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MODELLING THE BIOCHEMICAL PROCESSES OF THE ACTIVATED SLUDGE WASTEWATER TREATMENT

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ABSTRACT. Modelling and simulation of the activated sludge wastewater treatment processes proved to be very useful in the design, upgrade, control, evaluation and optimisation of wastewater treatment plants. This paper introduces existing activated sludge models and discusses empirical modelling techniques that can be used for the above tasks. Besides the description of the „traditional" Activated Sludge Models (ASMs), the paper suggests that Artificial Neural Network (ANN) models can successfully be used for many modelling applications, outperforming the ASMs in some aspects. Advantages and disadvantages of the different modelling techniques are also discussed.

Keywords: modelling, activated sludge, wastewater treatment, artificial neural networks

INTRODUCTION

Modelling and simulation can significantly contribute to the understanding and design of activated sludge wastewater treatment plants (WWTPs). A mathematical model of a WWTP, which is able to predict how the WWTP will react under various operating conditions, is an excellent tool for the design, analysis, control, forecasting and optimization of WWTPs, helping to assure high effluent quality.

A wastewater treatment plant model describes the biochemical and physical processes involved in the technical purification of wastewater. Through the biochemical processes the organic matter and nutrient content of the wastewater is eventually converted into carbon dioxide, nitrogen and a particulate fraction (cell material). The latter one can be removed from water by means of physical separation processes. Hence the activated sludge WWTP models usually consist of two interconnected sub-models: the activated sludge model and the settler model.

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MECHANISTIC WWTP MODELLING

Activated sludge models

Mechanistic (theoretical) models are based on the underlying physics and bio-chemistry governing the behaviour of the processes involved in activated sludge wastewater treatment. Emphasis is put on the modelling of conversion processes in the biological reactor and on the hydrodynamic modelling of the settler tanks, and less on the hydraulic modelling of the whole treatment plant. WWTP models usually do not describe explicitly flow propagation through the reactors, as in most of the cases treatment plant hydraulics are not sufficiently well known and can only be approximated. A commonly applied simplification is that the plant is considered as a few constant-volume-continuously-stirred-tank-reactors (CSTR) in series. In this way the mixing phenomena are modelled.

The modelling of the biochemical processes is based on several basic kinetic equations, describing bacterial growth, substrate utilization and the endogenous metabolism (decay) of bacteria, as well as the hydrolysis of entrapped organics. In the last 40 years several activated sludge models have been developed, describing the biochemical processes in a various manner [1, 2, 3]. The “state-of-the-art models” for activated sludge processes are considered to be the ASM1 – ASM3 models developed by the IWA Task Group [4]. These models incorporate carbon oxidation, nitrification, denitrification, while ASM2d also describes the biological and chemical phosphorus removal. The ASM models have been “updated” several times since the first coming out of the ASM1 and most of the problems identified in the earlier versions have been corrected. The models are based on COD units (use Chemical Oxygen Demand to define carbonaceous material); ASM3 has a total organic carbon (TOC) based version as well. These models are presented in detail elsewhere [4], here only a short description of ASM3 will be provided.

ASM3 was developed to correct some of the deficiencies of the earlier ASM1 and to include the advances in activated sludge modelling achieved in the decade following the publication of ASM1 [5]. It includes 12 biochemical processes and 13 components. Neither biological nor chemical phosphorus removal processes are included in ASM3. However, these can easily be added to it. Siegrist *et al*. (2002) [6] developed a relatively simple Bio-P module for ASM3 which was able to deliver accurate prediction both for a Swiss municipal WWTP and a pilot plant.

