

DYNAMIC SIMULATION OF WATER TREATMENT IN PULP AND PAPER INDUSTRY

Esko K. Juuso

Control Engineering Laboratory, Department of Process Engineering
P.O.Box 4300, 90014 University of Oulu, Finland

esko.juuso@oulu.fi ()

Abstract

This paper presents an overview of different modelling and simulation (M & S) methods used in water treatment. Special emphasis is on pulp and paper industry. In chemical water treatment, M & S is successfully used in control design. Hybrid models based on a cascade approach are needed in biological wastewater treatment 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.

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. The dosing control of chemicals is very demanding because the quality of water may fluctuate considerably and the effects of chemicals on the purification result are nonlinear. Chemicals are quite often dosed on the basis of the flow rate which does not always guarantee the adequate purification efficiency.

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 chem-

ical 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.

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

2 Modelling approach

2.1 Data-driven modelling

Linguistic equation (LE) models consist of two parts: *interactions* are handled with linear equations, and nonlinearities are taken into account by *membership definitions* [1]. 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_j is calculated the inverse functions of the polynomials [2].

Steady state LE models are represented by

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

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

$$y(t) + a_1 y(t-1) = b_1 u(t-n_k) + e(t). \quad (2)$$

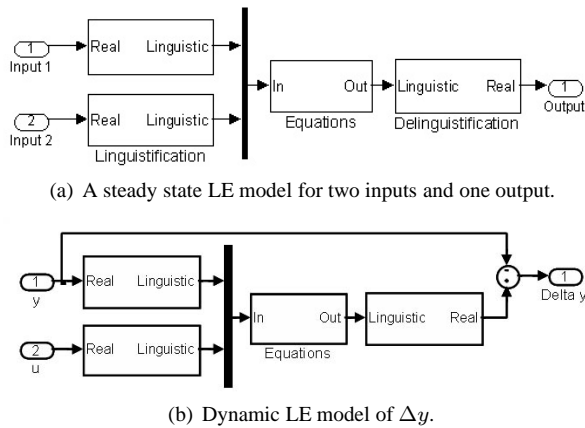


Fig. 1 LE models.

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:

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

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.

2.2 Mechanistic modelling

Mechanistic models have been developed for biological water treatment. Activated Sludge Models (AS models) 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 [3], is most commonly used. Afterwards, a large set of basis models has been formed: 1995 ASM2 [4], 1999 ASM2d and ASM3 [5], and 2001 ASM3-bio-P models. A review on the historical evolution of the activated sludge process can be found in [6]. 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 [7].

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 stoichiometric 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 [8] 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. [7]

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 an 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. feed-

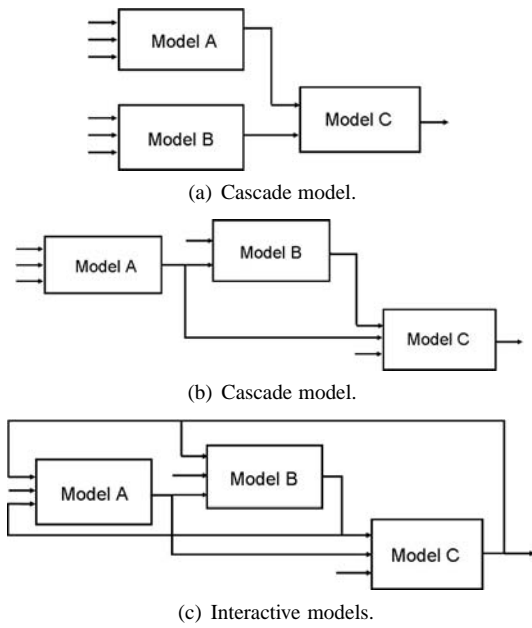


Fig. 2 Examples of cascade models.

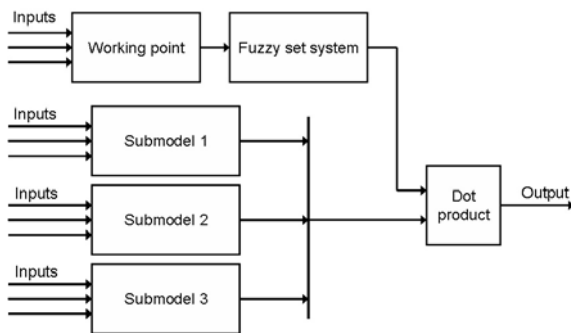


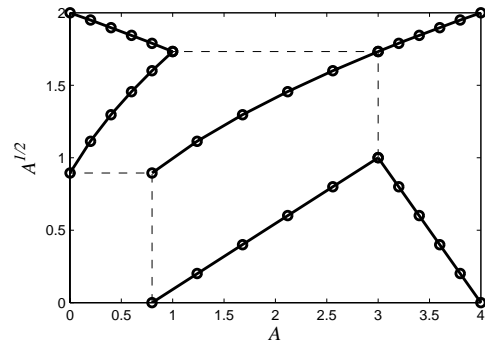
Fig. 3 A multimodel system with a fuzzy decision module.

back 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.

