# INTELLIGENT ANALYSERS AND DYNAMIC SIMULATION IN A BIOLOGICAL WATER TREATMENT PROCESS

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Abstract. This paper presents an overview of different modelling and simulation methods used in biological wastewater treatment in pulp and paper industry. A lot of process measurements are available, but measurement sets do not include sufficient information on special features of the influent nor on microbial composition of the sludge. Populations of microorganisms are highly important, e.g. sludge bulking cause especially poor treatment efficiency results when biosludge escapes from secondary clarification. Basic dynamic simulation is based on LE models, which have been earlier used in chemical water treatment. The models consist of two parts: interactions are handled with linear equations, and nonlinearities are taken into account by membership definitions. Activated Sludge Models provide a basis for phenomenological modelling and can be linked to process expertise. Hybrid models with a cascade approach are needed in biological wastewater treatment to cover different operating conditions. Operating conditions are detected with trend and deviation indices introduced in this paper. Indices can be used both in selecting modelling areas and in combining the submodels of the water treatment. Importance of the balance between load and nutrients clearly demonstrated, and effects of oxygen and temperature are detected. Uncertainty handling needs to be included, since the measurement material is rather sparse, especially for on features of the influent and microbial composition.

# **1** Introduction

In the pulp and paper industry, a huge amount of water flows through different processes. For environmental and economical reasons, the plant recycles the water as much as possible. Before recycling the water is purified to a certain degree. The chemical treatment is one of the purification methods. Chemical water treatment includes complex nonlinear phenomena such as coagulation and flocculation processes. The dosing control of chemicals is very demanding, and chemicals are quite often dosed on the basis of the flow rate which does not always guarantee the adequate purification efficiency. Modelling of these complicated processes is mainly data-based or empirical due to a lack of comprehensive physical models. Intelligent methods such as linguistic equations and neural networks can be applied for the modelling of nonlinear interactions between input and output variables. [1, 12, 13]

Waste water treatment within Finnish pulp and paper industry is most commonly done in an activated sludge plant, which is a complex biological process, where several physical, chemical, and microbiological mechanisms simultaneously affect purification results. Limits of the emissions are defined by authorities. A lot of process measurements are available, but measurement sets do not include sufficient information on special features of the influent nor on microbial composition of the sludge. Populations of microorganisms are highly important, e.g. sludge bulking cause especially poor treatment efficiency results when biosludge escapes from secondary clarification.

Process simulators are effective for developing, testing and tuning the controllers. Different control methods can be tested safely in changing process conditions without disturbing the process. Furthermore, the chemical dosage can be optimised and the quality of water can be analysed in the simulator. However, a reliable process model is essential for process simulations. For activated sludge plants, modelling is even more demanding since the condition of the biomass need to modelled as well. Mechanistic models have been two decades in active use. The first Activated Sludge Models (ASM) was presented in 1987 [10]. However, the use has been limited by complexity of the models. Lindblom [21] reduced the ASM1 to an activated sludge plant in pulp and paper industry.

Many variables are normally measured in a plant, but some of them are strongly cross-correlated. Data-based analysis have been used for variable selection [26, 23, 24]. Clustering data for detection of operating conditions has used in [7, 6] to get basis for specialised submodels. As the sludge settling properties have remarkable effects on the treatment results, modelling of the diluted sludge volume index (DSVI) is important [7]. In [6] models were used for predicting the chemical oxygen demand (COD) of the effluent in an activated sludge plant treating pulp and paper mill wastewater.

This paper presents an overview of different modelling and simulation methods used in biological water treatment, and combines these approaches into a hybrid procedure.

## 2 Modelling approach

Data-driven and mechanistic modelling need to be combined with cascade structures and uncertainty handling to obtain simulators for practical applications in biological wastewater treatment.

### 2.1 Data-driven intelligent modelling

Linguistic equation (LE) models consist of two parts: *interactions* are handled with linear equations, and nonlinearities are taken into account by *membership definitions* [14]. In the LE models, the nonlinear scaling is performed twice: first scaling from real values to the interval [-2, 2] before applying linguistic equations, and then scaling from the interval [-2, 2] to real values after applying linguistic equations (Fig. 1(a)). The linguistic level of the input variable  $x_i$  is calculated the inverse functions of the polynomials [15].

