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System process modelling report

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Publication date:
2005

Document Version
Publisher's PDF, also known as Version of record

System Process Modelling Report

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EU Research Training Network
HPRN - CT-2001 - 00200

Getting Systems Engineering into Regional Wastewater Treatment Strategies
WWT & SYSENG

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Document Release Date: March 2005
Version: Final
Project Deliverable: System Process Modelling Report

Lindblom, E.; Raduly, B. & Mikkelsen, P.S. (Eds.) (2005): System process modelling report. Environment & Resources DTU, Technical University of Denmark, 116 pp. incl. annexes.

This is a net-publication that can be downloaded from
http://www.er.dtu.dk/publications/fulltext/2005/MR2005-018.pdf

Published by:

Environment & Resources DTU
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Bygningstorvet, Building 115
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Acknowledgement:

The work leading forward to producing this report was funded by the European Commission through the Research Training Network "WWT&SYSENG: Getting Systems Engineering into Regional Wastewater Treatment Strategies", which runs from February 2002 to January 2006 (contract HPRN-CT-2001-00200).

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1. Introduction

The present ”System Process Modelling Report” (SPMR) is one of the main deliverables of the European Research Training Network called “WWT&SYSENG: Getting Systems Engineering into Regional Wastewater Treatment Strategies”, which runs from February 2002 to January 2006 and is funded by the European Community under the Human Potential Programme (contract HPRN-CT-2001-00200). The research area of the WWT&SYSENG Network is about developing the understanding and tools to control wastewater treatment processes and manage wastewater discharge into the environment, see further information on www.wwtsyseng.org.

The basis for the report was laid during a project training workshop held at the Technical University of Denmark from 17-19 September 2003. Each of the 9 WWY&SYSENG Young Researchers (YRs) attending the workshop prepared a short paper based on their own work prior to the workshop and presented it orally. Constructive comments were made by pre-assigned moderators and discussions of the presentation and paper followed. This was the first time several among the YRs presented orally to an international audience and discussed their work with peers. Senior researchers affiliated with the network furthermore reviewed the papers, and the YRs then revised their papers after the workshop. The revised papers are listed below and can be found as annexes to this report, numbered as shown.

	Young Researcher (principal author)	**Paper title**
1	Flavia Camilleri University of Strathclyde, UK	The ASM2d model: Implementation in MatLab and description of the processes
2	Farid Benazzi University of Strathclyde, UK	Application of extended Kalman filter to activated sludge process
3	Joanna Boguniewicz University of Pavia, Italy	A description of data collection – The hydrological and water quality modelling using GIS techniques
4	Marie O’Brien University of Strathclyde, UK	Predictive control of a simple waste water plant
5	Botond Raduly University of Pavia, Italy	Empirical modelling of wastewater treatment pro-cesses – an approach to model reduction and integration
6	Irina Comsa Imperial College, London, UK	Integrated model of the urban wastewater system into a river context
7	Bianca Chindris Technical University of Crete, Greece	Sewer networks: Water flow and quality modelling
8	Cristina Lazar Universitat Autonoma de Barcelona, Spain	Control of a WWT plant: Stating the problem
9	Gladys Tapia Universitat Autonoma de Barcelona, Spain	Dynamic and steady-state modelling of pilot-scale WWT plant using the ASM2d model

The aim of the System Process Modelling Report is to aid the YRs understand the regional wastewater system and the integration of the subsystems therein. To enhance learning and networking among YRs they were all involved in preparing the report. Groups of YRs were formed under the supervision of senior researchers from the network to review literature and prepare reports on individual components of the integrated system. Chapter 2 provides a review of system process modelling work related to integrated urban wastewater systems and is composed of these multi-authored contributions on 1) Environmental models, 2) Sewer network models, 3) Wastewater treatment plant models, 4) River water quality and river basin models, 5) Control interfaces, and 6) Integrated wastewater system models.

The third chapter of the report briefly discusses the status of the project, i.e. how the work of each of the YRs fits into the overview provided in Chapter 2 and what the future plans were after the workshop. Sections discussing the contributions and perspectives on 1) sewer modelling, 2) WWTP modelling, 3) river basin modelling, 4) control and 5) integrated wastewater system modelling have been edited and written by two YRs, Erik Lindblom and Botond Raduly, during a period in autumn 2004 where the latter visited DTU during a temporary leave from University of Pavia. Erik Lindblom and Botond Raduly furthermore edited the report in collaboration with Peter Steen Mikkelsen from DTU. Erik Lindblom was not yet involved in the WWT&SYSENG network at the time of the Copenhagen workshop and thus used the editing work as an opportunity to get acquainted with the work of other YRs in the network.

2. Review of system process modelling of integrated wastewater systems

2.1. Environmental models

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By simulating the processes that occur in nature, environmental models make possible the study of environmental systems and the assessment of the environment quality. From the output of these models we can draw conclusions regarding the state of the environment and we can forecast the short or long term deterioration or amelioration of it. Typically, mathematical models are used to study processes of great complexity. Since environmental systems are affected by a huge number of reactions and other factors yielding long time constants and non-linear behaviour, models often provide indispensable tools for the environmental science community.

Models are built in various areas of science and engineering to serve specific purposes. In disciplines concerned with water issues, environmental models most often eventually converge with questions related to recipient quality. By tracing different substances in the water system, the fate models can forecast pollutant levels in water bodies that could endanger certain aquatic species. With the help of environmental models oxygen depletion and eutrophication caused by long-term accumulation of nutrients can be forecasted. The benefits of such results are evident, since they can be used to minimise risks for e.g. partial extension of different aquatic species or the depopulation of the water body in question.

2.1.1 Pollutants

The endless list of pollutants in wastewater includes substances resulting from all kinds of human activities. To mention a few, faeces, urine, soaps, detergents, pesticides, herbicides, industrial and pharmaceutical product chemicals and heavy metals from roofs and hydrocarbons from traffic areas all contribute to pollution loads. It is impossible to model all of them and therefore necessary to identify the most important ones, from the water quality's point of view. Pollutants can be classified in many ways e.g. according to their phase, chemical nature, provenance or possible environmental effects. For modelling convenience pollutants are often divided into the following classes: sediments, oxygen-consuming organic matter, nutrients, heavy metals and man-made organic pollutants (Table 2.1). Water supply, urban drainage and wastewater treatment systems were originally designed to solve conventional problems (supply of potable water, flooding prevention and sanitation) and water quality research was focused on the modelling of organic matter and of nutrients. In more recent years, man-made xenobiotic organic compounds (XOCs) that are hormone-active and toxic to natural ecosystems are being of rising concern. Awareness of these is increasing because impacts on humans are reported, detection limits are decreasing, and new priority pollutants are being discovered.

Table 2.1. Examples of pollutants, their origin and environmental effects.

Pollutant type	**Examples of origin**	**Examples of environmental effect**
Sediments	Soil erosion, leaf litter, grass, building weathering, vehicle wear etc.	Changes in benthic communities, resuspension
Nutrients	Households, agriculture, atmosphere, detergents, animal excretion etc.	Eutrophication of surface water, algae blooms
Organic matter	Decaying organic matter, Sewer overflows, septic tank leafs	Oxygen depletion, negative impact on aquatic species
Heavy metals	Vehicle wear, roofs weathering, water pipes, illegal discharges	Acute aquatic toxicity and long-term accumulation in fishes
Xenobiotic organic compounds	Pesticides, herbicides, illegal discharge, septic tank leaks, pharmaceuticals	Aquatic toxicity, persistent and bioaccumulating

The origins of contamination can be divided into point and diffuse sources of pollution. Point source pollutions come from specific, identifiable sources such as a single smokestack or pipe. In contrast, diffuse pollutants originate from less defined sources such as agricultural and urban runoff. The type, which one assigns to a pollutant from a certain environmental or technical unit, depends on the assigning modeller. A scientist or engineer working with river basin models would for example most often regard combined sewer overflows as a diffuse pollution. Knowledge about locations and magnitudes of the possibly present overflow structures within the basin area is often missing. However, the modeller working with integrated wastewater system models considers the overflows as point-sources of pollution. The way how WWTP effluents are treated provides another example. On the one hand an industrial wastewater treatment plant, located beside a river, is considered as a point-source pollutant in a river quality model. On the other hand, if several WWTPs are encircled by a model system boundary and their expected environmental impacts are located far downstream, the effluents are treated as diffuse pollutants.

The different models used to solve wastewater-related problems have to describe a very wide range of processes that occur in the different subsystems of a wastewater system. The task is complex because in ecosystems there is a tight coupling between physical, chemical and biological processes, each with their characteristic spatial and temporal scales. A graphic showing the variety of processes to be modelled, together with their temporal and spatial scales is seen in Figure 2. (Lijklema,1998).

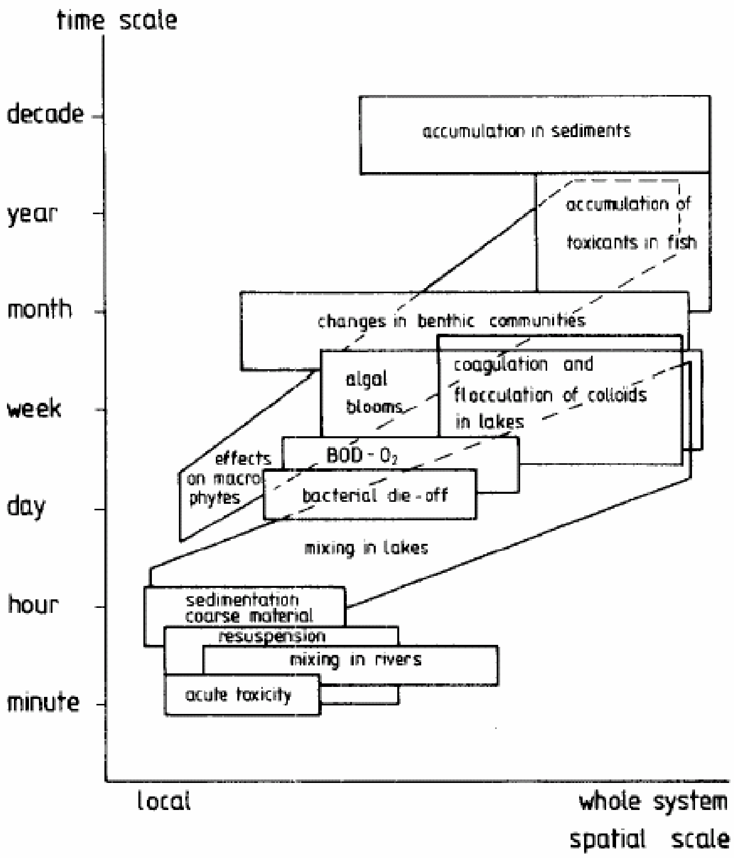

Figure 2.2. Relationship between process rates and spatial scale of effects.

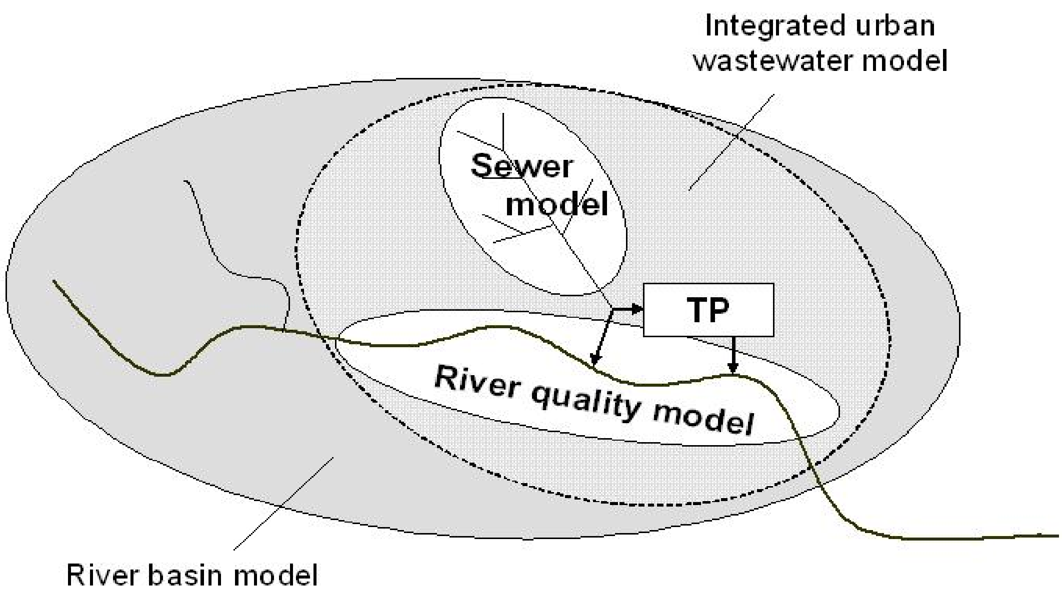

Figure 2.1. A schematic illustration of the different model scales applied in the WWT&SYSENG Research Training Network.

2.1.2 Model scales and pollutant sources

The goal of the WWT&SYSENG project is to further the understanding of large scale wastewater systems and their effect on the environment. The participants work with the following models: (1) sewer models; (2) wastewater treatment plant (WWTP) models; (3) river quality models; (4) integrated wastewater system models and (5) river basin models. The five types are illustrated in Figure 1. A summary of the WWT&SYSENG project is given in Butler *et al.* (2004).

The **sewer model** describes the sewer system, where wastewater and rainfall runoff is transported from the catchment area to the wastewater treatment plant. If the amount of runoff exceeds the given hydraulic capacity of the system, wastewater is discharged directly to the recipient via combined sewer overflows. Historically, the sewer system has been regarded just as a pipe structure transporting wastewater to the WWTP and receiving waters, thus many sewer models describe only the transport of the pollutants and neglect the conversion processes. Today it is clear that the network also acts as a biological/chemical reactor and much effort is put on appropriate descriptions of both the hydraulic processes and transformations of compounds within it. Examples of important sewer conversion are the respiration of oxygen, production of hydrogen sulphide and production of easily degradable substrate that is greatly needed for nutrient removal in the subsequent WWTP (Huisman *et al.,* 2003; Vollertsen and Hvitved-Jacobsen, 2000). Chapter 2.2 provides aspects on sewer system modelling.