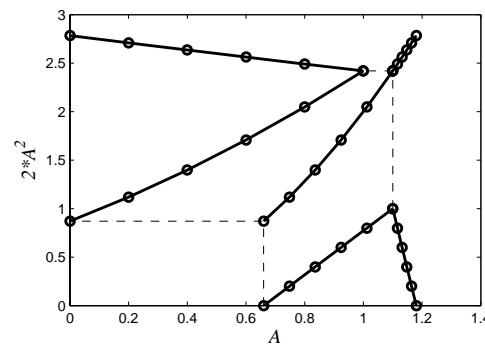
The submodels are developed by the case-based modelling approach. The multimodel system has several submodels and a fuzzy decision system for selecting a good model for each situation (Fig. 3). Linguistic equation Takagi-Sugeno type fuzzy models (LETS) belong to this class but with one limitation: the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

2.4 Uncertainty

Universal approximators for fuzzy functions can be constructed as extension principle extensions of con-



(a) Extension with a square root function.



(b) Extension with a second order polynomial.

Fig. 4 Examples of fuzzy extensions.

tinuous real-valued functions which continuously map fuzzy numbers into fuzzy numbers [9, 10]. The dynamic LE models with fuzzy inputs were introduced in forecasting of batch cooking in a pulp mill [11], and later adapted to dynamic modelling of a fluidised bed granulator used in production of pharmaceuticals [12], and dynamic simulation of a fed-batch enzyme fermentation process [13].

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 [14] 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 α levels should increase with growing fuzziness of the input.

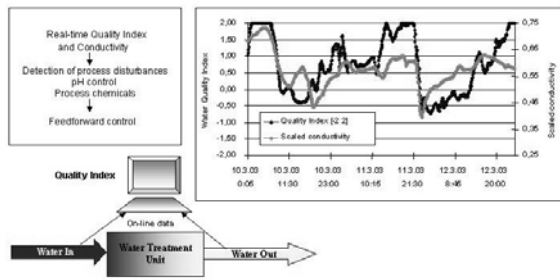


Fig. 5 Water quality indicator [16].

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 Water treatment

Modelling methods have been used first for simulation of chemical water treatment, and then extended to biological wastewater treatment.

3.1 Flotation

The chemical treatment is one of the purification methods. The dosing control of chemicals is very demanding because the quality of water may fluctuate considerably and the effects of chemicals on the purification result are nonlinear. Chemical water treatment includes complex nonlinear phenomena such as coagulation and flocculation processes. 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.

In the flotation unit, process water is treated with a polymer which reacts 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 . Effective time delays are taken into account in the models. Experimental design was used to evaluate the effect of chemicals dosage on the treatment results. Central composite circumscribed was chosen as the design method. Variables were tested at five different levels in order to evaluate the nonlinear effects. Two different designs were carried out at two capacity levels. In addition, the effect on the amount of dissolved air was tested. [15]

The quality and amount of incoming water can fluctuate greatly. 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

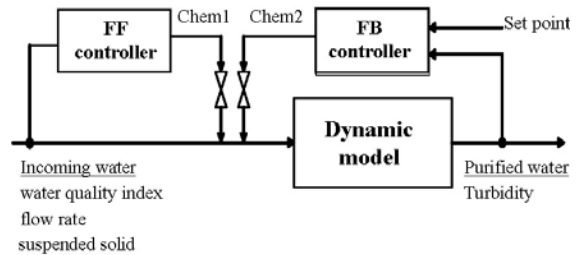


Fig. 6 Dynamic simulator with the feedforward and the adaptive feedback controllers [17].

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 (Fig. 5). If the error is negative the water quality is more impure than the average. 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. [15]

Process simulators are effective for developing, testing and tuning the controllers (Fig. 6). Different control methods can be tested safely in changing process conditions without disturbing the process [18]. 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. [17]

3.2 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.