Steady state LE models are represented by

$$x_{out} = f_{out} \left( -\frac{\sum_{j=1, j \neq out}^{m} A_{ij} f_j^{-1}(x_j) + B_i}{A_{iout}} \right)$$
(1)

where the functions  $f_j$  and  $f_{out}$  are membership definitions of input variables  $x_j$  and output  $x_{out}$ , respectively.

Rather simple input-output LE models, where the old value of the simulated variable and the current value of the control variable as inputs and the new value of the simulated variable as an output, can be used since nonlinearities are taken into account by membership definitions (Fig. 1(b)). For the default LE model, all the degrees of the polynomials in parametric models become very low, i.e. all the parametric models become the same

$$y(t) + a_1 y(t-1) = b_1 u(t-n_k) + e(t).$$
<sup>(2)</sup>

This model is a special case with three variables, y(t), y(t-1) and  $u(t-n_k)$ , the interaction matrix  $A = [1 a_1 - b_1]$  and the bias term B = 0.

The output, the derivative of the variable y, is integrated with numerical integration methods:

$$y = \int_0^T F(t, y, u) dt + y_0,$$
(3)

where T is the time period for integration, and  $y_0$  the initial condition. Usually, several values from the integration step or the previous steps are used in evaluating the new value. Step size control adapts the simulation to changing operating conditions.

In water treatment, dynamic LE approach has been used in modelling of flotation units, where the process water is treated with chemicals which react with extractives forming pitch sludge. The dynamic LE model is similar to the model shown in Figure 1(b): the outlet turbidity,  $x_{turb}(t + T_s)$ , is here calculated on the properties of incoming water, chemical dosages and previous calculated turbidity,  $x_{turb}(t)$ . The model is developed for steps equal to the sampling time,  $T_s$ . Normal process dat and some test campaigns based on experimental design [1].



Figure 1: LE models.

#### 2.2 Mechanistic modelling

Mechanistic models have been developed for biological water treatment. Activated Sludge Models (ASM) has been in active use in many fronts from industry to the science and many practical projects. The first model, which was presented in 1987 [10], is most commonly used. Afterwards, a large set of basis models has been formed: 1995 ASM2 [8], 1999 ASM2d and ASM3 [9], and 2001 ASM3-bio-P models. A review on the historical evolution of the activated sludge process can be found in [11]. Both white-box models for description of activated sludge processes and combining these models with knowledge-based information extraction tools have been described in a survey [5].

ASM1 was designed for modelling chemical oxygen demand (COD) and nitrogen removal in municipal waste water. ASM1 contains 13 variables, 8 processes and 19 parameters. The variables include seven COD components, four nitrogen components, dissolved oxygen, and alkalinity. The processes describe biomass growth and decay,

hydrolysis and ammonification. The parameter set includes 5 stochiometric and 14 kinetic parameters. Bisubstrate hypothesis deals COD in two parts: readily biodegradable substrate and slowly biodegradable substrate. When cells die, a part is assumed to be inactive residual, and the rest slowly biodegradable. Phosphorus can be modelled with Bio-P module, which is included in ASM2, ASM2d and ASM3-bio-P models.

For pulp and paper applications, AS models can be simplified. Lindblom [21] reduced the ASM1 to aerobic conditions and identified the parameters from a measurement campaign at a pulp and paper mill in Sweden. As five phosphorus components and three additional nitrogen components are included, the model contains 20 variables, 8 reactions and 26 parameters.

AS models are constructed through a step-wise procedure: model purpose definition, model selection, data collection, data reconciliation, calibration of the model parameters and model unfalsification. The model purpose, defined at the beginning of the procedure, influences the model selection, the data collection and the model calibration. In the model calibration a process engineering approach, i.e. based on understanding of the process and the model structure, is needed. [5]

Calibration of the models is challenging because of a large number of variables and parameters. Black-box, stochastic grey-box and hybrid models are useful in waste water applications for prediction of the influent load, for estimation of biomass activities and effluent quality parameters. These modelling methodologies thus complement the process knowledge included in white-box models with predictions based on data in areas where the white-box model assumptions are not valid or where white-box models do not provide accurate predictions.