The input of the treatment plant is one of the outputs from the sewer system. The **wastewater treatment plant model** describes the biochemical and physical processes involved in the technical purification of wastewater. These include biological processes where organic matter and nutrients in the wastewater are converted to a particulate fraction, which can be removed by means of physical separation processes. Since the activated sludge process is the most widely used wastewater treatment method, most WWTP models are concerned with this treatment system. A state-of-the-art description of treatment plant modelling is given in Chapter 2.3.

A **river quality model** contains mathematical descriptions of the physical-chemical-biological transformations and of hydraulic transport processes taking place in rivers. Water flow, mixing, sediment transport, reaeration and biochemical transformation processes of important river quality components are often incorporated in these models. Algal production, benthic processes, as well as kinetic algorithms for temperature variations may also be included in river quality models. River water quality models, integrated with the river basin models are discussed in Chapter 2.4. A **River basin model** describes a river with the surrounding catchment, it is basically the model of a river and its tributary streams coupled together and complemented with the catchment description. The river basin models can describe hydraulic and transport phenomena and in some cases, also river quality processes. The river basin scale models may also consider spatial variations, using GIS technologies, soil maps, land use maps etc. The input for a river basin model is meteorological data, characteristics of the catchment area, sewer overflows and WWTP effluents. River basin models are sometimes mixed up with river water quality models, although some of them do not include river quality processes. A summary of commonly applied river basin models is given in Chapter 2.4.

Control interfaces are becoming more and more common in wastewater treatment plants, sewer systems and river systems and consist of measurements, controller computations and manipulating actuators. Chapter 2.5 provides an overview and briefly discussed unit process control, limitations of control and supervisory (integrated) control.

Integrated wastewater system models combine the sewer, the WWTP and the river models. Unlike river basin models, the current integrated models are not linked with GIS systems and do not contain explicit description of the catchment areas. More about these models can be read in Chapter 2.6.

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2.2. Sewer Network Models

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[1]Technical University of Crete, [2]Imperial College, [3]University of Strathclyde

2.2.1 Introduction

The sewer system model is part of the global model, which integrates several sub-systems including the urban sewerage and wastewater treatment networks. Models of the sewer system are important while estimating the exact locations of combined sewer overflows (CSOs), the amount of pollutants in the sewer and also for evaluating control strategies.

There are several levels of complexity based on which, models of the sewer network are developed. The appropriate modelling approach depends, among other things, on the results that need to be obtained. Beyond the complexity level, a fundamental distinction between sewer models based on their information contents can be done. A sewer model may consider either (1) the quantity of the water flow (hydraulics) through the sewer network or (2) both the quantity and quality (pollution level) of the water, in an integrated way. Since this research project aims at developing control strategies that considers quantity and quality aspects, approach (2) above is adapted.

2.2.2 Literature review

The sewer network, a part of the urban wastewater system, was considered till the 1970's as only a means of conveyance of the wastewater towards the wastewater treatment plant or the receiving waters. Therefore, the mathematical models, developed between the 60's and 80's, have been focused mainly on design and/or simulation of the sewer network flows from a hydrological and hydraulic point of view (surface runoff and washoff and sewer flow). Further in time, increased knowledge about the negative impacts generated on receiving waters by combined sewer overflows, pushed the research towards a new direction. The sewer system models started to engage not only hydraulics, but also pollutant and sediment transport processes as well as biochemical transformations. New tendencies in control and optimisation strategies (for the sewer network only, for the sewer network and the WWTP and finally for the whole urban water system) lead to an increased model complexity. Meanwhile, the prevailing urge to further develop the management of comprehensive information about the drainage system boosted hydroinformatics, an area connecting drainage models with data management tools and graphic representations (GIS – geographical information systems). Models integrated with GIS technologies are further discussed in Section 2.4.

In the beginning, the mathematical models employed were predominantly empirical, while nowadays they are becoming mostly mechanistic. Equations used in flow models are frequently those known as the Saint-Venant equations, but this is not the only method to model the drainage system. There are also models employing the linear or non-linear reservoir method, hydrographs and other methods (Schlutter, 1999). Regarding quality models, the equations that describe the processes are based primarily on a set of advection/dispersion equations or on the representation of continuously stirred tank reactors (CSTRs). Biological and chemical in-sewer transformations are modelled by adding the corresponding reaction rates into the flow equations. Many of the biological processes that take place in-sewer are not completely understood and the adapted descriptions often mimic those used in traditional WWTP models (e.g. ASM1, ASM2d, ASM3 and AEROSEPT). Reviews and analysis of sewer system modelling can be found in Asheley *et al.,* (1999; 1996); Bertrand-Krajewski (2002); Bertrand-Krajewski *et al.,* (1993); Butler and Davies (2000), Huisman and Gujer (2003), Mourato *et al.,* (2003).

A great variety of software packages are today available on the market. Examples include HSPF, ILLUDAS, STORM, SWMM, MIKE-SWMM, FLUPOL (Bujon *et al.,* 1992), MOSQUITO, SIMPOL, MOUSE-TRAP (Crabtree *et al.,* 1995), Wallingford packages (HydroWorks, HydroWorks DM) (MarSaleck *et al.,* 1993), KOSIM and many others. Overview of software for simulation of sewer system is given by Ahyerre *et al.,* (1998); Gent *et al.,* (1996); Tech. University of Darmstadt (2001) and others.

As mentioned above, the mathematical modelling of water flow in sewer networks may address either the quantity of the water through the sewer network, or taking both the quantity and the quality of the water into account. Water quantity modelling reflects processes that take place in the different elements of the sewer network by use of known laws of hydraulics. Water quality modelling addresses the dynamic space-time distribution of the amount of pollutants within the sewer network and at its sinks as well as the sediment transport. It should be noted that water quality aspects include both pollutant concentrations, the sediment transport and physical, chemical and biological transformations, which all take place at the same time.

2.2.3 Model formulation: the sewer network flow

In the following, a summary of the model described in Chindris (2003) is given. A set of elements are used to build a combined sewer network model. In these elements, different processes take place, for example the water storage in the reservoirs or in the sewers and the merging of flows in the network nodes, etc. The elements are:

Link elements: There are two types of link models, namely hydrodynamic link elements and hydrological links elements. The hydrodynamic link element is used where a non-negligible storage of volume is caused in a sewer stretch by backwater or by flow regulation using throttle gates. The mathematical model applied for this element consists of the Saint-Venant equations, namely the continuity equation and the momentum equation, which describe quite accurately the dynamic behaviour of the flow along a sewer stretch. The hydrological links are used to model the link elements if the sewers have a relatively steep slope and if the spillback is less significant. The hydrological links are not strongly based on physical laws and are simpler than the hydrodynamic links. Consequently, their application requires parameter calibration with real data.

Reservoirs: The mathematical model applied for this element consists of a continuity equation. A reservoir can have an overflow capability if an overflow weir is present and the water height rises over the height of the weir. Under the assumption that there is no spillback downstream of the weir, the overflow is calculated by using an equation that combines the Poleni and the Toricelli formula.

Control gates: Control gates are used to control the flow in a combined sewer network, and they are usually placed at the end of the sewer stretches or at the low points of the reservoirs. In general, the outflow from a control gate is characterised by the upstream and downstream water levels of the control gate; but if there is no back pressure, it depends only on the upstream water level of the control gate.

Nodes: The processes, which take place in the nodes of a sewer network, are the propagation and the merging of flows, whereby the total inflow to the node is equal with the total outflow from the node.

2.2.4 Model formulation: the sewer sediment transport

The modelling of the water quality in a sewer network must first consider the phenomena, which occur before the sewer network (such as sediment build-up on the surface and sediment washoff from the surface), followed by the modelling of the processes within the sewer system (for example deposition and erosion).

Water and sediments are entering the pipe from upstream and are transported out of the pipe. There are two sediment processes that can occur in the pipe: (1) the sediments are deposited or (2) they are resuspended. Which of the two processes that occur (or none of them) in a certain pipe and at a certain moment depends on the level of the bed shear stress. The most common way to calculate the bed shear stress is to neglect the fact that there may be deposits on the bottom of the pipe increasing the bed shear stress. Generally, deposition depends on the hydraulic conditions, the characteristics of the sediments (particle sizes and weight), the bed shear stress, the available space for deposition and the concentration of suspended solids. Erosion depends on the sediment characteristics, the available space for erosion, and the discharge in the pipe.

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2.3. Wastewater treatment plant models

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The increase of sensitiveness to environmental problems in the last decades and the consequent more stringent environmental regulations adopted have had a high impact in the wastewater field. New limits on nutrient discharges introduced in the last years have resulted, for example, in the necessity to adapt the WWTPs to them. Additionally, a higher wastewater treatment process standard is required especially to prevent problems during critical load conditions. Thus, the introduction of control systems is often needed. This Subchapter is concerned with Wastewater Treatment Plant (WWTP) models and is organised as follows:

- Overview and generalities of WWT plant modelling
- Mechanistic models
- Data driven models
- Applications
- References

2.3.1 Overview and generalities of WWTP modelling

To find the optimal plant design and control combination, models and simulation software have begun to be used in the WWTP field in the last decades. This reproduces what happened 30 years before in the chemical processes sector and hopes for the same benefits. However, the main difference is the high complexity of WWT processes and plants which can reduce the efficiency of their modelling.

The WWTP performance is related to site specific conditions, which cannot be completely reproduced in a general model. Moreover, the influent characteristics are highly variable and often uncontrollable. Then, it is not totally possible to simulate the real situation. Regarding modelling of activated sludge (AS) systems, in which the greatest percentage of studies has been carried out, the situation is even worse:

- The biomass is composed by a large variety of microorganisms, which have their own growth parameters (often not completely known) and that react differently to variations of pH, temperature, dissolved oxygen, toxic substances and nutrients inside the plant and during the time. Simulating lumped biomass fractions (e.g. heterotrophs/autotrophs) is limiting.

- Not all processes involved in the AS treatment are completely clear: the influence of hydrolysis processes and biological phosphorus transformations need to be further studied.

The AS models presented by the IAWQ Task Group on Mathematical Modelling for Design and Operation for Biological Wastewater Treatment Processes are considered the state-of-the-art of AS modelling. Their application to the real world has to face the intrinsic problems of the WWTP modelling, particularly the huge variability of conversion factors, kinetic parameters and stoichiometric coefficients required by the models. In fact, in the literature a wide range of values is reported and only site measurement (not available for all the parameters/coefficients) can provide the real ones. Furthermore, also in the lucky case, in which it is possible to define their values, e.g. measurement noises and temperature variations have to be taken into consideration.

It is logical that the complex characteristics of the WWTP will result in complex models. One might think that the more complex the model is, the more properly it simulates the system, but this is not always true. An increased model complexity means formation of a larger cluster of parameters that must be estimated and thus, increased uncertainty. An example of this is the set of Monod functions used to model nutrient limitation in biological growth. Since the childhood of AS models (Dold *et al.,* 1980) to the biological phosphorus removal models of today (Henze *et al.,* 1999) the number of Monod factors in the growth equations have been increased significantly. Each of these includes one half-saturation constant that must bee estimated. Even if an ambitious experimental campaign is set up to identify these, the non linear characteristics of the functions anyhow involve that several sets of parameter values can give approximately the same results.

A common misunderstanding is that if a model does not predict reality exactly, it is useless. In truth, the demands on model performance must be correlated with the application. In control design for example, a model linearization is often required (Smets *et al.,* 2001). Although the linearization results in a significant information loss, these models have been proven to be useful.

The problem with physical identification of the kinetic and stoichiometric parameters for all the equations is partially avoided by choosing black box rather than mechanistic models. The choice between the two structural model forms is driven by different problem solving attitudes. Black box (or empirical) models represent the system through a mathematical function based only on input and output data. Since black box models are created using a set of training data, they sometimes suffice from having an enclosed validity region i.e. a well-calibrated black box model might describe one WWTP (or one type of input) well while giving poor results for others. Another drawback with empirical models is that it per definition is impossible to look inside their process formulations.

Because of the disadvantages with both the mechanistic and empirical approaches, grey-box models represent an alternative that several modellers have used. Grey box models combine the main process equations from the mechanistic models with empirical available data relationships and mathematical formulations from black box models. This kind of models, especially because of their use of mathematical estimation algorithms, is particularly suitable for automatic control purposes.

In reality completely mechanistic models do not exist, both because the equations used to represent the processes are in any case empirical (it has been shown how other equations, confronted with the Monod equation, are equally valid), and because in order to simplify a model that otherwise would be too complicated to understand, to verify and to validate with real data, simplifications, assumptions and approximations are always introduced.

Another trend of the last years has been to use stochastic analysis (data described in terms of statistical probability distributions) instead of deterministic data (single input and output). This has made the identification and verification of the models easier, whereas for deterministic models a stringent calibration is impossible. Moreover, pure deterministic models results often show deviations from the reality. The choice between deterministic or stochastic models depends on the scope of the model.

2.3.2 Mechanistic models

In 1983, the International Water Association (IWA) formed a task group, which were to promote development, and facilitate the application of, practical models for design and operation of biological wastewater treatment systems. The goal was firstly to review existing models and secondly to reach a consensus concerning the simplest one having the capability of realistic predictions of the performance of single sludge systems carrying out carbon oxidation, nitrification and denitrification. The final result, with many basic concepts adapted from the AS model defined in Dold (1980), was presented in 1987 as the IAWQ Activated Sludge Model No.1 (ASM1). Several versions and modifications of the original model have been developed since 1987. The Activated Sludge Model No. 2d was presented in 1999 and includes enhanced biological phosphorus removal (EBPR). Experiences from the ASM1 and ASM2d formed the bases for the Activated Sludge Model No.3 (ASM3), also presented in 1999. Still, the original ASM1 is probably the most widely used for describing WWT processes all over the world (Jeppsson, 1996; Roeleveld and van Loosdrecht, 2002). The ASM1 has proved to be a reliable tool for modelling nitrification-denitrification processes and has initiated further research in modelling and wastewater characterization. ASM1, ASM2, ASM2d and ASM3 are tastefully put together in Henze *et al.* (2000).

The activated sludge process is the most popular biological wastewater treatment method. In this a bacterial biomass suspension removes the pollutants from the treated wastewater. An activated sludge wastewater treatment plant (WWTP) can achieve removal of organic carbon substances, biological nitrogen removal and biological phosphorous removal. A very useful review on the historical evolution of the activated sludge process was carried out by Jeppsson (1996).

