Empirical Modelling Of Wastewater Treatment Processes – – An Approach to Model Reduction and Integration

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ABSTRACT

The aim of this project is to create an empirical model of a wastewater treatment plant (WWTP), which suits the requirements of integrated modelling. Such a model has to be simple enough in order not to increase too much the level of complexity and the computational demand when coupled with other submodels. The empirical model is identified using simulation data obtained from a mechanistic treatment plant model, this way a "model of the model" is obtained. The empirical modelling techniques used are Artificial Neural Networks (ANN) and Multivariate Polynomial Regression (MPR). As for the mechanistic model, an ASM3 coupled with a layer-based compressive gravity thickener is used.

KEYWORDS

Integrated water quality modelling, empirical modelling, activated sludge modelling.

INTRODUCTION

This project will use empirical surrogate models to integrate mechanistic models of the three major parts of the urban wastewater system (UWWS): the sewer system, the wastewater treatment plant, and the receiving water. Such a simulation model would make possible a combined evaluation of the three system components and could be used for research, for process control and optimisation and as support in planning and design of UWWS. The importance and utility of integrated modelling of the UWWS has become well-recognised in recent years. Integration of system components seems to become more and more common, new guidelines and regulations for water protection are stimulating the adoption of a holistic approach to water quality attainment at a basin scale of the system.

The present paper focuses on creating a wastewater treatment plant (WWTP) model in such a way, as to overcome the difficulties of model integration. These difficulties are identified as *model complexity* and *inconsistency* caused by the different state variables and timescales the submodels use. Our solution is to use empirical surrogate models to substitute for some of the mechanistic models, solving this way the problem of complexity and time-scale matching. We expect that the approach that we are developing will prove efficient enough to make integrated modelling more useful as a management tool.

The ultimate goal of this work is the integrated analysis and understanding of the dynamic behaviour of the UWW system, and the analysis and assessment of integrated control strategies having water quality as design criteria.

THE NEED FOR SIMPLE AND FAST MODELS

There are a few difficulties that are characteristic to integrated modelling. These difficulties have their origin in the fact, that the available submodels were not developed with the purpose to be later integrated. The main problems encountered are model complexity (consequently exaggerated computational demand and overparametrisation), different state variable sets used by the subsystems and differences in time resolution.

The individual components of the UWWS are modelled using complex mechanistic models. Each of these models is concerned about only one of the subsystems, often describing them with a considerable complexity. Linking the models together increases complexity further, resulting in overly detailed integrated models, which are hard to calibrate. Often these models are empirically underdetermined, being less accurate then simpler, but well calibrated models. Another disadvantage of overparametrisation is that it easily leads to the situation when the perspective is lost in details. Sometimes the combined models represent processes that are no longer important from the global system's perspective, but they contribute to the computational demand. One approach in handling this problem is that to use *simplified "surrogate" mechanistic models* instead of the detailed models of the subsystems. Results generated by a more detailed model can be used to calibrate the surrogate model. It is important to correctly identify the particularly significant processes that will be included in the simplified model, as well as which processes to omit (Haremoës and Madsen, 1999). A potential problem with this approach is that simplifying mechanistic models may eliminate their ability to simulate some performance features of the actual process.

Additional drawback of model complexity is that complex models with high computational demand are impractical for use in long-term simulations or in optimisation problems. Design and tuning of control strategies are typical optimisation problems, which require a high number of simulations, hence, short simulation times are desired (Meirlaen, 2002). The use of empirical models is proposed here, as an alternative to the complex mechanistic models.

The differences in time resolution constitute another barrier to model integration. The range of process time constants varies over a several orders of magnitude (seconds for the oxygen or flow dynamics in treatment plant and sewer, up to months for population dynamics in treatment plants and receiving water bodies). Integrated models should be able to estimate both the effect of an individual rain event, and the longer-term effects, such as accumulation of pollutants in the receiving water (Rauch et al., 2002).