## 2.3 Cascade modelling

The high number of parameters can be reduced with advanced modelling methods: the least angle regression is used for choosing appropriate coefficients in the response surface method, complete rule sets are not usually needed in fuzzy models, and regularisation methods reduce the number of the active connections in ANN models.

Cascade modelling divides the problem into sequential parts to further alleviate the problem of parameters (Fig. 2). The number of parameters is further reduced with principal components, e.g. Model A and/or Model B in Figure 2(a)) could produce principal components for Model C. Cascade modelling principle and linear models are essential in various fuzzy and neural methodologies as well. In Takagi-Sugeno (TS) fuzzy models are used for weighting local linear models. Radial basis networks are linear combinations of the outputs of the radial basis functions (RBF), e.g. in Figure 2(a) Model A and Model B could be radial basis functions and Model C the linear model. Generalised regression networks have a slightly different linear layer. In the learning vector quantisation (LVQ), a linear layer detects the classification classes by using subclass output of the competitive layer.

The output of a model can be used as a input of several models (Fig. 2(b)), and the models may also contain interactions or recycle flows (Fig. 2(c)). Feedback structures are needed in dynamic simulation, e.g. feedback connections in Elman networks can be generalised for interactive models (Fig. 2(c)). Neurofuzzy systems can be constructed as sequential combinations of neural and fuzzy parts, i.e. fuzzy set system provides inputs for a neural network, or neural preprocessing is used for inputs of a fuzzy set system. Variable grouping is important in cascade model structures.

The submodels are developed by the case-based modelling approach. The multimodel system has several submodels and a fuzzy decision system for selecting a good model for each situation (Fig. 3). Linguistic equation Takagi-Sugeno type fuzzy models (LETS) belong to this class but with one limitation: the fuzzy partition is defined with same variables as the models. As *LE* models are nonlinear, also these local models are nonlinear.



Figure 2: Examples of cascade models.

#### I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-35-3



Figure 3: A multimodel system with a fuzzy decision module.

#### 2.4 Uncertainty

Universal approximators for fuzzy functions can be constructed as extension principle extensions of continuous real-valued functions which continuously map fuzzy numbers into fuzzy numbers [2, 3]. The dynamic LE models with fuzzy inputs were introduced in forecasting of batch cooking in a pulp mill [16], and later adapted to dynamic modelling of a fluidised bed granulator used in production of pharmaceuticals [17], and dynamic simulation of a fed-batch enzyme fermentation process [18].



Figure 4: Examples of fuzzy extensions.

In this approach, LE models are extended to fuzzy inputs with this approach if the membership definitions, i.e. functions  $f_j^-$  and  $f_j^+$  and the corresponding inverse functions, are replaced by corresponding extension principle extensions of these functions. Square root functions (Fig. 4(a)) are used in the linguistification part (Fig. 1(b)).

The argument of the function  $f_{out}$  in (1) is obtained by fuzzy arithmetic. Only addition and subtraction are needed if the interaction coefficients are crisp. Fuzzy LE models with fuzzy inputs can be constructed by using multiplication and division as well. Fuzzy extension of the classical interval analysis [22] suits very well to these calculations. Finally, the delinguistication block uses also second order polynomials defined. An example is shown in Fig. 4(b).

Fuzzy extension results a nonlinear membership function for the output even if the membership function of the input is linear (Fig. 4). The number of  $\alpha$  levels should increase with growing fuzziness of the input.

Results of the fuzzy interval analysis have always maximal uncertainty as it takes the worst case. Negative associations between the input variables reduce the uncertainty considerably. In the calculations, this can be taken into account by using own membership functions for the upper and lower parts of the value range.

## **3** Intelligent analysers

Intelligent analysers are used as indirect measurements or for detecting operating conditions and trends.

## 3.1 Nonparametric models

Nonparametric models can be constructed as a weighted average of the neighbouring values. The smaller the neighbourhoods, the more complex or flexible model. Clustering methods suit well for constructing these models, e.g. self-organizing maps (SOM) were used in [7].