The activated sludge model no. 1

ASM1 was primarily developed for municipal activated sludge WWTPs and describes carbon and nitrogen removal, with simultaneous consumption of oxygen and nitrate as electron acceptors. Chemical oxygen demand (COD) was adopted as the measure of the concentration of organic matter. The model includes 13 components. The carbonaceous and nitrogenous material is divided based on biodegradability, solubility and viability while alkalinity is included to provide information whereby undue changes in pH can be predicted. The components are affected by 8 dynamic processes (in this section, process means the conversion of a component).

The 8 fundamental processes involved in ASM1 are: aerobic and anoxic growth of heterotrophs, aerobic growth of autotrophs, decay of biomasses, ammonification of organic nitrogen and hydrolysis of particulate organic matter. To facilitate modelling, readily biodegradable substrate is considered as the only substrate for growth of the heterotrophic biomass. Heterotrophic biomass is generated by growth on readily biodegradable substrate under either aerobic or anoxic conditions, but is assumed to stop under anaerobic conditions. Autotrophic biomass is generated by growth on ammonium nitrogen and inorganic carbon. On the other hand, biomass is lost by decay. This process acts to reduce the viability of the suspended solids in the bioreactor, and to account for respiration causing depletion of particulate material.

The activated sludge models no. 2 and 2d

The strong movement towards effluent criteria for both nitrogen and phosphorus initiated the development of a model describing phosphorus. ASM2 (Henze *et al.,* 1995) extends the capabilities of ASM1 to the description of phosphorus removal. In the model removal by chemical precipitation was also included. The publication of this model mentions that ASM2 allows description of bio-P processes, but that it does not include all phenomena that take place during the processes of phosphorus removal. The subsequent model ASM2d (Henze *et al.,* 1999) added the denitrifying activity of phosphorus accumulating organisms (PAOs), which should allow a better description of the dynamics of phosphate and nitrate. In ASM2d the PAOs are modelled with cell internal structure, where all organic storage products are lumped into one model component. The PAOs can only grow on cell internal organic storage material, the storage is only possible when fermentation products such as acetate are available in the environment, which means that storage will usually only be observed in anaerobic activated sludge tanks (Gernaey, 2003). Today, ASM2d has completely replaced ASM2.

The activated sludge model no. 3

The ASM3 (Gujer *et al.,* 1999) corrects some defects that have appeared during the usage of ASM1. The major difference between ASM1 and ASM3 is that the latter recognises the importance of storage of polymers in the heterotrophic active sludge conversions. It is assumed that all readily biodegradable substrate is first taken up and stored into an internal cell component prior to growth. The heterotrophic biomass is modelled with an internal cell structure, similar to the PAOs in ASM2d. In ASM3 the internal component is used for biomass growth. Nevertheless, in ASM1, the biomass growth occurs directly on external substrate. An advantage with ASM3 compared to ASM1 is that ASM3 is thought to be easier to calibrate than ASM1. This is achieved by converting the death-regeneration hypothesis into a growth-endogenous respiration model. Whereas in ASM1, effectively all state variables are directly influenced by the change of a parameter value, in ASM3 the direct influence is considerably lower thus simplifying parameter identification. Koch *et al.* (2000) concluded that both ASM1 and ASM3 are capable of describing the dynamic behaviour in common municipal WWTPs, whereas ASM3 performs better in situations where the storage of readily biodegradable substrate is significant or for WWTPs with substantial non-aerated zones.

2.3.3 Data driven models

Also referred to as empirical or black-box models, data driven models are models entirely identified based on input-output data, without reflecting any process knowledge in the model structure. These models are commonly used to model very complex systems, or when insufficient process knowledge is available. In the WWTP area, black-box models are useful in situations where the mechanistic models are not satisfactory (e.g. activated sludge sedimentation processes, description of simultaneous nitrification and denitrification, deterioration of sludge), or when insufficient data are available for the calibration. The advantage of black box models is that they can be identified without detailed knowledge about the processes; they are fast and usually perform well (in some cases better than mechanistic models). The disadvantage of these models is that their prediction capability is limited to the range of data used for identification, and that they do not allow for a better understanding of intrinsic process parameters.

Examples of black-box models include artificial neural networks (ANN), polynomial regression (PR) models, multivariate polynomial regression (MPR) models, stochastic models such as autoregressive (AR) models, autoregressive moving average (ARMA) models, ARMA models with external input (ARMAX), Box-Jenkins (transfer function) models or other multivariate statistical methods (MVS). The data set used for model identification can be simple input-output data or time series (in the case of stochastic models). In some cases a dynamical update of the model is possible using online measurement data.

Most of the above-mentioned modelling techniques have been successfully used to simulate different parts of the wastewater treatment plant, or to complement the knowledge summarised in white-box models. El-Din and Smith (2002) used a Box-Jenkins model to predict the behaviour of a primary settling tank, Erikksen et al. (2001) used MVS methods to predict influent COD load, Baeza at al. (2001) did the same using ANNs, just to name a few recent applications. Sometimes empirical models are used to predict some key parameters for the white-box models. Real-time control is another type of application, where fast black-box models can be used. The advantages of mechanistic and data driven models can be combined into hybrid or grey-box models. Hybrid modelling is a very promising field, where further research is needed. Cote *et al.* (1995) use ANNs to improve the prediction made by ASM1, Zhao *et al.* (1996, 1999) use a simplified ASM2d model in parallel with a neural network and Lee *et al.* (2002) described the hybrid neural network modelling of a full-scale industrial WWTP. Stochastic grey-box models are also widely used; in Carstensen *et al.* (1998) they are shown to perform better then mechanistic models for influent flow rate predictions.

2.3.4 Applications

The use of models will likely step by step take a central role in the understanding and simulation phases of processes and systems in several fields. This is particularly true in the wastewater sector where alternative methods (principally experimental analysis in laboratories or pilot plants) require much time and are often expensive. In order to be really efficient, however, a model needs to be developed related to the future use of the model itself, which, besides to influence the model structure, will influence its complexity. Below, principal model applications are reported

- Research: models are instruments that help to understand processes and to make hypothesis.
- Design: models are helpful in projecting new plants entirely or to improve existing ones.
- Control: the models are fundamental in founding the optimal control combination because it is possible to test different combinations for different input without act in and endanger the plant.

- Prediction: a model can foresee plant performance in case of probable future input disturbances in input and help in finding appropriate solutions.
- Performance analysis and diagnosis: operators can use models to understand reasons of abnormalities in the plant, as well as have a global vision of the plant performance.
- Education: models can be used as a tool useful both to explain WWT processes to students and to train plant operators.

It is foreseeable that in the future, WWTP models will take more and more space. They are suitable for taking a central role in all the phases of the life of a treatment plant: engineers need them in plant projecting, since the support of pilot plant experiments is often limited. During the plant operation phase, models help to indicate impacts of external disturbances on the plant, as well as the impact of operational decision, and allow to try several operation conditions in order to solve plant problems, to find the solution that gives the lowest environmental impact (saving more energy, producing less sludge, etc.) and to gear the plant to the new regulations.

2.3.5 References

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2.4. River water quality and river basin models

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2.4.1 Objectives

The Water Framework Directive (WFD), recently approved by the European Parliament, requires a holistic approach to water quality attainment at a river basin scale, which is based on biochemical and ecological water quality objectives. It specifically indicates that targeting of both diffuse and point source pollutions (see Section 2.2) are important. River catchments with their natural boundaries and hierarchical structure can be considered as integrators of many water-related interactions and therefore they represent an appropriate scale for ecohydrological modelling. For this reason, a general requirement for surface water was introduced on a basin scale. Integration of all the water quality problems at the river basin scale, and thus reaching the in-stream water quality objectives, is essential for the new WFD. Rivers have been used consistently as the principal pathway for disposal of industrial, domestic as well as agricultural wastewater. Assessments of river systems, focused on water quality, are becoming critical and thus there are clear motives for developing a basin-wide modelling framework.

2.4.2 Literature review

The purpose of this short literature review is to provide the reader with a general overview of river modelling as it pertains to the river basin. The application of modelling techniques to water quality problems at the basin scale has increased dramatically. Over the years, many models have been developed to help agencies to assess and control the quality of water bodies. Water quality simulation models have been developed by government agencies, academic institutions and consulting firms.

River quality models

A river as a natural aquatic ecosystem is made up of three compartments: the gas phase, the water phase and the sediment. A river quality model accounts for the processes within, and the interactions between, these compartments. The most widely known and used computer program for river quality modelling is the QUAL2E model developed by the US Environmental Protection Agency (EPA). It simulates dissolved oxygen and the many associated water quality parameters of the carbon, nitrogen, and phosphorus cycle in rivers in streams in conditions of steady streamflow and pollutant discharge. The limitations of the QUAL2 formulation become apparent when attempting conditions other than the steady-streamflow, constant-emission conditions for which it was developed. This problem, among others, initiated the development of the River Quality Model No. 1 (RWQM1) (Reichert *et al.,* 2001). The IWA task group on river water quality modelling was formed to create a scientific and technical base from which to formulate standardised, consistent river water quality models and guide-lines for their use. The result, RWQM1, is intended to serve as a framework for water quality models that overcome deficiencies in traditional water quality models, most particularly the failure to close mass balances between the water column and sediment. In addition, RWQM1 is intended to be compatible with the IWA activated sludge models (ASM1, ASM2d and ASM3) so that it can be straightforwardly linked to them (Rauch *et al.,* 1998). These models are constantly refined and updated to meet new and emerging problems of water pollution, such as eutrophication, acute and chronic toxicity, etc.

A river is affected by a variety of processes occurring in its surroundings and to handle the complex interactions caused by the increased influence of human activities on rivers, it is today mandatory to couple the river water quality models with those describing the river basins (Novotny *et al.,* 1994).

River basin models

A river basin consists of soil and water, dry areas, wet areas, rivers and lakes, surface water and ground water. In the past 30 years, the river basin modelling communities have employed parametric-based models. The most famous is the HSPF and all other, e.g. SWMM, CREAMS, STORM, ANSWERS, SWRRBWQ, are similar to HSPF. The models are used for river basin management, assessments and Total Maximum Daily Load (TMDL) calculations. It is seen that the physics-based, process-level contaminant and sediment transport and fluid flow models have the potential to further the understanding of the fundamental biological, chemical and physical factors that take place in nature. It is for this reason that the WFD research strategies clearly stated that the first principal physical models should be used in system assessment on a river basin scale.

Most of the river basin models presently available focus on mathematical descriptions of the physical-chemical-biological transformations and on the hydraulic processes. However, a large concern for the river basin modelling is also connected with spatial variations. Integration of Geographical Information System (GIS) technologies with hydraulic modelling software is a powerful solution to help water authorities to meet their responsibilities related to river catchments, urban drainage and water distribution. GIS facilitate the modelling of complex river basins and subsurface media because these models take into consideration spatial variability of the river basin. Several river basin models have been integrated with GIS; examples include the AGNPS (Agricultural Non-Point Source Pollution) model (Young *et al.,* 1987), the ANSWERS (Aerial Non-Point Source Watershed Response) model (Beasely *et al.,* 1977) and the SWAT (Soil and Water Assessment Tool) model (Arnold *et al.,* 1993). One of the drawbacks with using these models is the need for very large input data sets. However, spatial averaging can decrease the amount of required input data at the expense of output accuracy.

River basin models are used extensively in research as well as in the design and assessment of water quality management and measurement campaigns. There are numerous water quality software packages available both commercially and in the public domain. Many of these models have been specially designed for treating non-point source pollutants (e.g. SWAT) although they sometimes take into consideration point source pollutants (e.g. AGNPS). However, as it is in the latter example, these often assume that pollutants transported through a river system are conservative, i.e. the model does not allow for transformation of model component with time. Water quality models, such as QUAL2E and RWQM1, allow various biochemical reactions to be represented but they do not take into account spatial variations. Widely used models in river basin modelling are presented below.

HSPF – Hydrologic Simulation Program Fortran – is the US EPA program for simulation of river basin hydrology and water quality. HSPF incorporates the river basin scale Agricultural Runoff Model (ARM) and Non-Point Source (NPS) models into a basin scale analysis framework that include pollutant transport and transformations in stream channels. The result of this simulation package is quantity and quality of runoff from urban or agricultural river basins. Flow rates, sediment loads and nutrient and pesticide concentrations are predicted.

SWAT, a continuous daily time step model developed by Arnold *et al.* (1993), allows a basin to be divided into hundreds of sub river basins and also for analysis of long term (many years) impacts of management as well as timing of agricultural practices within the calendar year (i.e. crop rotations, irrigations or fertilizer application rates and timing). A GIS interface was developed to facilitate the use of digital spatial data. It uses spatial, hydrological and metrological data as basic model inputs. The interface software creates a sub basin description combining soils and land cover data with the sub basin coverage, which is then queried to create the input files required by SWAT. The interface also allows for output data to be viewed and analysed in ArcView as needed. The original SWAT simulator has been extended by Neitsch *et al.* (2002) with the aim of integrating water quality and quantity at a river basin scale. Water quality components from QUAL2E have also been incorporated.

BASINS – Better Assessment Science Integrating Point and Non-Point Sources – was originally released by the US EPA in 1996 (US EPA, 1999). It is a system developed to integrate GIS, national river basin and meteorologic data, and environmental assessment and tools into one convenient package. BASINS addresses three objectives: (1) to facilitate examination of environmental information; (2) to provide an integrated river basin and water quality modelling framework and (3) to support analysis of point and non-point source management alternatives (by means of the in-stream water quality model QUAL2E). BASINS supports the development of TMDL calculations, which require a river basin based approach that integrates both point and non-point sources. It can support the analysis of a variety of pollutants at multiple scales, using tools that range from simple to more sophisticated.

The model category of the Danish Hydraulic Institute (DHI) is named MIKE. MIKE SHE is one of the hydraulic models that were initially developed to integrate surface water and groundwater modelling capabilities. MIKE SHE simulates flow and transport of solutes and sediments in both these water environments. Areas of application include, but are not limited to, conjunctive water use, water resources management, irrigation management, wetland protection, surface and groundwater interaction and contaminant transport (DHI, 1999a). The water balance method at a river basin scale – MIKE BASIN – is structured as a network model. The model describes the interaction and balance between the demands and natural supply of water in river basins, groundwater as well as river water. Specific water demands, such as water abstraction for irrigation, urban water supply and reservoir operation, can be specified. Effects on water quality may also be analysed by the model.

In this chapter, we have focused on the most well known and most frequently applied models. This means that there exist a whole range of other models that may be well posed and applicable, but which we have not included in this compilation. However, this survey gives an idea of the variety of available water quality models.