MODELLING THE WWTP

Wastewater treatment plant models usually do not describe hydraulics and are merely concerned about the chemical and biochemical processes taking place in the treatment plant. Treatment plant hydraulics in most of the cases are not very well known and can only be approximated. That is why flow propagation through the reactors is not modelled explicitly. A commonly applied simplification is that the plant is considered as a few constant-volume-continuously-stirred-tank-reactors (CSTR) in series. This way the mixing phenomena are modelled. When the issue is the integrated model, the most important processes, in terms of their contribution to effluent quality) are the biochemical reactions taking place in the aeration basin together with the sedimentation in the clarifiers. The "state-of-the-art models" for activated sludge are considered to be the ASM1 – ASM3 models developed by the IAW (formerly IAWPRC) Task Group. These models include the processes of heterotrophic growth, nitrification, denitrification, and biological and chemical phosphorus removal processes. The ASM models has been "updated" several times since the first release of the ASM1 and most of the problems identified in the earlier versions has been corrected. The models are based on COD units, the ASM3 has a total organic carbon (TOC) - based version as well (Henze et al., 2000; Schütze et al., 2002).

The secondary clarifier is responsible for the treatment plant's performance, and plays a central role in the integrated wastewater management. The secondary clarifier serves to keep the biomass in the system while producing a high quality effluent. The clarifier is designed for a certain hydraulic and solids loading, over which it becomes overloaded and the sludge is washed out. This situation happens often during wet weather conditions, and as a consequence of it, the activated sludge becomes diluted, affecting the plant performance much longer then the causing rain's duration. In order to protect the plant from washing-out, the inlet flow to the treatment plant has to be limited to a maximum value, which does not causes too high sludge loss. A good settling model is needed which can describe the settling of particles and the thickening phenomena accurately in order to be able to predict the point where the clarifier gets overloaded (Harremöes et al., 1993; Capodaglio, 2002).

The clarifier models are based on settling functions, which evaluates the settling velocity of the particles, depending mainly on the solids concentration. Simple models consider only the vertical movement, but there are some two- and three-dimensional models as well, considered to be the state-of –the-art models. These models describe the settling phenomena somewhat closer to realty, but their level of complexity makes them unfit for integrated modelling. 3-D models are useful for final design and optimisation of settling tanks, to find the best geometric form and baffle arrangement. Biological processes, such as hydrolysis or denitrification, can be included in the models.

For the purpose of integrated modelling it is unnecessary to use such a sophisticated clarifier model. The most popular models are simple 1-D models based on the layer approach (e.g. the model proposed by *Takács et. al. 1991*), 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 model because they give a reasonable approximation of the sludge balance and of the sludge shift from the aeration tank to the secondary clarifier. These models can be calibrated with actual plant data. Conversion processes are not included in these models, being considered less important. Use of 2-D models might be possible as well, they can simulate the effluent suspended solids concentration better and 2-D models coupled with activated sludge models have already been applied in plant design. The increase in complexity these models induce limits their use in integrated water management (Ekama et al., 1997).

MODEL REDUCTION – THE MECHANISTIC APPROACH

As outlined above, existing treatment plant models are fairly complex and need to be simplified in order to make them useful for long-term simulations and optimisation problems. As the ASM models are mechanistic models (derived from more fundamental principles, i.e. based on the equations and laws of biological and biochemical transformations) the most plausible solution is to stay with these models, but to eliminate those equations, which are of minor influence to the simulation results. The models obtained by this knowledge-based reduction are the so-called *mechanistic surrogate models*, which are faster and less, but still sufficiently accurate.

