rm h}$	\mathbf{f}_{ns}
low	139	122	0.0027	0.00029	0.0012
high	712	340	0.0057	0.00043	0.0026

Table 1: Literature parameter ranges used for clarifier calibration

The final set of parameter limits and the optimal estimated parameter set produced by GA calibration of the one-dimensional mechanistic model of the primary clarifier are presented in Table 2.

Table 2: Primary clarifier parameter ranges and the optimal parameter set

parameter	Vo	V _o '	r _p	r_{h}	\mathbf{f}_{ns}	X_t
low	110	122	0.002	0.0001	0.03	800
high	370	340	0.01	0.001	0.70	1400
optimal set	233	165	0.0029	0.00078	80.0696	1229

Optimal parameters

As a result of calibration, the optimal parameters were: maximal theoretical settling velocity $V_o=233$ m/d, maximal practical settling velocity $V_o=165$ m/d, settling parameter characteristic of low solids concentration $r_p=0.0029$ m³/g, settling parameter characteristic of the hindered settling zone $r_h=0.00078$ m³/g, non-settleable fraction of influent suspended solids $f_{ns}=0.0696$, and threshold concentration $X_t=1229$ g/m³.

The optimal parameters fall within the literature parameter value range (Table 1), except the parameters related to the hindered settling (r_h) and the parameter related to the non-settleable fraction of influent suspended solids (f_{ns}). The discrepancy in the value of r_h might be due to the nature of the solids in the present study, or due to the long calibration data set used in the present study are different from the secondary clarifier solids studied by Takacs and Patry (1991) or the rice-straw pulp and paper process effluent used in the study by Sorour and Horan (1996).

The parameter related to the non-settleable fraction of the influent suspended solids was higher than the literature reported values, probably since primary clarifier overflow suspended solids concentrations are typically higher than those of secondary clarifiers (Takacs and Patry, 1991), and the influent suspended solids concentrations are lower, which leads to the conclusion that f_{ns} should be greater than the values for the secondary clarifiers reported in the literature.

Model fitness

The results of calibration and verification are summarized in Table 3 with the values of the objective function. Graphical presentations of the calibration and verification results for both the mechanistic and hybrid models for overflow suspended solids concentrations are shown in Figures 1 and 2 respectively, while the results of calibration and verification for both the mechanistic and

hybrid models for underflow suspended solids concentrations are shown in Figures 3 and 4. The figures show 3-day moving averages, because it is easier to see the model performance if there are fewer data points in the graphs.

The mechanistic model relative error for the calibration data was 0.27 for the overflow SS concentrations and 0.18 for the underflow SS concentration. The relative errors for the verification set were 0.24 for the overflow SS concentrations and 0.20 for the underflow SS concentrations. The similar error ranges for both the calibration and verification sets show that the sets were chosen properly. Since no literature reports exist on the calibration of full scale primary clarifiers treating pulp and paper wastewaters on long dynamic data sets, the model fitness in the present study cannot be compared to anything else.

Hybrid model

The basic neural network for the primary clarifier was designed to consist of three input and one output nodes. The input nodes were: influent flow rate, underflow flow rate and influent SS concentration. Two classes of neural networks were developed, each with a different output node. The output node was either overflow or underflow suspended solids concentration, depending on whether the neural network was used to learn the underflow or overflow SS concentration error function. Several more input nodes were added to the basic neural network within each class to find out which combination affected the model outputs the most. The additional options included primary clarifier pH, temperature and BOD₅ values in the clarifier overflow.

The results of the hybrid model calibration and verification are shown in Table 3. All the options include the basic network with an addition of one or more input nodes. The calibration errors are relative errors as described in the previous paragraphs. The last column in the table represents the number of hidden nodes in the neural network. Figures 1, 2, 3 and 4 show the mechanistic and hybrid model outputs compared to the real measured data for both calibration and verification data sets, as well as for the underflow and overflow suspended solids concentrations.

Overflow SS concentration

The relative error for the calibration data set for the overflow suspended solids concentration was higher than that for the underflow suspended solids concentration. It measured 0.27 for calibration and 0.24 for the verification data set versus 0.18 and 0. 20, respectively, for the underflow data sets (Figures 1 and 2, respectively). The error numerical values are shown in Table 3. The values indicated that the mechanistic model overflow suspended solids concentration outputs were not at the same accuracy level as the underflow suspended solids outputs, although the errors were similar. The reasons for the difference and the sources of the mechanistic model errors for the overflow SS concentration might be due to the model nature, to lab measurement error, to error in data interpolation, and to errors originating with data averaging.