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2.5. Control interfaces

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2.5.1 Structure of the overall control problem

The control engineering of wastewater treatment plants, sewer systems and river systems consists of measurements, controller computations and manipulating actuators. Related issues such as communication and signal processing are also of importance. The available data (measured or estimated) are generally used to maintain or control one or several process variables at fixed or otherwise desired values, which will have direct or indirect effects on the water quality. Prior to the introduction of automatic control within the wastewater treatment industry, the mechanical/biological (and to some extent chemical) plants were designed only to remove organic matter and suspended solids. This was largely a result of lacking instrumentation and automation capabilities. Obviously the introduction of computers for control purposes has also dramatically influenced the situation. Manual control was often sufficient for these simpler processes and type of operation but during the last decades, that situation has changed.

Some of the main achievements of control engineering (although an on-going process) regarding the wastewater industry are the improvements of the water quality (better effluent quality), more energy efficient use of the system, more effective disturbance rejection and improvement in stability and robustness of the processes. Other important aspects of control engineering are to reduce the costs of the treatment process by using less energy/chemicals, reducing the sludge production and the required manpower (as a result of introducing automation). One of the recent challenges is to introduce techniques for monitoring, diagnosis and control inspired by the chemical and petroleum process industries, such as time series analysis, multivariate analysis, cluster analysis, Fourier frequency analysis and wavelet-based time and frequency analyses.

2.5.2 Literature review

In this section, we will mention some of the main sensor types that are important for on-line measurements in the wastewater industry. The most fundamental sensors are related to measuring flow rates, pressure, temperature and liquid levels. There exist a number of different techniques to measure **liquid levels**. Level measurements can be obtained using floats with an internal electric switch, conductivity switches, (differential) pressure transducers, capacitance probes, sonic and ultrasonic level detection and bubblers (Vanrolleghem and Lee, 2003; Skrentner, 1988). It is also possible to use pressure cells and strain gauges to measure chemical levels in storage tanks.

Temperature is a classic parameter that can be measured with thermocouple, resistance temperature detectors (RTD), thermistors and thermal bulbs. Control of temperature is an important variable when considering anaerobic digesters, monitoring process conditions and equipment performance and for compensation in flow and level meters.

Pressure measurements are mainly used in wastewater treatment plants for alarm purposes in the aeration system and anaerobic digester (Marinaki *et al.*, 2003; Vanrolleghem and Lee, 2003). Tanks, pump discharges and compressed air distribution systems can benefit from the use of pressure meters. The most common sensors used to measure pressure are diaphragms, bellows and bourdons tubes. Pressure transmitters can be successfully applied to any wastewater process using isolation diaphragms.

Instruments for the monitoring **flow rates of liquid or gas** are omnipresent in wastewater treatment plants (Vanrolleghem and Lee, 2003). The different technologies used for flow meters in close conduit liquid flows are based on differential pressure, vortex shedding, mechanical (turbine and positive displacement), magnetic, sonic and ultrasonic methods. Depending on how the sensor is mounted, these technologies are used for different categories of meters, such as full bore, insert and clamp-on types. Gas-flow meters in closed conduit gas flows involve almost the same technologies as for liquid-flow meters embracing mass rate of cooling. Techniques used to measure gas flows include orifice plates, venture tubes, averaging pilot tubes, turbines and mass-flow meters. The most common flow sensors to measure open-channel flows are flumes and weirs. However, several variations are available, such as the Kennison nozzle, velocity area type, the Parshall flume and the Palmer-Bowlus flume.

Analytical instruments are increasingly being used in wastewater treatment for on-line measurements of different parameters. These include pH, concentration of suspended solids, turbidity, conductivity, respiration rate, concentration of chlorine residual, dissolved oxygen concentration (DO), concentration of total organic carbon (TOC), volatile fatty acids (VFA), chemical oxygen demand (COD), biological oxygen demand (BOD), gaseous products, sludge blanket level and various ion-specific analyses such as concentrations of ammonia, nitrate and phosphate. Such measurements are often essential for an efficient and robust control system. An excellent review with regard to sensors is given by Vanrolleghem and Lee (2003).

2.5.3 Unit process control

Essential sub-processes in wastewater treatment plants

Considering the dynamics of a typical biological WWT plant, the processes that occur within it may be divided according to the time scale of the dynamics: slow processes (days) – biomass growth; medium-scale processes (hours) – concentration dynamics and nutrient removal; fast processes (minutes) – flow and oxygen dynamics. The basic control should therefore deal with the flow and oxygen dynamics, the advanced process control should take care of the nutrient removal process and the concentration dynamics, while the supervisory control will take care of the biomass growth processes. Within each level the traditional "*divide et impera*" method can be applied, regarding each process unit as relatively independent. However, to avoid sub-optimisation the interactions among those units must then be taken into consideration.

The most important units to control in the bio-P process are the activated sludge reactor zones (anaerobic, anoxic or aerobic) and the secondary settlers. In the anaerobic zone the main reaction of interest is phosphorus release. The variables that have to be controlled are the P/COD ratio (should be low), the VFA concentration, the retention time and the NO_3 and DO levels, which should be as low as possible so as not to inhibit the P-release reaction. The concentration of VFA has proved to be very important for biological P removal. The content of readily biodegradable organic matter in the influent wastewater should be measured and if it is found to be too low (below a given set point for example), there are a number of ways of increasing the VFA concentration:

1. addition of products from the fermentation of sludge (e.g. use of pre-fermenters);
2. addition of external carbon sources such as CH_3COOH;
3. external supply of industrial H_2O containing readily biodegradable substrate;
4. increase hydrolysis/fermentation in the tank by increasing the retention time.

The return sludge, which is recirculated to the anaerobic zone should have a low nitrate concentration in order not to inhibit the phosphorus release. This points to the necessity of a well controlled denitrification process in the anoxic zone. The configurations adopted for the reactor zones may differ: there are systems with pre-denitrification and systems with post-denitrification. However, the requirements for good denitrification are:

1. keeping the DO level at a minimum by mixing and recirculation (given by a DO setpoint for the DO controller);
2. monitoring the carbon source level adding CH_3OH or C_2H_5OH when it gets too low;
3. manipulation of the retention time through the influent, recirculation and filter backwashing flow rates;
4. measuring the NO_3 at the outlet of the anoxic zone (should tend to 0);
5. possible redox potential and pH measurements: a low redox potential will favour denitrification and a pH between 7 and 9 is considered optimum for the reaction to take place. The low redox potential can be assured by the absence of DO and the pH can be adjusted by addition of bases.

The aerobic zone is perhaps the most complicated one to control, given the fact that there are three competitive reactions that have to happen virtually simultaneously: COD removal, nitrification and phosphorus uptake. Three types of bacteria with different growth rates are responsible for these reactions: heterotrophs, autotrophs and phosphorus accumulating organisms (PAOs). Another prerequisite is growth of proper floc-forming organisms and avoidance of extensive filamentous growth. The control must be oriented towards the:

1. DO level at various parts of the reactor through an adequate air flow rate, which may be distributed along the reactor and a good mixing. This is by far the most important control on the fast time scale, as DO is needed for all reactions to take place. Therefore, DO concentration should be high enough to support growth of adequate organisms, yet low enough for nitrate recirculation;
2. retention time, affected by the flow rate. This is important for reaction control, nitrification being the slowest reaction in a biological nutrient removal (BNR) process;
3. measurement of NO_3 and NH_4 concentrations. A high NO_3 concentration and a low NH_4 concentration indicate the completion of the nitrification reaction;
4. biomass growth rate and sludge wastage rate. These factors influence the total sludge mass. Flow properties are the key factors influencing sludge wastage rate. DO and substrate concentrations influence the type of bacterial growth. For

example, filamentous bacteria are generally favoured by low DO, low nutrient and low substrate concentration, which might lead to poor sludge settling properties;
5. return sludge flow rate, used to establish a good relation between sludge mass in the aerator and the settler;
6. possible chemical precipitation of phosphate if the phosphorus concentration measured at the outlet of the zone is too high.

In the secondary settler the main objectives to achieve are a good liquid-solid separation and a significant thickening of the sludge. This can be controlled by:

1. hydraulic propagation – a smooth influent flow rate is required;
2. hydraulic loading – influenced by the return sludge flow rate;
3. the floc properties – obtained in the reactor zones;
4. the presence or absence of biological reactions in the settler. There may occur substrate removal reactions in case oxygen is present, denitrification reactions if NO_3 levels are high enough and phosphorus release reactions if the PAOs get starved, the last two reactions mentioned being unwanted. The key control variable here is the return sludge flow rate.

Essential sub-processes in sewer systems

Control in the sewer system can be applied to regulate the basin filling volumes of a system with basins, or to treat the overflow in a system with or without basins. Basin filling control may imply either a regulation of the effluent flow rate from each basin to an interceptor or an adjustment of the flow rate to the treatment facility. The goals are an efficient use of the storage capacity of the system basins and/or avoiding an increased influent flow rate to the treatment plant, so that its secondary clarifier operation may be kept at an optimum even under heavy rain conditions.

The control loop for each of these objectives includes a sensor for the water level of the basin, a controller functioning according to a predetermined control algorithm and the actuator: a sluice-gate commanded by the controller. The control algorithm varies from case to case, depending on what is aimed at and the means of accomplishing it. The simplest one could be an "on-off" algorithm, for the opening and closing of the gate. The sluice-gate is often regulated using a set point corresponding to the desired water level in the storage basin.

Sewer overflow treatment is also a candidate for on-line control, its aims being COD and nutrient (N and P) removal. For a system with basins, there are two alternative methods that can be applied: sedimentation or precipitation and filtration. In the case of sedimentation, the process could be a sequential one: the basin is filled through an inlet pipe until a certain level is reached. This requires an opening valve commanded by a controller and a sensor for the water level. While the water remains in the basins, the COD, P and N concentrations should be monitored. When the desired concentrations are reached the water from the basin can be let out through a gate whose opening is commanded by the controller. Sediments should be removed and the cycle can then start over. If precipitation and filtration are used, the COD, P and N concentrations of the influent water should be measured and the precipitating reagent dosing be calculated accordingly by the controller. The set points for the reagent dispensing apparatus will be fixed based on the calculations. Control of precipitation could employ turbidity and pH measurements (precipitation is optimum in a certain pH interval and good precipitate formation can be monitored by measuring the water turbidity). After the precipitation is considered to be finished, water can be drained and the filtrate should be removed.

Recipient water monitoring

If an integrated system control approach is adopted, the possible oxygen depletion and eutrophication phenomena in the receiving water body should be detected. This implies some DO and (possibly) nutrient measurement points be set up in certain zones of the receiving water body, in the proximity of the treatment plant discharge point. The detected concentrations should be fed back to the treatment plant and appropriate actions be taken. One important thing to be taken into account is that the DO depletion consists of two effects: an immediate oxygen depletion happening in the polluted water volume that passes down the river and a delayed oxygen depletion associated with the degradation of the settled organic matter (either primary effect of organic material in the wastewater or secondary effect of high nutrient concentrations in the water promoting growth of organic matter that will eventually settle and decay). The detected DO concentrations therefore may be due to past events, which mean that the possible control algorithm to be used should also have an integral part.

2.5.4 Control limits study

Sensors, actuators and controllers

The sensors throughout the treatment process, sewer network and river system provide the information needed to perform control tasks. This information is provided by flow and level measurements (used in the treatment plant, the sewer and the river). Pressure and temperature measurements can be taken in the treatment plant. Quality measurements are also taken, mostly in the treatment plant, more so than the river and sewer. Actuators are the elements of the system that receive the control signal and perform the actual action. These actuators can be pumps, motors and valves in the sewer and in the treatment plant, as well as compressors and aerators, and weirs and gates in the river. The controller can be in the form of basic control in PLC's (programmable logic controllers) or higher control using complex control algorithms.

The limitations of this control are that it depends on the quality of the information being received from the sensors, and the quality of the response of the actuators. The quality of control can be degraded by a bad choice of sensors/actuators and by neglecting the instrumentation (wear and tear, as well as sensors being unclean after periods of time). Also, there is a lack of information as regards the river and the sewer network, in comparison to the treatment plant. Analysers used in quality measurements can have errors of up to ±5% of the actual value, similar errors can be expected from flow/level measurements. This error influences the quality of data being received by the controller, and the accuracy of its response. At the actuator side, the slew rate (delays due to mechanical effects) of the motors can cause inaccuracy in the control action. Most motors/compressors/pumps are designed for a specific working range, and badly chosen operating ranges for these motors can cause excessive wear and tear and hence errors in the control of the process.

2.5.5 Supervisory (integrated) control

The implementation of an integrated control system for the urban wastewater system, typically made up of a combined sewer network, wastewater treatment plants and the receiving water body, should aim at preserving the water quality of the receiving water body. Two kinds of pollution aspects should be taken into account: the short-term acute effect and the long-term accumulative effects. The main problems that appear in the case of urban water pollution are the DO depletion, the accumulation of nutrients, which may lead to eutrophication and bacterial contamination.

One of the main objectives is the minimisation of the transient pollution events. Basically, this may be accomplished by controlling the combined sewer overflow volumes, reducing the COD and nutrient concentrations in the wastewater, and monitoring the DO levels both of the wastewater and of the receiving water. For the design of the supervisory control of the integrated system, a top-down approach should be more efficient. The system can be split into three units: the combined sewer system, the treatment plant(s) and the receiving water body. These shall have to be interconnected using certain input-output variables. Each of the units can be considered separately as a system that can be further split into sub-units. The possible interconnection sequences should be:

1. combined sewer system - receiving water;
2. combined sewer system - treatment plant(s) - receiving water.

Both of the alternatives have to be considered, as there are cases when the input flow to the sewer system is so high that proper treatment of the entire volume of wastewater becomes impossible and the polluted water has to be discharged directly into the river.

The inputs to the combined sewer system are the urban wastewater flow rate, effects of rain events and urban drainage, leakage, loads of the pollutants considered (suggested: COD, N, P) and the DO concentration. The outputs from the sewer system should be the flow rate and the pollutant loads, which in turn will be used as inputs to the treatment plant and possibly to the receiving water. The output from the treatment plant will be an effluent flow rate, DO, COD and nutrients concentrations in the effluent. These will be used for feedback to the sewer system and as inputs to the receiving water. Their effects on the receiving water will be analysed through DO and nutrient concentration measurements and used as feedback to the treatment plant.