The complete ASM3 model uses 13 differential equations to dynamically model activated sludge systems. Two equations have been identified as "useless" (in the sense that their lack does not affect the performance of the model): the direct calculation of gaseous nitrogen and that of total suspended solids (TSS). These states are used only to close the mass balances and can be omitted

(Direct caculation of TSS may be included in the last tank on the reactor line, to predict the input for the secondary clarifier. This way we can get rid of the two unit-converters between the settler tank and bioreactor). The equation of alkalinity is also subject to elimination, as alkalinity does not seem to be a limiting factor for the processes modelled. Replacing the oxygen dynamics by an on/off function is a frequently used reduction method as well, but seriously reduces the model performance. Any further simplification of the model causes big losses in model accuracy (Meirlaen, 2002).

The secondary clarifier model should not be simplified too much, the commonly used layer-based clarifier model is already too simple. On the contrary, it is desirable to model compression in the settler model, to simulate the thickening of activated sludge, thus to be able to perform more accurate predictions of the sludge blanket level. As a conclusion, one could say that a considerable simplification of the treatment plant model could be achieved only at the expense of model accuracy. In addition, even in the case of a radical model reduction the gain in calculation time might be insufficient to justify the errors introduced by the simplifications.

A MODEL REDUCTION STRATEGY USING EMPIRICAL MODELS

In many cases, when a system is too complicated to predict from fundamental principles, we resort to empirical modelling. Literally, this means modelling based on experience. In practice, an empirical mathematical model is an equation whose coefficients are adjusted to match a given set of data.

In current work being carried out at the University of Pavia, we analyse the possibility of using empirical models instead of simplified surrogate models in order to obtain simple, fast and accurate models. These empirical models would be more for the purpose of integration. We use two different empirical methods in order to find a model, such that if we gave it values for the input variables, it would predict what the output would be. We believe the Artificial Neural Networks and Multivariate Polynomial Regression to be the two best methods to model the complex and highly nonlinear wastewater system. The methods are described in detail elsewhere, below is just a brief presentation of them, as well as a short comparison to other methods.

Artificial Neural Networks (ANN) are mathematical structures that imitate structures of the nervous system in a highly abstract way. An ANN consists in a collection of nodes and links between the nodes, each node representing a neuron. The nodes are organised in layers. An input layer, together with an output layer and one or more hidden layers forms an ANN. These highly interconnected simple processing elements offer an alternative to traditional approaches in computing. ANNs are able to learn from large sets of examples, and can generalise from the examples. The process of learning from examples is called training.

Neural networks are particularly useful for function-approximating problems, which have lots of training data available, but to which hard and fast rules cannot easily be applied. Trained with sufficient data, they can adequately describe multivariate systems with nonlinear dynamics, such as the biochemical processes in the biological wastewater treatment.

Multivariate Polynomial Regression (MPR) is a mathematical technique that identifies a polynomial equation that describes the relationship between input and output data. This determination is called fitting the model. The procedure is similar to the multilinear regression (MLR), but unlike MLR models, the MPR models are able to describe nonlinear behaviour including interaction. Interactions are where the sensitivity of an outcome to an independent variable depends upon the level of another independent variable. To describe complex response surface shapes, higher exponents are needed in the equation terms. As the number of variables and/or exponents increases, the models start to get too complicated. One way to limit model complexity is to weed out individual terms that don't contribute to the predictive ability of the model. The statistical technique of regression includes methods to determine which terms are significant. The resulting model will use a number of terms which is sufficient and enough to describe the input/output relationship (Vaccari and Wojciechowski, 1995).

The main advantages of MPR over ANN are that the resulting model is an explicit equation, which can be easily communicated or used for further analysis, and that it is parsimonious. On the other hand ANN fits better for very high-dimensional tasks and does not "explode" outside data ranges.

Using empirical models instead of fundamental or mechanistic models has several advantages. First, these models are able to describe system behaviour without fully understanding the system's processes, by only using the input and output data. This advantage does not apply to the current application, as we "model the model", namely the empirical models are created using the results obtained by running the mechanistic model. However, once the model found (by training an ANN or fitting the equations using MPR) the computational capacity needed for future predictions is very low. Thus, the models obtained are optimal to be integrated with other submodels, as they do not increase too much the overall computational demand of the integrated model. These empirical models are fast enough to be used in real-time applications, such us the integrated control of wastewater treatment plants. They allow for a fast consideration of long term effects and are easy to use for optimisation studies.