The compounds present in the wastewater are divided in 13 categories; these constitute the state variables of ASM3:

S_{ALK} - alkalinity of the wastewater [mole HCO_3^-/m^3]
S_I - inert soluble organic material [g COD/m^3]

S_S - readily biodegradable organic substrates [g COD/m^3]
S_{N2} - di-nitrogen [g N_2/ m^3]
S_{NH4} - ammonium plus ammonia nitrogen [g N/ m^3]
S_{NOX} - nitrate plus nitrite nitrogen [g N/ m^3]
S_{O2} - dissolved oxygen [g COD/m^3]
T_{SS} - total suspended solids (the same as XSS) [g/m3]
X_A - nitrifying organisms [g COD/m^3]
X_H - heterotrophic organisms [g COD/m^3]
X_I - inert particulate organic material [g COD/m^3]
X_S - slowly biodegradable substrates [g COD/m^3]
X_{SS} - suspended solids [g/m^3]
X_{STO} - organics stored by heterotrophic organisms [g COD/m^3]

There are a total of 12 biochemical processes modelled in ASM3. Figure 1 presents in a schematic way how the different compounds participate in the conversion processes. The kinetic expressions of the conversion processes are presented in detail by Henze et al. [4], here only a list of them is provided:

- hydrolysis of organic matter in readily available soluble substrate
- anoxic and aerobic storage of soluble substrate
- growth of heterotrophic organisms under aerobic and anoxic conditions
- endogenous respiration of the heterotrophic organisms under aerobic and anoxic conditions
- aerobic growth of autotrophic organisms
- aerobic and anaerobic endogenous respiration of the autotrophic organisms
- aerobic and anaerobic endogenous respiration of the storage products

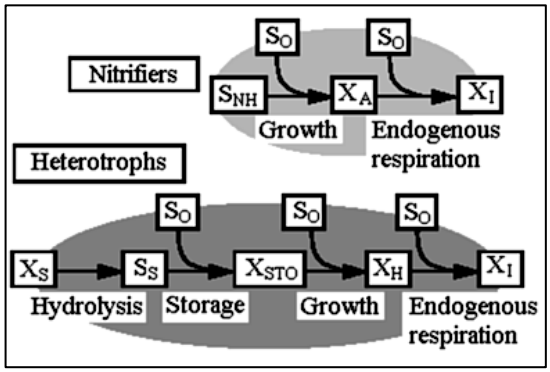

Figure 1. Flow of COD in ASM3 (redrawn from Henze *et al.,* 2000). The heterotrophic biomass includes cell internal organic storage products. Endogenous respiration is modelled for aerobic and anoxic conditions, both for the biomass and the storage products.

Settler models

Without a settler model the mass balance of an activated sludge WWTP using biomass recirculation cannot be closed. The clarifier models are based on settling functions, which evaluates the settling velocity of the particles, depending mainly on the solids concentration. The most popular models are simple 1-D models based on the layer approach (frequently the model proposed by Takács *et al.* [7]). These models describe settling and thickening with an acceptable level of accuracy and have a low computational demand. 1-D models are adequate for coupling with the activated sludge models because they give a reasonable approximation of the sludge balance and of the sludge shift from the aeration tank to the secondary clarifier. Conversion processes are typically not included in these models, being considered less important [8].

In practice clarifier models are implemented using the layer approach, which is a method for applying the flux theory in computer code. The settler tank is divided in horizontal layers and the differential form of the mass conservation equation is solved in each layer. The sludge coming from the activated sludge tanks usually enters the 5^{th} layer of the clarifier.

The problem of model complexity

The problem of model complexity rises from the belief that the more detailed a model is, the more accurate its prediction capability will be. Thus models were developed to include more and more knowledge for a better description of the phenomena modelled. Consequently models become more and more complicated, with too many parameters, and thus hard to calibrate, hence overparametrisation occur [9].

Another drawback of model complexity is the high computational demand of the too detailed models. WWTP models have to describe a wide range of processes with a varying timescale of the phenomena described (from seconds for the airflow rate in WWTPs to seasons for the temperature), resulting in a very stiff system of differential equations which is hard to solve numerically. Model stiffness is further worsened by the introduction of control loops, which stand in the way of using stiff numerical solvers and increase simulation time even more [10].