Models can be used for each of the units in order to predict their behaviour under different load conditions and try to minimise the effects of disturbances like considerable variations in the flow rates, increased pollutant loads or decreased DO concentration. A global system controller can be built based on these models.

2.5.6 References

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2.6. Integrated wastewater system models

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2.6.1 Introduction and objectives

The global model of a wastewater system consists of an integrated structure made up by multiple sub-systems. Together, these aim at describing a "whole" unit. In this context, a particular watercourse and its surrounding catchment area represent the "whole". The catchment area is divided into urban and rural areas. The wastewater system, characterising urban areas, consists of the sewer network (including urban flooding) (see sewer network models), the wastewater treatment plant (see wastewater treatment plant models) and the receiving waters (see river models). All these models of the sub-systems are integrated in order to build a global model. However, the model will be a simplified one, not only because each sub-system model is simplified in comparison with the reality, but also because the very fractionation into sub-systems represents a simplification.

Nevertheless, the advantages offered by the realisation of a global model of the wastewater system are outstanding. An integrated wastewater system model could provide new perspectives on water and wastewater management, new possibilities to adapt control actions at holistic levels in order to improve the performance of the urban wastewater system. The consequences are increased water quality in receiving watercourses, new panoramas for environmental modelling, and many others benefits.

The WWT&SYSENG network has as its aim to provide a global simulation model of the wastewater system, to provide case studies and to circumstantiate a current modelling framework. The objectives of the work involved in the global modelling of the network can briefly be presented as follows:

- investigate the actual state-of-the-art in the separate modelling of each sub-system;
- analyse the actual state-of-the-art in integrated urban wastewater system and river basin modelling;
- select the most applicable software available for the partners of the research network;
- design the collaboration between the partners (it is already agreed that the members of the network will use their own software and make this available for the others);
- develop simulation models for each sub-system and the global integrated simulation model;
- collaborate, exchange know-how, and assess better solutions for development of an integrated wastewater system model, one mission of this network;
- as a sine qua non, the development of the global model implies a thorough knowledge of the entire system from a theoretical point of view as well as an applicable model framework.

2.6.2 Literature review

The integrated approach of the global water/wastewater system, in particular of the urban wastewater system, is not a novelty (Harremoës, 2002). There were a few visionary suggestions being advanced as early as the 70's; one of the earliest was made by Beck (1976), who foresaw the possibility of assessing the performance of a whole system using integrated models. A first integrated model was used by Gujer et al. (1982). However, intense efforts were focused mainly on the modelling of the individual parts of the urban wastewater system (Butler and Davies, 2000). During the 90's, the perspectives conferred by an integrated model were being carefully appraised. Due to the apparent merits, many research teams (mainly in Europe) began to develop such integrated models, which were based on various versions of the available software packages for each individual sub-system. State-of-the-art integrated modelling concepts were presented by Rauch *et al.* (2002) and Schuetze *et al.* (2002). A main difficulty occurring during the integration process of two or more models, the various state variables in each sub-model, was overcome by Vanrolleghem *et al*. (1999), Schuetze (1998) and Fronteau *et al*. (1997) through the development of conversion factors. More recently, the same problem was solved by Meirlaen *et al.* (2002) by re-defining similar state variables sets using the River Water Quality Model No.1 (Vanrolleghem *et al.*, 2000).

As an exhaustive presentation of the models and simulation tools available or under development is beyond the scope of this report, only the most relevant software packages available for integrated modelling of the urban wastewater system are presented.

1. SIMBA® was developed at ifak Magdeburg, in collaboration with Otterpohl Wasserkonzepte, Germany. It runs on the MATLAB™/SIMULINK™ simulation platform. Sewer systems, treatment plants, and river models are available. SIMBA® is particularly suitable for on-line simulation and control applications. In MATLAB^{TM} / SIMILINK^{TM}, the user can add his/her own models. SIMBA® has been utilised in an integrated case study.

2. The Integrated Catchment Simulator (ICS) was developed by the Danish Hydraulic Institute (DHI) and the Water Research Centre and was funded by the EU project "Technology Validation Project" (TVP) (Mark and Williams, 2000). This simulation tool sets up integrated models such as MOUSE for sewers, MIKE 11 for rivers and STOAT for wastewater treatment plants. ICS has like SIMBA® been employed in real case studies. A simultaneous simulator for the integrated system is available (Taylor *et al.*, 2000).

3. WEST® was developed at the Universities of Ghent and Brussels, Belgium (Meirlaen *et al.*, 2000). This model emerged as a continuation of earlier research focused on a series of simulation studies on integrated modelling, carried out at the above mentioned universities. WEST® has been further developed by Meirlaen *et al.,* (2002) into a simultaneous simulation tool for the integrated urban wastewater system model.

Research on integrated modelling of the urban wastewater system has been carried out at Imperial College London (Schuetze, 1998; Reda, 1996), by Rauch and Harremoës who developed an integrated simulation model (Harremoës and Rauch, 1996; Rauch &

Harremoës, 1997), and by the EU COST workgroup (COST682 – "Integrated wastewater Management", being continued nowadays with COST624 – "Optimum Management of Wastewater systems") (Schilling *et al.*, 1996; Vanrolleghem *et al.,* 1999).

2.6.3 Models

Sub-systems models have been analysed separately in earlier subchapters. In Section 2.2 sewer system modelling was discussed. The state of the art in WWTP modelling was presented in Section 2.3 while common river basin models were presented in Section 2.4. Regarding the available integrated models, within the WWT&SYSENG network, there are apparently two; more specifically one is being presently in use (originating from Imperial College London, UK) while the other is (at present in the prospectus phase) being designed at the University of Strathclyde, UK. In this report, the one currently in use will be briefly presented.

The integrated model SYNOPSIS (software package for synchronous optimisation and simulation of the urban wastewater system), is a simulation tool describing the urban wastewater system, developed at Imperial College London in the 90's (Schuetze, 1998; Schuetze *et al.,* 2002). This simulation tool has a quasi-parallel integrated model of the sewer and wastewater treatment plant and models the receiving river in series.

The purpose of the simulation tool is to represent the impact of control on the performance of urban wastewater systems. One of the main objectives of the original work was to evaluate/analyse the potential of integrated control. This tool has two simulation modes available: stand-alone simulation and simulation-optimisation. The model is dynamic, unsteady and deterministic. The constituent models of SYNOPSIS are modified versions of: KOSIM (sewer model), Lessard and Beck's model (wastewater treatment plant) and a river model developed by Lijklema *et al.,* (1996), implemented in the DUFLOW program. Auxiliary routines model the river catchment runoff. Furthermore various conversions between the state variables of the integrated models are being described.

The control strategies are simulated using a module that involves control actions on the sewer and wastewater treatment plant, employing information on system state from the sewer, treatment plant and different upstream locations in the river. Another module deals with optimisation of parameters describing the control strategy. The optimisation procedures adopted in SYNOPSIS are the Controlled Random Search (CRS), a genetic algorithm and Powell's method applicable for local optimisation. In addition to the input data for the stand-alone simulation mode, such as catchment characteristics, dry-weather flow and concentration definition, parameters of biological processes and of the control strategy, the optimisation-simulation mode requires specific input data, such as definition of the objective function, selection of optimisation procedures, parameters of the chosen optimisation procedure and so on.

The outputs provided by SYNOPSIS can take various forms e.g. tables and time-series plots for the principal variables of the whole system (sewer, treatment plant, and river), summary information and 3-D plots presenting the assessment criteria versus any combination of two parameters.

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3. Status for the project

3.1. Contributions and perspectives in sewer modelling

Historically, the sewer system has been regarded just as a pipe structure transporting wastewater to the WWTP and receiving waters. Today, it is clear that the network also acts as a biological/chemical reactor and much effort is put on appropriate descriptions of both the hydraulic processes and transformations of compounds within it. At the Technical University of Crete (TUC), see Chindris (2003), the development of a sewer model that considers both quantity and quality of the wastewater is discussed. A sewer module is a must for studying the integrated wastewater system. Applications of the developed model include testing and optimisation of control strategies with the global aim of improving the performance of the WWTP and thus minimising wastewater pollution in the river.

Examples of important sewer conversion are the respiration of oxygen, production of hydrogen sulphide and production of easily degradable substrate that is greatly needed for nutrient removal in the subsequent WWTP (Huisman *et al.,* 2003; Vollertsen and Hvitved-Jacobsen, 2000). It has also been reported that sewers affect the fate of XOCs in the urban water cycle. Growing evidence suggests that a major fraction of volatile organic pollutants discharged to municipal sewers are emitted prior to reaching downstream treatment plants and thus, volatilisation must be regarded in environmental models. In Lindblom *et al.,* (2004), an approach on how some processes affecting hazardous chemicals in sewers can be modelled is discussed. At the Technical University of Denmark (DTU), work related to quality modelling of the sewer system has been initiated. Pollutant generation, e.g. hazardous chemicals in wastewater originating from surface wash-out will also be considered. It is recognised that a good collaboration with Lund University (LU), that works with a WWTP influent generator (see below), can be established.

3.2. Contributions and perspectives in WWTP modelling

In the Chemical Engineering Department of Autonomous University of Barcelona (UAB) an A2/O scheme pilot plant placed in this department is modelled. Sets of experimental data measured in experiments with the pilot plant are simulated using activated sludge model No. 2d (ASM2d) and Takacs settling model (Tapia et al., 2003). Steady state and un-steady state simulations were fitted to experimental data quite well. Moreover an extensive study of sensitivity and identifiability was done as well. WWTP modelling based on the ASM2d model has also been conducted at the Industrial Control Centre in Strathclyde (Camilleri et al., 2003).

University of Pavia (PU) is assessing the possibility of using data-driven models to substitute for the whole mechanistic treatment plant model or for different parts of it. The methods used are artificial neural networks and multivariate polynomial regression and are presented in Ráduly *et al.,* (2003). The work aims to formulate simpler models, which are more suitable for integration with other sub-models.

At DTU, modelling of WWTPs is also carried out, but with somewhat different goals (Lindblom *et al.,* 2004). The fate of hazardous chemicals in the urban wastewater system is of rising concern and although municipal WWTPs in general are not designed to remove specific substances present at low concentrations, they sometimes have a high capability to do so. At DTU, it is recognised that transformation processes in an activated sludge treatment plant are similar to those in the environment, except at a higher rate. Consequently, to develop descriptive mechanistic models for the fate of chemicals in the integrated wastewater system, a feasible first step is to gain knowledge about the pathways in municipal WWTPs. At DTU, modelling and model development will be carried out concurrently with dynamic full-scale experiments. Outcomes will on the one hand be a calibrated WWTP model of the ASM1 type to optimise the experiments and on the other hand increased knowledge about how operational parameters such as sludge retention time influence process rates.

3.3. Contributions and perspectives in river basin modelling

The river basin management system studies in the network can help to develop methodologies for applied case studies and reorganisation of water quality management systems according to the basic EU water framework directive. For the development of action plans model tools are needed. Some of the worldwide software, such as SWAT and QUAL2E will be implemented and applied to case studies. Until present, the basic activities have been based on analysis of river basin modelling tools for the training program. From now, analysis of integrated models and simulations on a river basin scale will be performed for various scenarios. Moreover, an integrated water quality modelling approach requires a river water quality model that can be connected directly to, and is compatible with, typical activated sludge wastewater treatment models (Reichert *et al.,* 2001). Work concerned with comparing and integrating state variables, reaction rates etc between the various models is therefore inevitable.

One paper, presented at the Copenhagen workshop (Boguniewicz, 2003), covers some of the areas discussed in Chapter 2.4. Namely, usage of the SWAT program for water quality modelling and application of the GIS technology in a case study at the lake Pusiano river basin, Italy, is discussed in the paper. It considers the work done in that areas, reflecting that the majority of the work done until now has been focusing on collecting, collating and quality checking of data to resemble a database, which is used to develop an analysis tool for studying water quality. The majority of the work has been carried out with GIS, and it has been used to collect, store and elaborate spatial data. There are still some problems with data collection, uncertainties in flow measurements at some gauging stations and with additional measurement locations to collect water quality data.

At PU, future work will include formatting data to create inputs for the SWAT program. A version of the QUAL2E water quality model, mainly considering nitrogen and phosphorus have been implemented. The model will be calibrated and validated with real data from the Pusiano catchment. Additional water quality monitoring at the river Lambro will be initiated; the sampling, together with the model, will be used for predicting nutrient dynamics along the river Lambro and the surrounding river basin of the Pusiano catchment.

3.4. Contributions and perspectives in control

As explained in Section 2.5, one of the objectives in control of a wastewater treatment plant is to obtain efficient data from the plant. Significant problems appear due to noisy signals, when measuring information from sensors. Many signals are degraded with noise that can be removed using filters. The Extended Kalman Filter (EKF) can be the perfect tool for providing an estimate of the missing information from noisy measurements (Benazzi *et al.*, 2003). One of the applications, so far, consists of applying an EKF to a biological wastewater treatment process in order to control the dissolved oxygen (DO) and the substrate (S) with proportional integral (PI) controllers based on the estimates provided by the filter. This EKF is also convenient when used for online real-time processing because of the minimum storage data required.

Another application of control in wastewater treatment covers the area of predictive control (O'Brien *et al.*, 2003). This is an advanced form of control that uses past information about the system (past inputs, past outputs, etc.) to perform better control. Thus the rainfall data, and the quality data of wastewater systems, as well as rivers and sewer networks, could be used to improve the control actions done on the system. Predictive control could also be used to reduce actuator wear and tear, by avoiding the actuator limitations through predictions of possible future actuator actions. Another benefit of predictive control is that it allows control of a multivariable system, without any complex tuning. Predictive control is, in most cases, a high level controller, with PLC's (programmable logic controllers) doing some basic logic and providing set points and PI controllers doing some simple control at a lower level to the predictive controller. Using predictive control on top of traditional control provides improved performance.

Botond Raduly's (Raduly et al., 2003) paper presented an alternative approach to the traditional mechanistic-based model control, namely the use of empirical models. Their use brings the simplicity and rapidity in an integrated model so that it can be used for real time control needs. Areas of the integrated urban water system, where the use of empirical models could have a potential benefit will be investigated.

Cristina Lazar's (Lazar, 2003) paper dealt with the control problem for a wastewater treatment plant and made a review of the most common techniques of plant control, showing both the traditional and the newer model-based control trends.

