An overview of the posters presented at Watermatex 2000. III: Model selection and calibration/ optimal experimental design

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Abstract This paper presents an overview of the posters presented in sessions 7 and 8 of the Watermatex 2000 conference. These posters present two aspects of modelling biological processes – model selection and calibration. Special attention is given to the papers on OED (Optimal Experimental Design), which is a method of optimising the data collection for model selection and calibration. The presence of these presentations at the conference highlights the continuing significance of modelling and stresses the requirement of improvements in modelling techniques. The papers provide some contribution to this end.

Water Science and Technology **Vol 43 No 7 pp 387–389**

Introduction

Models are used for the design and operation of biological processes. With tightening economic and environmental restrictions, the importance of optimal design and operation is increasing. This results in a continuing emphasis on the importance of the models, their selection and calibration. It is therefore not surprising that papers on these topics continually appear at international conferences.

Two sessions were devoted to modelling at Watermatex 2000. Various techniques available to achieve model selection and calibration were presented. They range from techniques using traditional unstructured, *ad hoc* techniques to more formalised approaches such as OED (Optimal Experimental Design). OED is a technique used to design experiments in order to be able to extract the maximum amount of information with a minimum effort. Depending on the goal of the study, different design criteria can be used: (1) to perform optimal model-selection from a list of candidate models, (2) to assign optimal values to model parameters, or (3) a combination of (1) and (2). Due to the recent popularisation of OED, it achieved status as a separate session at the conference.

In this review, the papers discussing model selection are reviewed first. Whilst OED can also be used for model selection it was not presented in the poster papers at the conference. Therefore this aspect is not discussed here. The papers discussing model calibration are reviewed next with particular emphasis on those using the OED techniques.

Model selection

The most important factor in selecting a model is the aim of the model. A model that is used to describe particular process dynamics will need to be more complex than one that is used for control purposes. Liu and Beck (2000) required a model of the transport and mixing of both solute and particulate matter in the activated sludge system so that nitrification could be adequately described in their system. Yamanaka *et al.* (2000) compare a mechanistic and a black box model in order to adequately predict sewerage stormwater inflow. Vaes and Berlamont (2000) discuss the physical characterisation of reservoirs.

Table 1 Comparison of experiments aimed at parameter estimation for the Monod kinetics. A "+" denotes high, a "–" denotes low, and a "±" denotes medium

	Batch	Continuous	Fed-batch
Saving effort, time, material	+	–	±
Ease of implementation	+	±	±
Parameter estimation quality	–	±	±
Parameter transferability to other operations	–	±	+
Balanced growth guaranteed	±	+	±
Opportunities for experiment design	_	±	+

Table 2 Model calibration techniques used by the authors

	Model	Calibration method	Remarks
Simeonov (2000)	Anaerobic WWT	Optimisation	
Kim *et al.* (2000)	IAWQ ASM1	Genetic algorithm	This was formulated as a type of optimisation problem
Vaes and Belamont (2000)	Reservoir model	Optimisation	Discusses the importance of the events used to obtain the data

Model calibration

Important factors in model calibration include the aim of the model, the data available or that can be made available, and the calibration technique that will be used.

The papers on OED deal in more detail with the former two factors. The study of Zec *et al*. (2000) shows that better parameter estimates can be obtained if the purpose of the model is taken into account. Vaes *et al.* (2000) investigated the possible simplifications of rainfall input series. These simplifications can be different for different applications. The simplifications that were applied are design storms, short selected rainfall series and modified single storm events. Sometimes simplified models appearing in combination with long term simulations seemed to be optimal.

Where will the data come from (on-line measurements or laboratory analyses)? How good is the data? How do we ensure that it provides enough information to calibrate the model? Versyck and Van Impe (2000) investigated this. To determine kinetic parameters for the Monod growth model, different modes of operation of bioreactors (continuous, batch and fed-batch) were applied. Different remarks and drawbacks on all 3 modes of operation are discussed. These are shown in Table 1.

The ability to collect sufficient good data was focused on by Liu and Beck (2000) who present a mobile process control laboratory that can be deployed to a field site and used to collect on-line data.

The papers of Simeonov (2000), Kim *et al.* (2000), and Vaes and Berlamont (2000) present three different techniques for the calibration of three different types of models. They are summarised in Table 2. It is evident that most techniques are based on optimisation procedures.

Conclusions

This paper has highlighted the importance of modelling in biological process design and operation. It reviews poster papers presented at Watermatex 2000 that discuss techniques used for model selection and calibration. Particular emphasis is placed on papers that use OED for model calibration. OED can be used to improve both model selection and calibration because the techniques are often more time efficient and produce more reliable and justifiable results than traditional techniques.

References

In: Proceedings of the 5th IWA international symposium on systems analysis and computing in water quality management (Watermatex 2000), Gent, Belgium, September 18–20, 2000 (preprint book).

Kim, S., Kim, C., Kim, J. and Ko, J. (2000). *Genetic algorithms for the uncertainty analysis of IAWQ-activated sludge model No. 1*. 8.48–8.55.

Liu, R. and Beck, M.B. (2000). *Solute and particulate transport characterization in the activated sludge process.* 8.33–8.39.

Simeonov, I.S. (2000). *Methodology for parameters estimation of non-linear models of anaerobic wastewater treatment processes in stirred tank bioreactors*. 8.40–8.47.

Vaes, G. and Berlamont, J. (2000). *Physically based calibration of reservoir models*. 8.56–8.63.

Vaes, G., Willems, P. and Berlamont, J. (2000). *Rainfall input requirements for urban drainage modelling*. 7.44–7.47.

Versyck, K.J.E. and Van Impe, J.F.M. (2000). *Review on operation modes in bioreactor experiments aimed at parameter estimation of the Monod growth kinetics*. 7.28–7.35.

Yamanaka, O., Nagaiwa, A., Yamada, F., Matsubara, S. and Nakada, M. (2000). *Sewerage stormwater inflow prediction based on system identification method with Hammerstein type of nonlinear model.* 8.64–8.71

Zec, M., Hvala, N. and Strmcnik, S. (2000). *Planning of the measurements used for parameter estimation of the simple activated sludge model. 7.*36–7.43.