EMPIRICAL WWTP MODELLING

Unlike mechanistic models, empirical models do not use *a priori* knowledge of the underlying processes, but they are identified from input-output data (measured data). Empirical models address in a radical way the problems of mechanistic models, namely the high complexity and low simulation

speed. Data-based models may have a better practical value because of the infinite complexity of the underlying phenomena: according to the empiricists it is not needed to exactly know the phenomena, it is enough to have good input/output response. As to the simulation speed, empirical models consist of simple algebraic equations, and thus they may be several orders of magnitude faster than their mechanistic counterparts.

Among the empirical modelling techniques artificial neural networks (ANN) are more frequently used for WWTP modelling [11, 12, 13]. A neural network model consists of a set of parallel interconnected simple computational units, called neurons. Such a model resembles the brain in two aspects: (1) knowledge is acquired by the neurons through a learning process and (2) inter-neuron connection strengths, known as synaptic weights, are used to store the knowledge [14]. The learning process encompasses the adjustment of the weights of each processing unit, and can be seen as teaching the network to yield a particular response to a specific input [15]. Learning is accomplished by using a so called “training algorithm” that is a mathematical formulation of the rules that determine the magnitude of weight adjustment. If properly trained, the ANN is able to generalize from the examples used for training.

RESULTS AND DISCUSSION

The ANN modelling of the activated sludge processes has several specific aspects that are not commonly listed amongst ANN training instructions. As ANN modelling of WWTP plants is a relatively unknown field, we conducted a number of experiments in order to assess the effect of different ANN-related parameters on the prediction of the activated sludge variables

As a result of our series of experiments, three important aspects of ANN modelling of the activated sludge processes have been recognized. These aspects concern the composition of input dataset, the length of the training data set, and the network architecture.

a) Length of the training dataset: as many of the activated sludge biochemical processes have low dynamics, the data used for training has to cover several months. In case when temperature effects have also to be considered, one have to use at least half year of training data: this is the time needed for the wastewater’s temperature to change from it’s minimum to it’s maximum value (winter-summer). For a good training one should cover the whole temperature range, so that the ANN could learn from a representative sample. When artificially generated influent data is used for training, the temperature profile can also be modified in a way that the temperature profile that is normally observed over a complete year is squeezed into a six months period. This leads to better predictions.

b) Composition of input dataset: our experiments show that good prediction accuracy can be reached only by using a moving window of the past records of the input variables (Figure 2). This sliding window defines the number of lagged input variables (from the past moments T...T-n) used for the prediction of the output in a moment T. In this way the ANN can get information about the "history" of the activated sludge and thus it can consider the actual state of the system. For example the concentration of micro-organisms at a given time is influenced by the substrate concentrations of the past. The size of the moving window required is correlated to the speed of the activated sludge population dynamics.

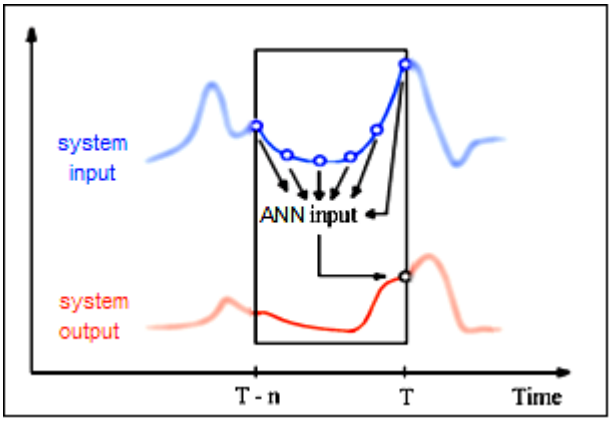

Figure 2. Prediction using a moving window of lagged input variables.