LU has worked with formulating and defining a WWTP benchmark model for application in integrated wastewater system control. The work has been of great value for many of the network since the validated models have been provided to the young researchers. Work with a substantially extended benchmark system, including both monitoring and control strategy benchmarking of entire WWTPs including the sludge train is ongoing. Recently, the group has initiated the development of a general model for influent wastewater generation including household and industry wastewater, infiltration effects, stormwater, sewer system impacts, rain and first-flush and weekend effects.

University of Strathclyde has shown a keen interest in the benchmarking work. In the past, much effort has been directed towards understanding of the WWTP processes and how Kalman filtering techniques can be applied to them (see Benazzi *et al.,* 2003).

Future work will involve a deeper understanding about the benchmark simulation model. As an implication of using this standardised simulation platform, result evaluation and model development is simplified. The collaboration between Lund and Strathclyde will be highlighted.

3.5. Contributions and perspectives in integrated wastewater system modelling

The integrated model of the urban wastewater system represents the major aim for three research projects presently carried out in the WWT&SYSENG network framework, as follows:

Imperial College (IC) is carrying out further developments of the SYNOPSIS simulation tool. Their main objective is to develop a fully parallelised integrated model of the urban wastewater system in a river context in order to apply integrated control strategies. To do so, a river quality model will be selected and implement. Taking into account the integrated control perspective it has initially been decided to improve the representation of nitrogen compounds in the treatment plant model. The wastewater treatment plant model implemented into SYNOPSIS was developed in the 1980's (Lessard, 1989). Further modifications, especially concerning the secondary clarifier, have later been conducted by Vazquez-Sanchez (1996). Currently, the developments are centred on the implementation of a new sub-module, coping with the denitrification process, together with an up-grade of the secondary clarifier model.

The new model of the denitrification process will offer better flexibility within the treatment plant model. For consistency with earlier versions of SYNOPSIS, a simplified version of ASM1 (Lessard, 1989) is being developed to include denitrification. This new module is introduced into the wastewater treatment plant, and in turn, the integrated simulation model. Furthermore, the up-grade of the secondary clarifier consists, in fact, of a simplification of the mathematical representation of the processes occurring in the secondary clarifier. The original Lessard model for the secondary clarifier has an elevated level of complexity. A simpler one-dimensional model, the well known Takacs' model, will be further implemented. For further details see Comsa and Butler (2003) annexed to this report.

The research carried out at UP is about integrated analysis and understanding of the dynamics of the urban wastewater system. It covers analysis and assessment of integrated control strategies with water quality as the main design criteria. To accomplish model integration, empirical surrogate models, which will substitute some deterministic parts of the integrated model, are being developed. The ultimate aim of this approach is to solve problems of complexity and time scale matching typical for large models describing greatly differing phenomena. The empirical surrogate models will be developed using data sets from a complex deterministic model, which has been calibrated and tested with real data. The main empirical methods that have been chosen to develop the model are Artificial Neural Networks and Multivariate Polynomial Regression. A brief description of these two methods is presented in Raduly *et al.,* (2003), annexed to the report. The first stage of this research is to develop of a deterministic model for the treatment plant, which will be based on ASM3. The biological phosphorus removal will not be considered due to lack of data. The model employed for the secondary clarifier is the compressive gravity thickening model.

During the last five months, DTU has been formulating the project "integrated modelling of xenobiotic organic compounds in the urban wastewater system", where xenobiotic organic compound (XOC) is a lumped name for man-made organic substances originating from e.g. care products, pharmaceuticals and chemicals. The existing water quality models, which have been introduced in Chapter 2, are not concerned with specific organic compounds and cannot be applied directly to establish the pathways of XOCs. In the urban wastewater system, XOCs are affected by on the one hand physico-chemical processes such as sorption/desorption, volatilisation/ stripping and on the other hand by biological processes such as sorption. Physical processes, such as sedimentation and increased advection, have a secondary impact via the physico-chemical processes. Thus, to describe the pathways of XOCs in the urban wastewater system, it makes sense to integrate model approaches based on the micro scale with larger scale physical ones. A summary of proposed model extensions are found in Lindblom *et al.,* (2004); it is clear that this research will profit from contributions by all other young researcher.

3.6. Summary

The future work towards the development of the integrated wastewater system model will continue to stress a continuous exchange of ideas and concepts between the partners within the WWT&SYSENG network. Possible case studies, different integrated control strategies and already developed simulation tools for different sub-systems of the global system will be regarded. Table 3.1 below gives an overview of the focus of each of the YRs employed within the WWT&SYSENG project.

Table: Research focus of the YRs employed under the WWT&SYSENG network.

YR	Components	Techniques	Model Platform	Objectives
Flavia Camilleri	WWT +River	Optimisation	Matlab/Simulink	Minimise WWT effluent on river
Joanna Boguniewicz	River basin	Deterministic modelling	GIS,SWAT,QUAL2E	Improve water quality
Cristina Lazar	WWT with Integrated models	Control	Matlab/Simulink	Improve WWT operation
Farid Benazzi	Integrated models	Control/Estimation	Matlab/Simulink	Estimate variables to improve control
Marie O'Brian	Integrated models	Predictive control	Matlab/Simulink	Improve control using prediction
Botond Ráduly	WWT + River	ASM+ANN	Matlab/Simulink	Improve modelling
Irina Comsa	Integrated models	Optimisation, Control	SYNOPSIS	Improve water quality
Gladys Tapia	WWT	Deterministic model control	Matlab/Simulink	Improve WWT operation
Bianca Chindris	Sewer + WWT	Optimisation control	KANSIM	Improve WWT operation
Erik Lindblom	Sewer + WWTP+River	Deterministic stochastic models	Matlab/Simulink	Understanding organic pollution dynamic
Krist Gernaey	WWT	Deterministic and stochastic models, benchmarking	Matlab/Simulink	Improve WWTP operation

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4. Acknowledgement

The work leading forward to producing this report was funded by the European Community through the Research Training Network "WWT&SYSENG: Getting Systems Engineering into Regional Wastewater Treatment Strategies", which runs from February 2002 to January 2006 (contract HPRN-CT-2001-00200).

THE ASM2D MODEL: IMPLEMENTATION IN MATLAB AND DESCRIPTION OF THE PROCESSES

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Abstract
Nowadays the water problem is one of the most urgent issues that the world has to face. One aspect of this global worry is the poor quality of the water bodies. In this context the application of an optimal control system of the wastewater network assumes an important and fundamental role. How is it possible to find the optimal control solution? It is necessary to use software that can test several control combinations in a short period of time.
The research explained in this report has been carried out to develop, on the base of the ASM2d model, a simulation program for a wastewater treatment plant. Several processes have been simulated to test the efficiency of the first version of this program. Together with the main results obtained and the analysis of them, the reader will find also proposals for changes in the program which are likely to be developed in future versions.

INTRODUCTION

The water problem is going to be a big issue of the new century. In 2001 the European Commission published the list of the 37 big European cities (most of which are in Member States) which, after ten years of the European Union's urban wastewater Directive, still discharged their wastewater untreated and/or many other effluents without adequate treatment. The application of an adequate and optimal control to the existing wastewater treatment plants and to new plants will be a means to reduce the impact of the water discharged from the treatment plants into the receiving waters. Moreover, this takes a greater meaning if the wastewater treatment plant is thought of as an integral part of an *integrated water management* system.

This paper discusses the development of a computer programme of a simplified wastewater treatment plant model in order to be able to apply and test different combinations of system control. The first part of this project is reported in this paper, showing the implementation of a wastewater treatment plant model in simulation software, applying it to a CFSTR reactor and testing its performance through the simulation of different wastewater treatment plant processes. This has been done mainly with the aim to demonstrate and explain sanitary engineering processes to who is not familiar with them. Moreover, having set several initial and boundary conditions during the simulation phase, it has allowed seeing if the program was able to react properly to the changes of the system.

The computer language which has been chosen is Matlab/Simulink in order to combine simulation and control design. The model chosen to write the program is the ASM2d model, which is one of the most complete model of the models nowadays available.
In this paper the reader will find a brief description of ASM2d, of its implementation in Matlab, the description of the most significant simulations results and then the conclusion, in which the program advantages/disadvantages and problems are reported.

AIM OF THE PAPER

In this initial phase, our research was lacking of experimental data or data from a real treatment plant. Therefore, we have not been able to test the program applying it to a real activated sludge system. Moreover in this phase of the project, the necessity to explain, both theoretically and graphically, which are the activated sludge processes and how they function, has been felt and seen as a fundamental step to allow a common scientific knowledge base. Then what the reader will find in this paper is the demonstration of how the processes and the ASM2d model equations work under a hypothetical point of view, that is without the problems and noises that are usually present in a real treatment plant.

THE ASM2D MODEL

The ASM2d model belongs to the family of the Activated Sludge Models (they are ASM1, ASM2, ASM2d, ASM3 and they differentiate each other for the processes and the components involved) produced by the IWA task group *on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment.* The reasons of their success are essentially two; firstly, to have unified the language used for the wastewater treatment processes and, not less important, to be the base for several simulation software.

Considering the mass balance of a general component C in an activated sludge tank:

$$V\frac{dC}{dt} = Q*C_i - Q*C_e \pm V*r \qquad (1)$$

where: **C**= concentration of the component; **Ci**, **Ce** = concentration of the component respectively in the influent and in the effluent; **Q** = flow; **V** = volume of the tank;

practically, the models give the reaction terms ***r*** for all the components considered in them, through the following formula

$$r_i = \sum_j v_{ij} * p_j \qquad (2)$$

where p_j is the j^{th} process and v_{ij} represents the stochiometric coefficients.

The same formula can be written in a matrix formulation:

$$\mathbf{r=A'*p} \qquad (3)$$

where **r** is the reaction terms vector, **A** is a the matrix of the coefficient and **p** is the processes vector. In ASM2d **r** has dimension 19*1 (the model studies the behaviour of 19 components); **A** has dimension 21*19; **p** has dimension 21*1 (21 processes are considered). See in appendix 1 which are the 19 components and 21 processes considered in ASM2d.

The reaction terms in this way obtained are necessary to study the behaviour during the time of the components inside the activated sludge tank, through their mass balances.

THE COMPUTER PROGRAMME

The aim of the first version of a simulation program is to test its adaptability to the model chosen through the simulation of model processes and to check the coherence of the results with what the theory teaches. To do this, the processes have been regrouped related to their logical and possible coexistence, and for their simulation the treatment plant has been schematized through just one tank, which simulates a CFSTR reactor.

The model has been written in Matlab language, through the use of S-function, and the simulation has been done in Simulink (Figure 3 in Appendix2). However, we would like to stress the fact the program, especially its Simulink application, has to be more developed both on the basis of the results obtained in this phase and to be able to represent most properly a wastewater treatment plant (for example, through the introduction of different tanks for different processes, aeration, secondary clarifier, etc.).

The basic version of the Matlab program does not involve biomass recycle and external input variables. The following modifications have been introduced:

1. The aerobic conditions have been simulated through the zero setting of the oxygen derivative term at the end of the derivative section of the program (end of *case 1*).
   ```
   (sys(1)=0;%in order to let O2 constant)
   ```
2. To institute the anoxic conditions two different methodologies were used to take into consideration the different aims of the simulations for different processes and their different equations:
   a) For the denitrification process the most interesting thing was to show the transfer from aerobic to anoxic conditions, that is to be able to see the formation of the nitrate firstly and then their transformation in nitrogen. To achieve this, the following command has been introduced at the end of the derivative section (end of case 1):
   ```
     if  x(5)<10  %The anoxic conditions are instituted when
   %Sno3 is greater    than 10 gN/m3, otherwise the aerobic
   %conditions are present in the tank.
     sys(1)=0;in order to let O2 constant
       end
   ```
   b) For the phosphorus accumulating organism processes, the anoxic conditions, since they have been simulated separately from the other conditions, have been set giving a fixed value for the nitrate, which is equal to $10gN/m^3$.
3. The biomass recycle was simulated by simply increasing the concentration of the microorganism in the influent. This has been done because, without recycle of biomass, the initial biomass is destined to wash out completely with the effluent and there is not biomass inside the tank to remove the substrate, as also the simulation has shown.

SIMULATION AND RESULTS

During the simulation phase, all the processes included in the ASM2d model have been simulated, in according with the following subdivision:

A. Organic substrates removal in aerobic condition and processes related to it;
B. Nitrification process;
C. Denitrification (including Nitrification);
D. Organic substrate removal, Nitrification, Denitrification and all the processes associated to the heterotrophic and autotrophic organisms;
E. Phosphorus accumulating organism processes;
F. Precipitation and redissolution of Phosphorus.

For every processes group, different simulations have been done by changing the boundary and the initial conditions (for example: case with and without biomass recycle, higher initial substrate, etc.), in order to see how those influence the total behaviour. Moreover, it has been interesting to see in every process group how the introduction of the biomass decay and/or of the hydrolysis processes changes the final steady state conditions.

The parameters and the concentrations used for the simulation have been chosen as follow: the kinetic parameters and the input concentrations are the ones advised in ASM2d model; the initial concentrations have been obtained from the input concentrations considering typical removal efficiency.

In this paper, since it is not possible to show all the simulations, the most important (under a kinetic/biological point of view) will be explained.

The first one is the <u>**ORGANIC SUBSTRATE REMOVAL IN AEROBIC CONDITIONS**</u> **(A.)**(Fig1a,b) for different θ (hydraulic retention time) set.
First it is possible to note some general observations:

- the *oxygen* (S_{O2}) remains constant in according to the modification of the program;
- both the *soluble substrate* (S_A and S_F) are completely removed, that means that they are used by the biomass for their growth. As a result of the biomass growth, and giving evidence of this, the steady state value for the biomass in fig.1a is higher than its input concentration. However, it has to be stressed the fact that this growth can be seen just from this concentrations difference and not from the slope of the line, which is influenced mostly from the washout of the biomass due to its high initial condition;
- the *slowly biodegradable substrate* (X_S), which arrives in the tank with the influent and which is also one product of the biomass lysis for figure 1b, is accumulated because hydrolysis is not considered in these two simulations.