Model Type	Input nodes	Suspended solids	Calibration error	Verification error	# of hidden nodes
	_				
Mechanistic					
	N/A	overflow	0.27	0.24	N/A
	N/A	underflow	0.18	0.20	N/A
Hybrid					
	basic NN	overflow	0.25	0.32	9
		underflow	0.16	0.20	5
	pН	overflow	0.25	0.35	9
	*	underflow	0.16	0.23	3
	BOD ₅	overflow	0.24	0.33	8
		underflow	0.21	0.20	4
	Temp	overflow	0.23	0.32	10
		underflow	0.16	0.24	2
	pH, BOD₅, temp	overflow	0.29	0.34	2
	1 / 0/ 1	underflow	0.16	0.22	2
	pH, BOD ₅	overflow	0.24	0.35	6
	1, 5	underflow	0.15	0.21	5
	pH, temp	overflow	0.24	0.29	5
	I , I	underflow	0.16	0.22	3
	BOD ₅ , temp	overflow	0.29	0.34	2
		underflow	0.16	0.24	2

Table 3: Port Alberni Mill primary clarifier model relative errors

Mechanistic model nature.

The one-dimensional models do not fully describe the clarification process because they do not consider all the complex hydrodynamic processes and turbulence occurring in the clarification portion of the settler. The model also does not compensate for differing suspended solids characteristics, except through the parameters in the settling velocity function. However, these parameters do not capture directly the shape of the particles, which is different in the primary and secondary clarifiers. The one-dimensional mechanistic model is known to represent the thickening process better than the clarification process, so that the modelled underflow suspended solids concentrations are expected to be closer to their real measured counterparts than those of the overflow suspended solids concentrations (Vitasovic, 1989; Jeppsson, 1996).

Lab measurements.

The measurement error for the overflow suspended solids concentrations was higher than that for the underflow suspended solids. The samples taken for the lab measurements were of the same volume, but the solids concentrations for the overflow and underflow samples differed by 3 orders of magnitude (60 vs. 50,000 mg/L). This fact might have caused much higher lab measurement error for the overflow suspended solids concentrations than that for the underflow SS concentration. Thus, the accuracy of the measured overflow concentrations could be lower than that of the underflow suspended solids concentrations. According to data given in Standard Methods for the Examination of Water and Wastewater (1992), the relative error for the total suspended solids measurement for concentrations close to the overflow suspended solids concentration is 17% (less than 5% for the underflow SS concentration). Consequently, the accuracy of the presented results should be considered in the light of the accuracy of the measured data.

Data interpolation

The original data base used for calibration and verification was not complete, so that some data reconstruction had to be done. The reconstruction may not have been accurate enough for all the missing frames, because insufficient correlated data were available. As opposed to the underflow SS concentration discussed later, it was much more difficult to clearly see this impact on the overflow SS concentration. However, since the impact on the underflow suspended solids was shown and the model is more sensitive for the overflow suspended solids concentration this source of the error is likely to exist

Data averaging

The input data used consisted of one-day averages that neglected all within-day variations that might have caused changes clearly reflected in the output variables. It was not possible to assess the extent of this source of error.



Figure 1: Primary clairfier overflow SS - Calibration.



Figure 2: Primary clarifier overflow SS - Verification



Figure 3: Primary clarifier underflow SS - calibration.



Figure 4: Primary clarifier underflow SS - verfication

The relative error for the verification data set was in the same range as for the calibration set (0.24 vs 0.27, Table 3), which meant that the calibration and verification sets represented the same data population. The hybrid model did not improve the mechanistic model response. In fact, the addition of a neural network actually increased the relative error. The hybrid model followed the trend better in some regions, but not sufficiently to help draw any conclusion.

Table 3 indicates that the hybrid model did not improve the mechanistic model response regardless of the neural network applied. There might have been three reasons for such an outcome: an inadequate length of the data sets, problems in extrapolating conditions of the verification data set, or a lack of information in the error function that was useful for neural networks.

The length of the data sets was not the most probable cause, because the same length data sets showed adequate results for the secondary clarifier hybrid model discussed later. Even though a statistical analysis showed similar characteristics for both the calibration and the verification data set, and the mechanistic model response was similar on both the calibration and the verification set, the presence of noise present in the data could have introduced extrapolating conditions. However, considering the hybrid model success for the secondary clarifier, the most probable reason might have been that the mechanistic model residuals used to train the neural network did not contain any valuable information for the neural network, i.e. the mechanistic model extracted all of the valuable information on the process carried by the measured data. This might lead to the conclusion that the one-dimensional clarifier model has limitations for application to a primary clarifier treating pulp and paper primary solids and the data available in the present study.