The prediction capability of the different ANNs is compared in Figure 3. Results clearly indicate that increasing the number of past records leads to better prediction. Practically the correlation coefficients for all 6 predicted variables are higher than 0.9 when using at least 8 past values of the influent variables. At the same time a considerable difference in the predictability of individual effluent variables can be observed. Biochemical oxygen demand (BOD_5) and total suspended solids (X_{SS}) can be easily predicted from just a few inputs, and have about the same correlation coefficients when using a moving window with a size equal to or larger than 2 hours. In the case of COD and total nitrogen (TN) the correlation coefficients increase continuously with the size of the past horizon covered by the delayed values. The good predictability of effluent X_{SS} and BOD_5 suggests that the reactions and mechanisms responsible for the concentration of these variables are less complicated than the other processes so the ANN can easier identify the input-output relations. Indeed, the X_{SS} concentration in the effluent depends mainly on the efficiency of the settling process in the

secondary clarifier and less on the biochemical reactions in the bioreactor. Hence it is affected very much by the flow rate to the treatment plant and gives sudden response to flow rate changes. The same holds for BOD_5, which is strongly related to the output X_{SS} concentration. The reactions of COD and N-products are more complex and take more time, hence the prediction of these variables is more difficult.

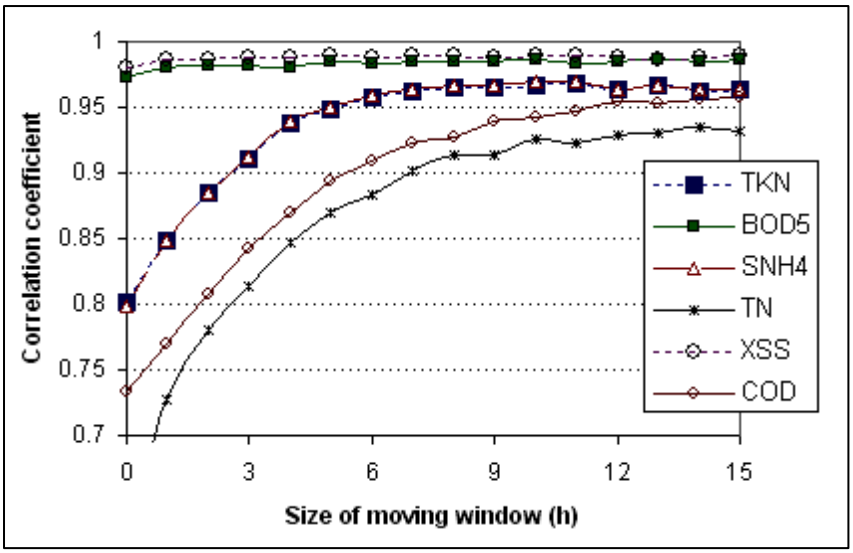

Figure 3. Prediction accuracy vs. size of moving window of lagged input variables.

c) Network architecture: the use of the sliding windows of past input variables results in an increase of input nodes. Thus the ANNs with good prediction capacity were all very big, consisting of a total of about 200 neurons. Our results (Table 1) show that network architecture does not have a drastic effect on prediction accuracy (unless the number of neurons in the hidden layer is extremely small). ANNs with only one hidden layer seem to predict slightly worse than ANNs with 2 hidden layers. With respect to learning speed, one can state that ANNs with two hidden layers learn faster than one-layered ANNs with the same number of neurons. The gain in learning speed is increasing together with increasing ANN complexity, reaching 40% in the case of ANNs with 35 hidden nodes. One may note that the time needed for training rises fast with increasing number of hidden nodes, while the prediction gets only slightly more accurate. Thus, the use of too large ANNs is not recommended, and a two-layered configuration should be preferred against a single hidden layer in the interest of minimizing the length of the ANN training phase.

Table 1. Influence of network architecture on ANN performance.