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 in-

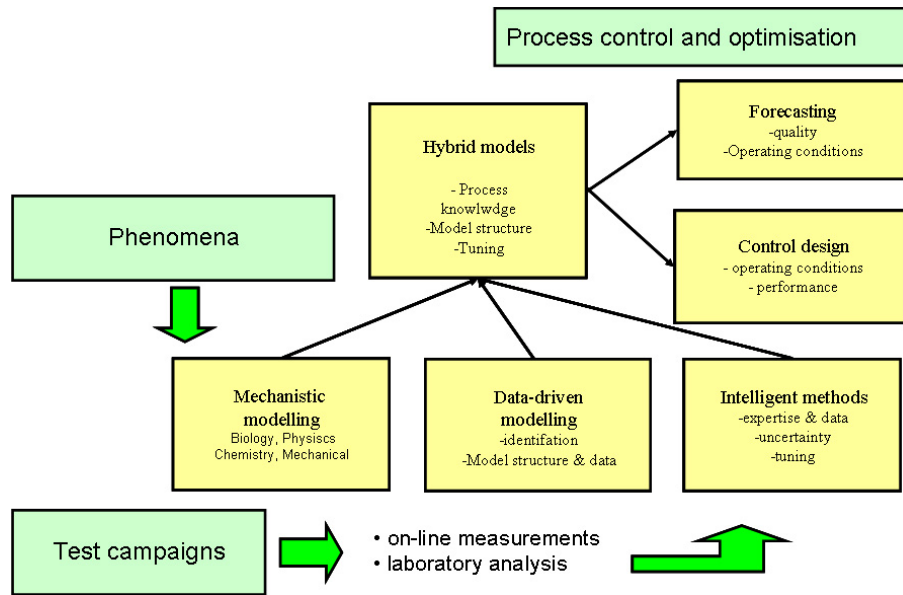


Fig. 8 Work packages of project Control and optimisation in biological water treatment (BioConOpt).

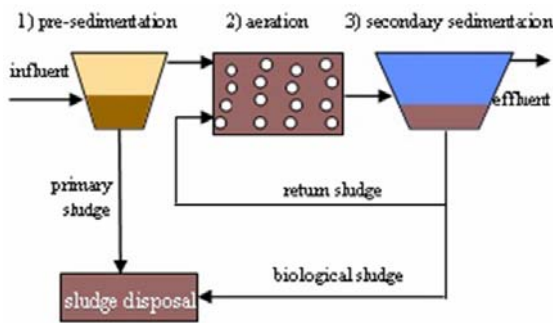


Fig. 7 Activated sludge plant.

dex (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 cause 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.

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.

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 [19, 20, 21]. Clustering data for detection of operating conditions has been used in [22, 23].

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. The multimodel system shown in Fig. 3 should be based on the biomass population. Then the individual dynamic models can be developed by using similar structures as in flotation 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 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.