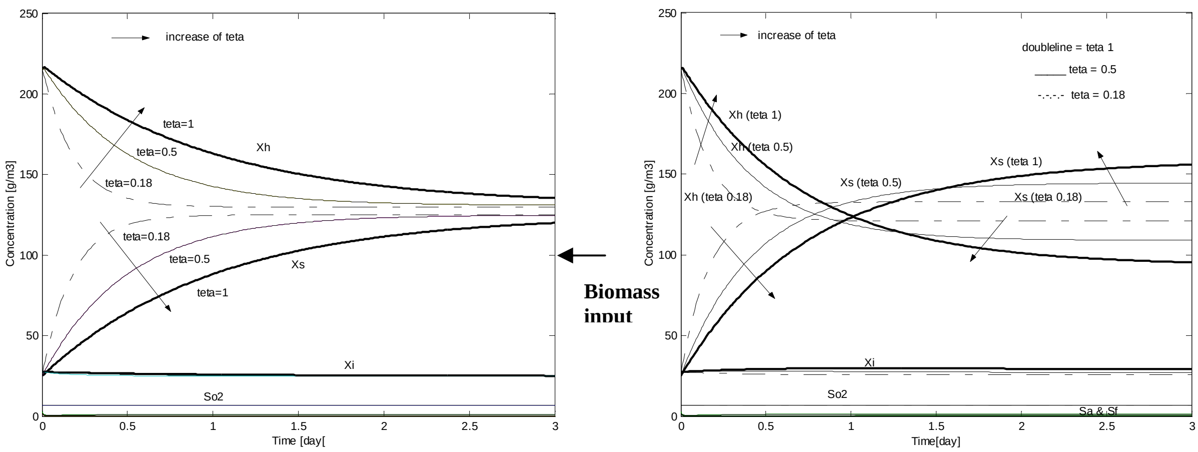

Fig.1a,b: Study of different behaviour under different values of theta (hydraulic retention time).
1a: **Processes: Aerobic growth on S_F; Aerobic growth S_A**; Biomass recycles made setting input concentration at 100 gCOD/m^3. Constant oxygen supply (7g/m^3).
1b: **Processes: Aerobic growth on S_F; Aerobic growth S_A; Lysis of heterotrophic organism**; Biomass recycles made setting input concentration at 100 gCOD/m^3. Constant oxygen supply (7g/m^3).

Examining the differences given by changes in theta, in the simulation graphs there is an increase of the time required to reach the steady state conditions in correspondence to the increase of theta, both for the *biomass* (X_H) and for the *slowly biodegradable substrate* (X_S). As a consequence of the immediate removal of soluble substrate, it is not possible to see in the graphs the increase of the amount of soluble substrate that should be removed in correspondence of higher theta, in steady state condition and supposing the reaction term constant (admissible supposition since the reaction term variations are in normal condition not so high).
When the biomass decay is introduced (fig 1.b) it is possible to observe:

- the biomass concentration decreases and it more significantly happens with higher theta, because the biomass remains longer in the reactor so it is subjected longer to the reduction processes;

- simultaneously the slowly biodegradable substrate (that is the larger product of the biomass decay) increases.

Another group of simulations has been done to simulate the Nitrification and Denitrification processes. The most complete graph is that one which reports all the three main biological processes together, that is the heterotrophic and autotrophic organism's processes. The processes which have been considered are: **HYDROLYSIS PROCESSES, HETEROTROPHIC ORGANISMS PROCESSES (AEROBIC GROWTH, DENITRIFICATION, FERMENTATION, LYSIS) AND NYTRIFING ORGANISM GROWTH AND LYSIS (D.)** (Fig. 2)

Beginning with the biological nitrification (in the ASM2d model it is assumed to be one step, that is from the ammonium to the nitrate, without the formation of nitrite), it is possible to observe that in the aerobic conditions the complete removal of the ammonium is reached: as soon as the anoxic conditions are instituted the ammonium begins to increase again due to its concentration in the influent. The removal of the ammonium is related with the formation and increase of the nitrate, whose concentration in input is equal to zero.

In the anoxic conditions the nitrate is transformed into nitrogen through the denitrification and the nitrogen line has a higher slope than in the aerobic conditions (the increase of nitrogen in the aerobic conditions is due to its influent concentration). This process is due to the heterotrophic organisms, as well as the removal of the substrate in the aerobic conditions (aerobic growth of heterotrophic organisms), but their growth is again hidden behind the washout phenomena.

Finally the readily biodegradable substrate (S_F) and the fermentation products (S_A) are completely removed in the aerobic and anoxic conditions; in the anaerobic conditions the only processes that affect their concentration are the anaerobic hydrolysis and the fermentation. The anaerobic hydrolysis results in the transformation of the slowly biodegradable substrate (X_S) entering with the influent into S_F; but the most influential process in these conditions is the fermentation, which results in a high increase of fermentation products concentration -S_A- (in the model the fermentation is hypothesized as a simple transformation process from readily biodegradable substrate (S_F) to fermentation products (S_A)).

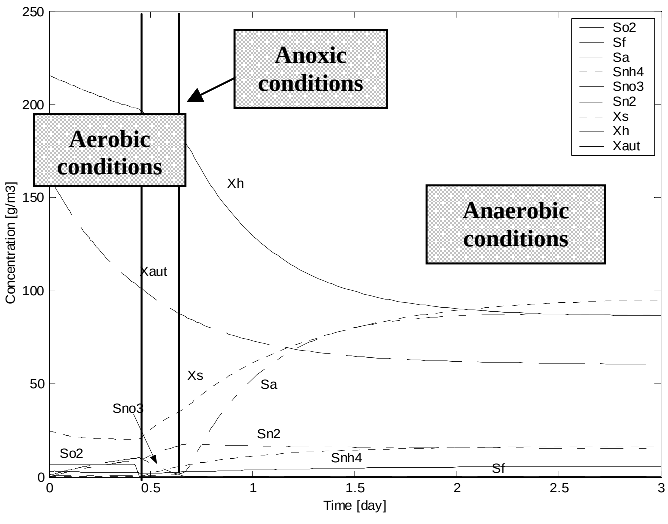

Figure 2: Processes: Hydrolysis processes; Heterotrophic organisms processes(growth on S_F and S_A; dentrification with S_F and S_A; Fermentation; lysis); Nytrifing organism (autotrophic organism) growth and lysis. The biomass recycles is made setting X_{Hu}=100, X_{AUTu}=65. Constant oxygen supply (7g/m^3) until value of NO_3 <10 g/m^3.

Other processes have also been simulated: for the **PHOSPHORUS ACCUMULATING ORGANISMS (PAO) PROCESSES (E.)** the simulation step has been divided in four phases:

1. aerobic conditions: aerobic storage of poly-phosphate, which is the cell internal inorganic storage product of PAO (X_{PP}) and aerobic growth of PAO;
2. anoxic conditions: anoxic storage of X_{PP} and anoxic growth of PAO;
3. anaerobic conditions: storage of the cell internal storage product of the phosphate accumulating organism (X_{PHA});
4. lysis of X_{PAO}, X_{PP} and X_{PHA}.

As for the other simulations, here X_{PAO}'s, X_{PP}'s and X_{PHA}'s recycle has been introduced setting higher values for their input concentration.

It is important to point out that the storage of X_{PHA} process is likely to happen in anaerobic conditions (which are stress condition for the biomass), but the model does not exclude its possible existence also in aerobic/anoxic conditions, since experimental observations have shown that the storage of Xpha can occur also in these conditions.

In aerobic and anoxic conditions the simulation has shown that the complete removal of the phosphorus is reached, together with an increase of the "final" X_{PP} concentration related to its input. X_{PHA} is completely removed because it is consumed by the PAO whose growth is verified by a higher final concentration than the input. Also for those processes, the washout effect can hide these results, which are visible only with a comparison between the final concentrations and the input.
In anaerobic conditions the storage of X_{PHA} has been simulated and, in order to be able to see the process behaviour, the soluble organic material (S_A) has been set as a constant (sys(3)=0). The results are an increase of X_{PHA}, a decrease of X_{PP} and an increase of S_{PO4}.

The last series of processes regard the <u>**CHEMICAL PRECIPITATION OF PHOSPHATES**</u> **(F.)**, which involves the precipitation and the redissolution of salts formed by metal with orthophosphate/polyophosphate. The model assumes that the Metal is iron, the Metal-hydroxide (X_{MeOH}) is the ferric-hydroxide ($Fe(OH)_3$) and the salt formed (X_{MeP}) is ferric-phosphate ($FePO_4$). In order to see the process results in a better way, higher concentration of phosphorus have been set (S_{PO4i}=36 g/m^3; S_{PO4u}=36g/m^3) and the metal is supposed to be added in the tank during all the time (X_{MeOHi} = 27 g/m^3 and its constant supply (`sys(18)=0;`)). The simulations have shown what was foreseeable, that is the increase of ferric phosphate and of total suspended solids, as well as a decrease of phosphate. The redissolution has a smaller effect than the precipitation.

MODEL SIMPLIFICATION

Some processes are more important in some conditions than in other and a simplification to the program could be made if some processes are neglected. For example:

i. The hydrolysis process has a stronger influence in aerobic conditions, whereas in anoxic and anaerobic conditions its influence is reduced by two different reduction factors (they are: η_{NO3}= anoxic hydrolysis reduction factor=0.6; η_{fe} = anaerobic hydrolysis reduction factor=0.4). In anaerobic conditions, especially if also the fermentation is considered, the hydrolysis could be neglected.
ii. The phosphorus-accumulating organisms have shown a similar behaviour in anoxic and aerobic conditions.
iii. Further study and experimental tests should be done to verify if the ferric-phosphate redissolution can be neglected in comparison with the precipitation and washout phenomena influence.

CONCLUSIONS

This paper summarizes the research made into the use of ASM2d model as a tool for control studies and for demonstrating different processes. It can be used as a useful tool for the representation of the activated sludge processes.

Future developments should be based in improvements of the Simulink model, with the introduction for example of biomass recycle and the continuous supply of components that allow the existence of the processes (like for example the oxygen in aerobic conditions, or the metal hydroxide for the precipitation of phosphorus). Also the simulation of the treatment plant through more different tanks is advised.

Improvements should be carried out also in the program if all the processes have to be simulated together (for example, modifications in order to avoid the error given by the zero value of the oxygen in the denominator of some equation terms).

Regarding the initial wastewater characterization, it is important to point out the difficulty to have values for all the parameters, like for example the initial concentrations that should be extracted by the steady state conditions of previous simulations or by real treatment plants. The overestimated initial conditions, for example, have resulted in the hiding of some parameters growth due to the prevalence of washout phenomena. Moreover the problem is also to find values that are suitable for the simulation of several or all processes together.

Finally the author would like to stress the fact that the aim of the program shown is not to find the exact concentrations in the effluent, but to give an indication of the behaviour of the system by changing boundary conditions. This is because we are not looking for a program that could compare simulated data with experimental data, but an instrument which could estimate the performance of one kind of control rather than another one.

Flavia Camilleri acknowledges the financial support provided through the European Community's Human Potential Programme under contract HPRN-CT-2001-00200[WWT & SYSENG].

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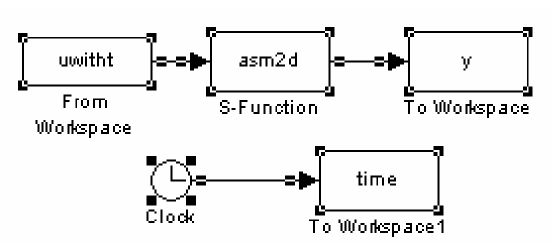
APPENDIX 1: Components and processes of ASM2d

Soluble components	**Particulate components**
S_A= Fermentation product	X_{AUT} = Nitrifying Organisms
S_{ALK} = Alkalinity of the wastewater	X_H = Heterotrophic organisms
S_F = Fermentable, readily biodegradable organic substrates	X_I= inert particulate organic material
S_I = inert soluble organic material	X_{MEOH}= Metal hydroxides
S_{N2} = Dinitrogen	X_{MeP} = Metal Phosphate (MePO4)
S_{NH4} = Ammonium plus Ammonia Nitrogen	X_{PAO} = Phosphate accumulating organisms
S_{NO3} = Nitrate plus Nitrogen (NO_3^-+NO_2^- -N)	X_{PHA} = the cell internal storage product of phosphorus accumulating organisms
S_{O2}= Dissolved oxygen	X_{PP} = Poly-Phosphate
S_{PO4}=Inorganic soluble phosphorus	X_S = Slowly biodegradable substrates
S_S= Readily biodegradable substrate (not explicitly considered in the model. It is the sum of S_A and S_F)	X_{TSS}=total suspended solids

	Processes	**Processes numeration**
Hydrolysis processes	Aerobic hydrolysis	p1
	Anoxic hydrolysis	p2
	Anaerobic hydrolysis	p3
Heterotrophic organisms: X_H	Growth on fermentable substrate, S_F	p4
	Growth on fermentation product, S_A	p5
	Denetrification with fermentable substrates, S_F	p6
	Denetrification with fermentation products, S_A	p7
	Fermentation	p8
	Lysis	p9
Phosphorus accumulating organisms (PAO): X_{PAO}	Storage of X_{PHA}	p10
	Aerobic storage of X_{PP}	p11
	Anoxic storage of X_{PP}	p12
	Aerobic growth on X_{PHA}	p13
	Anoxic growth on X_{PHA}	p14
	Lysis of X_{PAO}	p15
	Lysis of X_{PP}	p16
	Lysis of X_{PHA}	p17
Nitrifying organisms	aerobic growth of X_{AUT}	p18
	Lysis of X_{AUT}	p19
Simultaneous precipitation of phosphorus with ferric hydroxide $Fe(OH)_3$	Precipitation	p20
	Reddisolution	p21

APPENDIX 2: Fig.3: The Simulink model



Application of Extended Kalman Filter to Activated Sludge Process

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Abstract

Control of dynamics systems need a perfect understanding of its behaviour and it is not always possible for some complex or simple applications to measure all variables that we want to control. The Extended Kalman Filter (EKF) is supposed to be the perfect tool to provide an estimate for deducing the missing information from indirect and noisy measurement.

In this paper an EKF is applied to a biological wastewater treatment process in order to control the dissolved oxygen (DO) and the Substrate (S) with proportional integral (PI) controllers based on estimates provided by the EKF. The EKF approach is to apply a standard Kalman Filter (for the linear model) to the non-linear model with additive white noise and continually update the linearization around the previous state estimates. Simulation results and comparison between the Kalman Filter (KF) and the EKF are given to demonstrate that the KF is a powerful tool for linear models and to also prove the robustness of the EKF for non-linear models. This filter is also convenient for online real-time processing because of the minimum storage data required.

Keywords

Activated Sludge Process, Control; Extended Kalman Filter; Kalman Filter; Linearization; Wastewater Treatment plant.