No. of hidden nodes		Training time (s)	Mean R^2
Layer 1	Layer 2		
20	-	161	*0.972*
25	-	198	*0.973*
35	-	272	*0.973*
14	6	150	*0.973*
15	10	171	*0.973*
20	15	215	*0.975*

The prediction accuracy of a well-built ANN can be satisfactory for many model applications. The mean prediction accuracy of our best performing ANN are presented in Table 2.

Table 2. ANN prediction performance indicators, relative to the mechanistic model predictions.

Predicted variable	BOD_5	X_{SS}	COD	S_{NH4}	TKN	TN
R^2	0.990	0.990	0.978	0.975	0.975	0.958
Mean relative error (%)	1.27	1.35	1.62	2.59	2.52	2.97

A sequence of simulated effluent concentration variables obtained with the two modeling approaches is provided in Figure 4. The simulation results presented in Figure 4 illustrate that the ANN performs quite well for effluent COD and BOD_5 prediction, whereas results are a little bit less good for effluent TN and S_{NH4} predictions. Diurnal effluent pollutant concentration variations are well predicted by the ANN, resulting for example in sharp effluent ammonia (S_{NH4}) peaks on dry weather days. These peaks are caused by the variable ammonia load of the household wastewater; they occur twice a day (early morning and late afternoon) in concordance with household habits.

On day 6493 a rain event is visible, and as can be seen, the capacity of the activated sludge plant to remove pollutants is exceeded at peak influent flow rate and both model approaches are able to predict this. During the rain event the increased hydraulic load of the WWTP causes activated sludge losses through the secondary clarifier, the bioreactors being “washed out”. Thus increased amount of organic material will be present in the effluent (see BOD and COD peaks).

The simulation speed of this ANN is about 0.8 years/sec, while training took 5 minutes. The total time needed for training data generation, training, simulation and additional processing is below 13 minutes all together. This is about 16 times less than the time needed for simulation with the mechanistic

model (~7 hours in this case). Solving the numerous differential equations of the complex activated sludge processes is very compute-demanding, leading to very long simulation times. The ANNs are not operating with differential equations, thus they do not present a simulation slow-down. For model applications where simulation speed is essential and the prediction accuracy of the ANN model is considered to be adequate, the ANN model is the preferable choice over the mechanistic model of the WWTP [12].

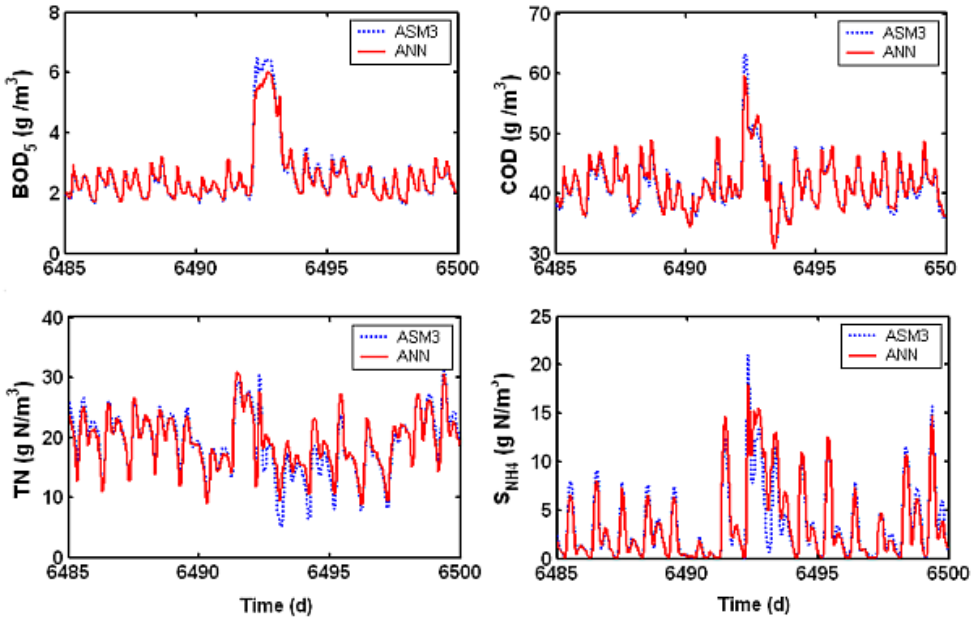

Figure 4. Prediction of wastewater parameters with the mechanistic ASM3-based model and the ANN model of the WWTP.