5 References

- [1] E. K. Juuso. Fuzzy control in process industry: The linguistic equation approach. In H. B. Verbruggen, H.-J. Zimmermann, and R. Babuska, editors, *Fuzzy Algorithms for Control, International Series in Intelligent Technologies*, pages 243–300. Kluwer, Boston, 1999.
- [2] E. K. Juuso. Integration of intelligent systems in development of smart adaptive systems. *International Journal of Approximate Reasoning*, 35:307–337, 2004.
- [3] M. Henze, C. P. L. Grady Jr., W. Gujer, G. V. R. Marais, and T. Matsuo. Activated sludge model no. 1., iawq scientific and technical report no. 1. London, UK, 1987.
- [4] M. Henze, W. Gujer, T. Mino, T. Matsuo, M. C. M. Wentzel, and G. V. R. Marais. Activated sludge model no. 2., iwa scientific and technical report no. 3. London, UK, 1995.
- [5] M. Henze, W. Gujer, T. Mino, T. Matsuo, M. C. M. Wentzel, G. V. R. Marais, and M. C. M. van Loosdrecht. Activated sludge model no. 2d, asm2d. *Water Sci. Technol.*, 39(1):165–182, 1999.
- [6] U. Jeppsson. *Modelling aspects of wastewater treatment processes. Ph.D. Thesis*. Lund Institute of Technology, Lund, Sweden, 1996. Available from <http://www.iea.lth.se/publications>.
- [7] K. V. Gernaey, M. C. M. van Loosdrecht, M. Henze, M. Lind, and S. B. Jørgensen. Activated sludge wastewater treatment plant modelling and simulation: state of the art. *Environmental Modelling & Software*, 19:763–783, 2004.
- [8] E. Lindblom. *Dynamic modelling of nutrient deficient wastewater treatment process. M.Sc. Thesis*. Lund University, Lund, Sweden, 2003. TEIE-5175.
- [9] J. J. Buckley and T. Feuring. Universal approximators for fuzzy functions. *Fuzzy Sets and Systems*, 113:411–415, 2000.
- [10] J. J. Buckley and Y. Hayashi. Can neural nets be universal approximators for fuzzy functions? *Fuzzy Sets and Systems*, 101:323–330, 1999.
- [11] E. K. Juuso. Forecasting batch cooking results with intelligent dynamic simulation. In *Proceedings of the 6th EUROSIM Congress on Modelling and Simulation, Ljubljana, Slovenia, 9-13 Sept., 2007*, volume 2, page 8 pp. University of Ljubljana, Ljubljana, Slovenia, 2007.
- [12] E. K. Juuso. Intelligent modelling of a fluidised bed granulator used in production of pharmaceuticals. In *Conference Proceedings of SIMS 2007 - The 48th Scandinavian Conference on Simulation and Modeling, Göteborg (Särö), 3031 October, 2007*, pages 101–108. Linköping University Electronic Press, Linköping, Sweden, 2007.
- [13] E. K. Juuso. Intelligent dynamic simulation of a fed-batch enzyme fermentation process. In *Tenth International Conference on Computer Modelling and Simulation, EUROSIM/UKSim, Cambridge, UK, April 13, 2008*. The Institute of Electrical and Electronics Engineers IEEE, 2008.
- [14] R. E. Moore. *Interval Analysis*. Prentice Hall, Englewood Cliffs, NJ, 1966.
- [15] I. Ainali, M. Piironen, and E. Juuso. Intelligent water quality indicator for chemical water treatment unit. In *Proceedings of SIMS 2002 - the 43rd Scandinavian Conference on Simulation and Modelling, September 26-27, 2002, Oulu, Finland*, pages 247–252. Oulu, 2002.
- [16] E. K. Juuso. Applications of smart adaptive system in pulp and paper industry. In *Proceedings of Eunate 2004 - European Symposium on Intelligent Technologies, Hybrid Systems and their implementation on Smart Adaptive Systems, June 10-12, 2004, Aachen, Germany*, pages 21–33. Wissenschaftsverlag Mainz, Aachen, 2004.
- [17] I. Joensuu, M. Piironen, and E. Juuso. Dynamic simulator for dosing of water treatment chemicals. In *Proceedings of European Symposium on Computer Aided Process Engineering-15 (Escape-15), Barcelona, Spain, May 29 - June 1, 2005, Computer-aided chemical engineering, 20A*, pages 301–306. Elsevier, Amsterdam, 2005.
- [18] I. Joensuu, M. Piironen, and E. Juuso. Adaptive feedback controller for dosage of water treatment chemicals. In *Proceedings of AFNC'04 - the 2nd IFAC Workshop on Advanced Fuzzy/Neural, September 16-17, 2004, Oulu, Finland*, pages 127–131. Finnish Automation Society, Helsinki, 2004.
- [19] P. Teppola, S.-P. Mujunen, and P. Minkkinen. Partial least squares modeling of an activated sludge plant: A case study. *Chemometrics and Intelligent Laboratory Systems*, 38(2):197–208, 1997.
- [20] S.-P. Mujunen, P. Minkkinen, P. Teppola, and R.-S. Wirkkala. Modeling of activated sludge plants treatment efficiency with pls: a process analytical case study. *Chemometrics and Intelligent Laboratory Systems*, 41(1):83–94, 1998.
- [21] K. P. Oliveira-Esquerre, M. Mori, and R. E. Bruns. Simulation of an industrial wastewater treatment plant using artificial neural networks and principal component analysis. *Brazilian Journal of Chemical Engineering*, 19(4):365–370, 2002.
- [22] M. Heikkinen, T. Latvala, E. Juuso, and Y. Hiltunen. Som based modelling for an activated sludge treatment process. In *Tenth International Conference on Computer Modelling and Simulation, EUROSIM/UKSim, Cambridge, UK, April 13, 2008*. The Institute of Electrical and Electronics Engineers IEEE, 2008.
- [23] M. Heikkinen, T. Heikkinen, and Y. Hiltunen. Modelling of activated sludge treatment process in a pulp mill using neural networks. In *The 6th International Conference on Computing, Communications and Control Technologies: CCCT 2008, Orlando, Florida, USA, June 29th July 2nd 2008*. 2008.

6 Acknowledgements

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