## 3.2 Model-based indicators

The basic dynamic flotation model is the core of the quality indicator. In addition, it contains two parts; one for selecting the proper submodel and the other for calculation the impurity level. Selection of the most suitable submodel is based on the error between measured (on-line) and predicted outlet turbidity and membership functions of errors. These parameters define the weighting coefficient for each submodel. If the error is positive the water quality is more pure than the average value. If the error is negative the water quality is more impure than the average (normal) water quality was defined using on-line data for a long period (one month). Cationic demand seems to correlate strongly with impurity levels of inlet water. [1]

Process simulators are effective for developing, testing and tuning the controllers. Different control methods can be tested safely in changing process conditions without disturbing the process [12]. The dynamic simulator contains a dynamic linguistic equation (LE) model for the flotation basin, controllers for two chemicals and a soft sensor for the detection of incoming water quality. The faster effecting chemical is controlled by an adaptive feedback LE controller. More slowly affecting chemical is controlled by a feedforward controller. The quality indicator is an essential part of the control system since the quality and amount of incoming water can fluctuate greatly. [13]

## 3.3 Trend analysis

Temporal reasoning is a very valuable tool to diagnose and control slow processes. Manual process supervision relies heavily on visual monitoring of characteristic shapes of changes in process variables, especially their trends. Although humans are very good at visually detecting such patterns, for control system software it is a difficult problem. The formal framework for the extraction and representation of process trends with triangular episodic representations developed in [4] has been applied in fermentation process data analysis [25]. Trend index . Trend analysis was applied to a pilot scale fermentation process in [20]. More methods for trend analysis are reviewed in [19].

Trend analysis provides useful indirect measurements for high level control. For any variable *j*, a *trend index*  $I_j^T(k)$  is calculated from the scaled values  $X_j$  by a linguistic equation

$$I_j^T(k) = \frac{1}{n_S + 1} \sum_{i=k-n_S}^k X_j(i) - \frac{1}{n_L + 1} \sum_{i=k-n_L}^k X_j(i),$$
(4)

which is based on the means obtained for a short and a long time period, defined by delays  $n_s$  and  $n_L$ , respectively. The index value is in the linguistic range [-2, 2] representing the strength of both decrease and increase of the variable  $x_j$ . The derivative of the index  $I_j^T(k)$ , denoted as  $\Delta I_j^T(k)$ , is used for analysing triangular episodic representations. Severity of the situation can be evaluated by a *deviation index* 

$$I_{j}^{D}(k) = \frac{1}{3} (X_{j}(k) + I_{j}^{T}(k) + \Delta I_{j}^{T}(k)).$$
(5)

This index has its highest absolute values, when the difference to the set point is very large and is getting still larger with a fast increasing speed.

# 4 Activated sludge plant

Biological water treatment depends strongly on changes in inlet water quality. Changes in biological state influence on the purification result and subsequent process phases. The objective of the project is to develop a model based optimisation and control concept for detecting process conditions and comparing control actions to improve process operation. On-line measurements and laboratory analysis are combined to build indirect measurements and intelligent dynamic models. Uncertainty handling is an essential part of the models. The concept is tested in connection to industrial purification processes.

### 4.1 Measurements

Influent quality depends on suspended solids (SS), chemical oxygen demand (COD), biological oxygen demand (BOD) and concentrations of nitrogen and phosphorus. In pulp and paper industry, additional nitrogen and/or phosphorus dosing is needed to keep the biomass in good condition. Changes in biomass population may cause sludge bulking which is seen as deterioration of sludge settling properties, described with sludge volume index (SVI) or diluted sludge volume index (DSVI). For example, if there is lack of oxygen or nutrients compared to biomass population, filamentous sludge leads into poor settling properties.

Changes in activated sludge process are slow, especially recovering from the bulking state to normal operation takes time. There significant seasonal effects, e.g. temperature is typically some degrees lower in winter time. On the other hand, cooling problems may case temperature rise in summer time. In addition pH, dissolved oxygen profile have obvious effects to the biomass population. Considerable changes of influent quality can be seen in conductivity.



Figure 5: Activated sludge plant.

The control variables such as sludge age, COD/nutrient rate, sludge loading, and recycle ratio can be derived from the measurements. The treatment efficiency is assessed by reduction of total nitrogen, total phosphorus, and total COD. Effective time delays should be taken into account, and an additional challenge is that these time delays are varying. Naturally, the delays depend on the flow rates, but also the changes of kinetics have their effects.