CONCLUSIONS

While mechanistic modelling of activated sludge WWTPs is well-estabilished by now and models can readily be found, there is little known about empirical modelling in this field. Our experiments show that ANN modelling is a powerful tool for reproducing the input/output relationships of WWTPs. Static backpropagation neural networks performed well, even if the modeled system was of great complexity. It has been shown that the composition of input data set has the biggest influence on the ANNs prediction accuracy, while network architecture has only a moderate effect on it. This means that predefined ANN architecture and training settings can be used for the modelling of different

WWTP layouts, making the ANN modelling available also for modelers with no background in neural networks. The resulting ANNs are good enough to replace the original WWTP model in many modelling applications and bring a significant increase in simulation speed. Possible application areas include WWTP performance prediction over a long period of time, for example in the frame of evaluating plant designs, and sub-model substitution in integrated urban water quality modelling.

EXPERIMENTAL SECTION

The parameters examined during the ANN tests were: type of learning algorithm, network architecture, length of training data, sample frequency of training data and components of the input data. Several hundreds of ANNs have been evaluated during the test, in terms of prediction capability, training time and simulation speed. In all of the cases static feedforward backpropagation ANNs were trained to predict six wastewater parameters: BOD_5, TN, total Kjeldahl nitrogen (TKN), dissolved ammonium (SNH_4), X_{SS} and COD. The ANNs had always tan-sigmoid transfer functions in all nodes, except the output neurons, where linear transfer functions have been used. Neural Network toolbox of Matlab 7.3 (The Mathworks, Inc.) has been used for the development, testing and application of the different ANNs. All of the learning algorithms of the named toolbox have been tested, and the scaled conjugate gradient algorithms were found to give the best results. Early stopping and Bayesian regularization were used for more efficient training and for avoiding overfitting. The 0.85 value of the performance parameter ratio was found to be best suitable for the given task.

Since it is very difficult to find good quality WWTP influent and effluent data, the influent and effluent files of the International Water Association's Benchmark Simulation Plant no. 1 (BSM1) have been used for ANN training purposes. The BSM1 has a five-compartment reactor: the first two compartments, 1000 m^3 each, are non-aerated and fully mixed. The last three compartments have a volume of 1333 m^3 each, and are aerated. In the last compartment the dissolved oxygen level is maintained at 2 mg/l with the use of a PI controller. The BSM1 layout has no primary clarifier, the input to the plant is considered to be one that has already undergone primary treatment. The secondary settler tank has a volume of 6000 m^3 and a surface area of 1500 m^2. The feed point to the settler is 2.2 m from the bottom. The complete specifications of the BSM1 plant layout can be found in Copp, 2002 [16]. For long-term simulation phases the BSM1 was fed with influent data created with an influent disturbance scenario generator [17].

The specifications of the best performing ANN of our test series are given in Table 3.

Table 3. Configuration of the best performer ANN.

ANN type	Static, feedforward, backpropagation
Training algorithm	Conjugate gradient with Polak-Ribiere updates
Initial weights	Random Gaussian distribution
Stopping criterion	Cross-validation
Number of neurons	145 / 35 / 25 / 6
Neuron types	Tan-sig / Tan-sig / Tan-sig / Linear
Input window size	20 hours
Data processing	Zero-mean normalization [-1,+1]
Training/validation	6 / 1 (every 7^{th} sample used for validation)
Optimization	Regularization, PPR = 0.85

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