A further model improvement might be achieved by either adopting a multi-dimensional model, and/or developing additional neural networks with input nodes featuring data not available in the present study.

Underflow SS concentration

The mechanistic model response for the underflow suspended solids concentration was good, taking into account the duration of the data set and the variability of the model input data. The relative model errors were 18% for the calibration and 20% for verification data set (Table 3). The measured plant output data and the model predictions for the calibration and verification sets are shown in Figures 3 and 4, respectively. The model followed the real data trend well, although it was inclined to emphasize the extremes. The fact that the relative error for the verification data set (20%) was in the same range as for the calibration (18%), indicated that the sets were chosen properly, i.e. represented the same data population. The possible sources of the model errors are data interpolation, mechanistic model nature, and data averaging.

Data interpolation

As already discussed, the data reconstruction may not have been accurate enough, so that some incorrect model input data could have caused inaccurate mechanistic model response. Examples of the impact of inaccurately reconstructed data on the model accuracy can be identified in the regions corresponding to time periods in the vicinity of days 35000, 35080 and 35200 (Figure 4).

Mechanistic model nature

As already discussed, the one-dimensional model used does not describe all the complex hydraulics of the settling tanks, but has been shown to be capable of relatively accurate prediction of underflow suspended solids concentrations. However, the model does not compensate for the different suspended solids nature in pulp mill wastewater relative to municipal activated sludge.

Data averaging

As discussed in the paragraph on the model response to the overflow SS concentrations.

The hybrid model was not a significant improvement over the mechanistic model, although it followed the measured data trend better in some regions. The reasons for the hybrid model inability to improve the mechanistic model were already discussed with the reference to the overflow suspended solids concentrations.

Primary clarifier model calibration was useful as additional evidence (along with the Port Alice Mill results) to support some findings related to the secondary clarifier model. Considering different model behaviour on the primary and secondary clarifier data sets, a reasonable hypothesis may be established that the model behaviour depends on the nature of the influent suspended solids. A detailed discussion of the mechanistic and hybrid models, as well as a comparison between primary and secondary clarifier results and their consequences is provided in a subsequent report on the secondary clarifier results and conclusions.

MANAGEMENT APPLICATIONS

The results reported here represent those from the first stage of a larger project to develop simulators for pulp and paper wastewater treatment systems. To ensure compliance with water quality regulations, pulp and paper mills have been trying to optimize their wastewater treatment facilities, and, if necessary, to extend their treatment systems with new components. Optimization and design of the systems can be significantly improved with a better understanding of the treatment process behaviour and the influence of various operating conditions on the process. Even though each treatment step is important, the secondary treatment process is critical to successful wastewater treatment, because it has the greatest impact on the reduction of contaminants. It is the most complex process and the most difficult to operate and control. Understanding the behaviour of this process is the most important element in optimizing the performance of a wastewater treatment system and achieving the treatment objectives.

The development of a mathematical model is a widely used approach for attaining a better understanding of a process. A comprehensive mathematical model could be a valuable tool in simulating variations in the system caused by changes in treatment plant operational conditions and the pulp and paper process. A model, capable of coping with the processes and components of substrate and biomass occurring in the system, makes it possible to develop a simulator that is able to predict the behaviour of the activated sludge system under dynamic conditions. The simulator could serve as a technical aid for design, control, optimization, training, performance analysis, research, and education.

CONCLUSIONS

The mechanistic model showed good accuracy for predicting both the underflow and overflow suspended long term solids concentrations in a pulp and paper wastewater treatment plant primary clarifier. The relative error over the whole data set was 0.25 for the overflow SS concentration and 0.20 for the underflow suspended solids concentration. The major sources of the mechanistic model error for the overflow suspended solids were attributed to the mechanistic model nature and its inability to account for suspended solids of differing nature. A hybrid model did not improve the mechanistic model response. The major reason was identified as insufficient information contained in the mechanistic model residuals to train the neural network.

A one-dimensional clarifier model parameter set for a primary clarifier treating pulp and paper wastewaters was determined by using long term dynamic, full scale data and a sophisticated calibration technique. The present study approach was an advantage compared to the literature examples.

In addition to determining the behaviour and parameter values of a one-dimensional mechanistic model, the primary clarifier model calibration was useful as it indicated that the model behaviour depended on the nature of the influent suspended solids. A detailed discussion of the mechanistic and hybrid models, as well as a comparison between primary and secondary clarifier results and their consequences will be provided in the section on the secondary clarifier results and conclusions.

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