As compared to the mechanistic models, ANN or MPR models are of reduced spatial and temporal scale. In this specific case, the wastewater treatment plant becomes a point, there is no nitrification/denitrification tank or secondary clarifier with many layers, but only a simple model which gives a prompt answer to the input variables. The problems related to the time-scale are skipped, because the new models can be developed to match the time scale desired (Christodoulatos, Vaccari, 1993; Vaccari and Wojciechowski, 1995).

"MODELLING THE MODEL"

In this approach, the first step is to create a good mechanistic model, which has to be calibrated and tested. This is then used to generate data sets for use in developing the empirical models. The empirical models will be identified and fitted to the test data, and validated with independent data sets.

This approach will be developed initially using the wastewater treatment plant portion of the UWWS. The modelling objective is to create a model of a biological wastewater treatment plant that is simple enough to permit fast simulation and can be easily integrated with the other parts of subsystem.

The mechanistic treatment plant model is based on an ASM3 model, which is considered to be the state-of-the-art model in the field. Biological phosphorus removal is not included, because no data are available for calibration (there are just a few treatment plants in Italy with biological P removal) and partly because of the increase in complexity that phosphorus removal requires. Considering the phosphorus accumulating organisms (PAO-s) and the storage/growth/lysis processes they participate in, P removal doubles the number of equations in the model. Phosphorus removal can be added to the model later if necessary (Henze et al., 2000).

For more flexibility, the mechanistic model has separated tanks for nitrification and denitrification. These tanks will be coupled with the clarifier. For the secondary clarifier a compressive gravity thickening model is used. This model is similar to the other 1-D settling models, but includes compression effects. Thus the sludge blanket's level can be predicted. This is very useful in optimisation studies, where the hydraulic overload/underload margin has to be estimated with a high accuracy. This advantage was considered more important then the small increase in complexity caused by the extra compression gradient term (Vaccari and Uchrin, 1989).

Modelling work will is carried out in MATLAB™/SIMULINK™ environment. This allows for advanced flexibility, the model can be used later for integration with other mechanistic models if needed. A flexible architecture is necessary for different modelling studies.

The data for calibration is being collected from full size wastewater treatment plants and surface waters using submersible UV-VIS spectrometers. The calibrated model will be then tested with another set of data. After testing, this mechanistic model will be used to simulate a large number of different scenarios. The results of simulations will constitute the training data for the ANN and for the MPR. The obtained ANN or MPR models then can be linked with the river and sewer model and can be used in real-time applications or for evaluation of longer-term effects.

FUTURE PERSPECTIVES

It is not questionable that a holistic approach of the urban wastewater system is desired for an efficient wastewater management. Such a holistic approach calls for the use of integrated models. There will still be a need for improved mechanistic models, either for direct integration or integration via surrogate empirical models. Integration with geographical information systems will be (or it already is) another step to the basin-scale river management. Integrated models of future will probably combine the urban wastewater system with detailed watershed models, modelling point-source and diffuse pollution as well as infiltration and groundwater quality.

These very detailed, comprehensive models will not be suitable for the purpose of integrated control for a long time, mainly because of their exaggerated computational demand and the large amount of adjustable parameters they need for calibration. One may say, that the advance in computer technology will bring the solution of the computational demand in a few years. We have to realise that the main obstacle in the way of the widespread application of integrated models is mainly model complexity (beside of the administrative fragmentation, characteristic to the water management of the past) and less the lack of computational capacity. None of the fastest computers will solve the problem of overparametrisation and excessive data demand. Real-time control needs fast and simple models, and empirical models offer a good alternative instead of simplified surrogate models.

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