## 4.2 Intelligent modelling

Modelling methods used first in chemical water treatment [1, 12, 13] have been extended to biological wastewater treatment. The nonlinear scaling approach presented in [15] is the basis of these models. Measurements were extracted from databases of the pulp mill of Stora Enso Fine Paper in Oulu [7]. The data set used in this study contains measurements for almost four years with one day resolution.

The model consists of three interactive models (Fig. 2(c)): Model A calculates the load from the inflow, COD and suspended solids (Fig. 6). The load, nutrients, oxygen and temperature shown in Figure 6 are used in the model of the sludge settling. The load and the nutrients should be balanced, i.e. the difference of the load and nutrient level should be close to zero (Fig. 7). Too high nutrient level compared to the load causes poor settling seen as an increase of the DSVI, which continues as an oscillating behaviour, see days from 250 to 480 in Figure 7. On the other hand too low nutrient level causes problems in settling. Even short periods of high load can be seen in the DSVI, see days from 600 to 800 in Figure 7. The nutrient levels have decreased during the years (Fig. 6).

The normal levels are the best also for the temperature and the oxygen: too high and low temperatures affect to the biomass; too low oxygen levels are harmful and too high levels mean excess energy consumption. Very low levels of oxygen (days from 780 to 1000) were followed by a long period poor settling (days from 920 to 1020) and low COD reduction (days from 950 to 1050).

The multimodel system shown in Figure 3 should be based on the biomass population, which is here assessed by DSVI. Smooth transitions between the submodels are handled with fuzzy reasoning by using the degrees of membership obtained from the difference Load - Nutrients. Also oxygen and temperature levels are used in the model.

The COD and BOD reduction depend strongly on the biomass: the lowest reduction results from poor settling properties, see days from 950 to 1050, first 40 days and some days during the oscillating behaviour.

The individual dynamic models can be developed by using similar structures as in flotation models. Effective time delays are taken into account in these models. Uncertainty handling needs to be included, since the measurement material is rather sparse, especially for on features of the influent and microbial composition.

### 4.3 Intelligent analysers

Some changes have drastic effects on the purification process. As these changes are slow, an early detection is important. Changes in load, load-nutrient balance and settling are detected with the indices (4) and (5). Interpolation is needed since the measurements are sparse and the time between measurements varies. Outliers are removed before interpolation. The index value is in the range [-2, 2] representing the strength of both decrease and increase of the variable  $x_j$ . Also the weights of the submodels are calculated from the indices. The same approach can be use in calculating indices for any process or laboratory measurement.

The analysis with one day resolution provides indication for the main changes in operating conditions. However, some measurements, which are available with one hour resolution, have drastic variations within day periods. These will be included in further studies.



Figure 6: Levels of working point variables: load, nutrients, oxygen and temperature.



Figure 7: Load-nutrient balance, diluted sludge volume index (DSVI) and treatment results.

### 4.4 Hybrid models

Hybrid models are needed to cover different operating conditions (Fig. 8). Mechanistic models provide material understanding the phenomena but the number of variables and parameters is too high for parameter identification. Data-driven models can be developed only for specific operating conditions. Dynamic models do not provide any information about important variables if the training material contains several operating conditions. Therefore, detection of these conditions based on clustering has been the main topic in the beginning of the BioConOpt project. These approaches provide basis for indirect measurements of the biomass properties.



Figure 8: Work packages of project Control and optimisation in biological water treatment (BioConOpt).

## 5 Conclusions

Modelling and simulation approaches used in chemical water treatment can be extended to biological wastewater treatment. Mechanistic modelling provides understanding of the phenomena. Hybrid models based on a cascade approach are needed to cover different operating conditions. Uncertainty handling needs to be included, since the measurement material is rather sparse, especially for on features of the influent and microbial composition. Changes in operating conditions can be detected with new trend and deviation indices. Indices can be used both in selecting modelling areas and in combining the submodels of the water treatment.

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## 7 Acknowledgements

This research was supported by the Finnish Funding Agency for Technology and Innovation (Tekes), Kemira Oyj, Stora Enso Oyj and UPM-Kymmene Oyj.