1 INTRODUCTION

The wastewater treatment plant (WWTP) is at the heart of the process dealing with domestic, industrial and agricultural waste. In most countries and cities, the wastewater is treated in biological treatments plants rather than receiving physical treatment (like sedimentation or filtration) or chemical treatment (like precipitation or flocculation) (Metcalf, 2003]. Due to the measurement difficulties involved in measuring variables in a biochemical process, we will therefore use the EKF to estimate the states of one of the most common wastewater treatment process which is the activated sludge technology. The activated sludge process (ASP) has a very complicated and non-linear dynamics. Most ASP plants are only controlled (DO, nitrate, chemical dosing, return activated sludge and so on) using PID controller. The performance of these controllers over varying load condition is not satisfactory. In addition the ASP suffers from poor instrumentation. Hence, to control the process, it is required to use observers or estimators to estimates the states which are not measured or remove the noise from those which are measured. This paper is concerned with the application of EKF in order to smooth the measurement and investigate the possible performance improvement using a more advanced controller (Katebi, 1999), (Olsson, 1976).

This paper reports on the design of the EKF implemented with the ASP and will be organised as follow: In section 2, the ASP is briefly described. Section 3, introduces the KF and compare the outputs with the non-linear model. Section 4, presents the design of the EKF. In section 5, the performance of the EKF and the PI control are demonstrated via simulation study. General conclusion ends the paper.

2 BIOLOGICAL WWTP

The studied biological system is an ASP which consists basically of a series of activated sludge tanks in which different conditions (anaerobic, anoxic and aerobic) are used to promote the nutrient removal process. A typical activated sludge treatment process with one anaerobic tank, one anoxic tank, one aerobic tank and a secondary clarifier is represented in Figure 1. The activated sludge processes are biological processes that allow removal of pollutants from the wastewater, principally those ones that are in soluble form and those that are biodegradable in a period that is technologically acceptable.

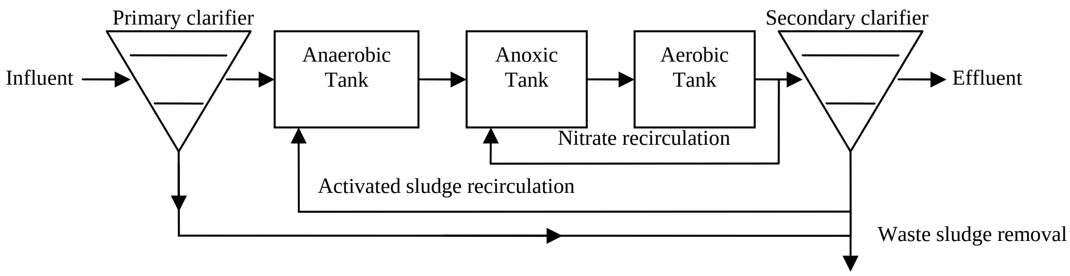

Figure 1: Activated sludge treatment process

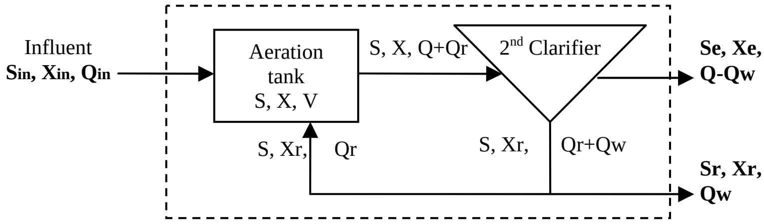

Figure 2: Activated Sludge Reactor

In this paper an aerobic process will be used as shown in Figure 2. This comprises an aeration tank and a secondary clarifier that is necessary for the settling of the biomass and its recycling. Where Q represents the secondary influent flowrate; Q_r the return sludge flowrate; Q_w the waste activated-sludge flowrate and X_e the effluent suspended solids. The mass balance on the aerator and the settler gives the following set of non-linear differential equations (Nejjari, 1997):

$$\dot{X}(t) = \mu(t)X(t) - D(t)(1+r)X(t) + rD(t)X_r(t) \tag{1}$$

$$\dot{S}(t) = -\frac{\mu(t)}{Y}X(t) - D(t)(1+r)S(t) + D(t)S_{in} \tag{2}$$

$$\dot{C}(t) = -\frac{K_o\mu(t)X(t)}{Y} - D(t)(1+r)C(t) + K_{La}(C_s - C(t)) + D(t)C_{in} \tag{3}$$

$$\dot{X}r(t) = D(t).(1+r).X(t) - D(t).(\beta + r)Xr(t) \tag{4}$$

Where X(t), S(t), C(t) and X_r(t) are the states representing the biomass, the substrate, the dissolved oxygen and the recycled biomass concentration respectively. The parameters r ($r=Q_r/Q$) and β ($\beta=Q_w/Q$) represent the ratio of recycled flow to influent flow and the ratio of waste flow to the influent flow, respectively. S_{in} corresponds to the substrate in the feed stream; the biomass growth is described by the specific growth rate, μ ($\mu=r_g/X$) and the yield of cell mass, Y. The constants Cs, and K_{La}, represents the dissolved oxygen saturation concentration and the oxygen transfer rate coefficient ($K_{la} = \alpha.W$ with $\alpha>0$ and W=air flow rate) and K_o is a switching constant (DO switch). We assume that the specific growth rate is referred as multiple Monod kinetics (Olsson, 1976), depending on substrate and dissolved oxygen concentrations:

$$\mu = \mu_{max}\frac{S}{K_s + S} * \frac{C}{K_c + C}$$

Where μ_{max} is the maximum specific growth rate, K_s is the affinity constant and K_c is the saturation constant. The parameters taken from Nejjari model (Nejjari, 1997) are given on section 5.

3 The Kalman Filter

The KF is one of the most widely used methods for tracking and estimation due to its, optimality and robustness (Welch, 2002). The KF addresses the general problem of estimating the states x of a process that is governed by the linear stochastic difference equations

$$\dot{\mathbf{x}}(t) = \mathbf{Ax}(t) + \mathbf{Bu}(t) + \mathbf{w}(t) \tag{5}$$

with a measurement $\mathbf{y}_v$ that is

$$\mathbf{y}_v(t) = \mathbf{Cx}(t) + \mathbf{v}(t) \tag{6}$$

where w(t) is the *n*-dimensional process noise vector which is assumed to be a zero-mean, Gaussian distributed, random noise process with the n*n covariance matrix Q(t) and where $\underline{v}$(t) is the *m*-dimensional measurement noise vector which

is assumed to be a zero-mean, Gaussian distributed, random noise process with variance R(t). The process noise and the measurement noise are assumed to be uncorrelated.
The estimate of the state is denoted by $\hat{\mathbf{x}}(t)$ and the ‘a priori’ state estimate is denoted by $\hat{\mathbf{x}}(t)^-$ (the super minus). The ‘a priori’ estimation error covariance matrix of the states is denoted by $\mathbf{P}(t)^-$ and the ‘a posteriori’ estimation error covariance matrix is denoted by P(t) and is given by

$$\mathbf{P}(t) = E\{(\mathbf{x}(t) - \hat{\mathbf{x}}(t))(\mathbf{x}(t) - \hat{\mathbf{x}}(t))^T\}$$

where E represents the expectation process. Note that P(t) is a *n* x *n* symmetric, positive-definite matrix. The diagonal terms of the estimation error covariance matrix represent the variances (i.e. the square of the standard deviations) of the estimation errors of the state (Skaar, 1994).

The Time Update Equations (7 & 8) are used for predicting the current state and covariance matrix, used at time t+1 to predict the previous state.
The Measurement Update Equations (9, 10 &11) are used for correcting the errors made in the Time Update equations.
The KF time update equations are given by:

$$\hat{\mathbf{x}}(t)^- = \mathbf{A}(t).\hat{\mathbf{x}}(t) + \mathbf{Bu}(t) \quad \text{(Project the state ahead)} \quad (7)$$

$$\mathbf{P}(t)^- = \mathbf{A}(t).\mathbf{P}(t).\mathbf{A}(t)^T + \mathbf{Q}(t) \quad \text{(Project the error covariance ahead)} \quad (8)$$

and the KF measurement update equations are:

$$\mathbf{K}(t) = \mathbf{P}(t)^- \mathbf{C}(t)^{\mathrm{T}} (\mathbf{C}(t).\mathbf{P}(t)^- \mathbf{C}(t)^{\mathrm{T}} + \mathbf{R})^{-1} \quad \text{(Compute the Kalman Gain)} \quad (9)$$

$$\hat{\mathbf{x}}(t) = \hat{\mathbf{x}}(t)^- + \mathbf{K}(t).(\mathbf{y}_v(t) - \mathbf{C}\hat{\mathbf{x}}(t)^-) \quad \text{(Update estimate with measurement } \mathbf{y}_v\text{)} \quad (10)$$

$$\mathbf{P}(t) = (\mathbf{I} - \mathbf{K}(t)\mathbf{C}(t))\mathbf{P}(t)^- \quad \text{(Compute error covariance for update estimate)} \quad (11)$$

where the n*n matrix A in the difference equation (5) relates the states at time t. The n*l matrix B relates the optional input control u to the states x. The n*m matrix C in the measurement equation (6) relates the states to the measurement y_v. Note that in this case the A and B matrix never changed (they are not updated). The n*m matrix K in equation (10) is the Kalman gain or blending factor that minimizes the a posteriori error covariance P(t) (Brown, 1997).

In this paper, a linear KF has been applied to an ASP as represented by Figure 3. To test the performance of the KF (inner of the filter represented in Figure 4) in a region around the operating point, we increased the inputs level from 0% (d=0.08 1/h for the dilution rate and W=90 m^3/h for the air flow rate) to 50% (d=0.124 1/h and W=135 m^3/h) as shown in Table 1. The simulation results which compare the KF and non-linear outputs are display on Figure 5 and have been simulated using Matlab software. Table 1 also presents the error (%) between the non-linear outputs and the estimated outputs from the KF.

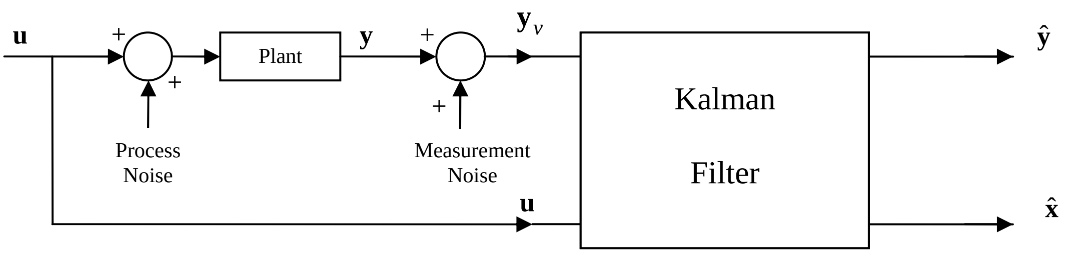

Figure 3: Linear KF implemented with the plant

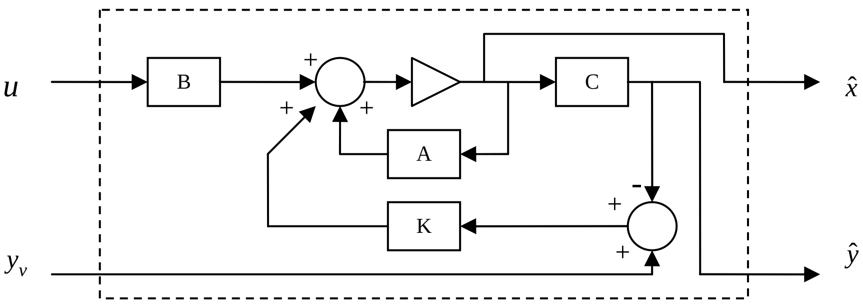

Figure 4: Inner Kalman Filter

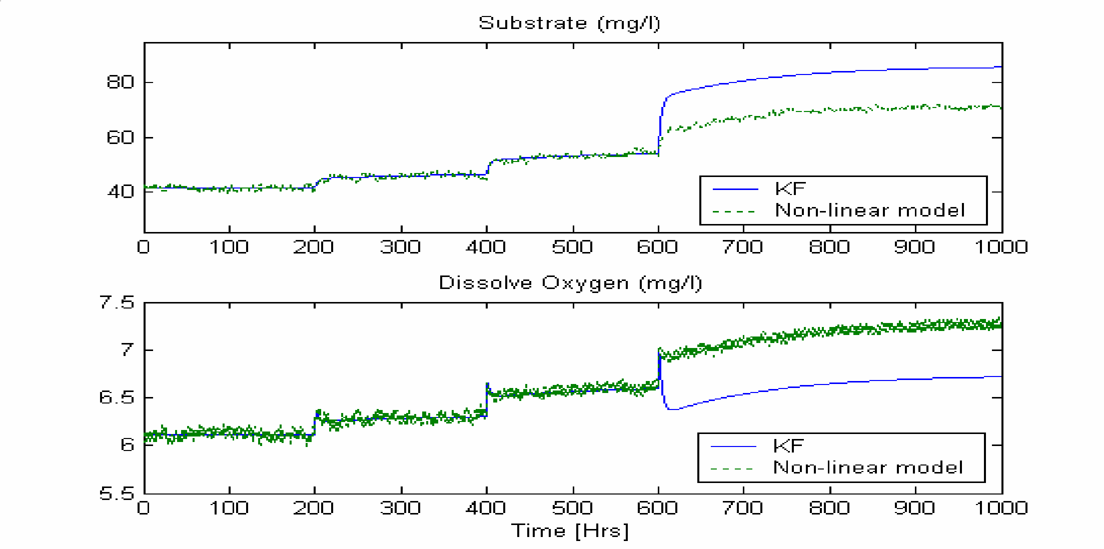

Figure 5: Estimated KF outputs compared with the non-linear outputs

	0<t≤200 (hrs)	200<t≤400 (hrs)	400<t≤600 (hrs)	600<t≤1000 (hrs)
δu (%)	0	10	25	50
Output change from Css (mg/L)	0	0.2	0.4	0.7
Output change from Sss (mg/L)	0	3	8	15
DO Error between $\mathbf{y}_v$ and $\hat{\mathbf{y}}$ (%)	0 %	3.13 %	5.89 %	10.81 %
Substrate error between $\mathbf{y}_v$ and $\hat{\mathbf{y}}$	0 %	6.25 %	13.8 %	17.65 %

Table1: KF and non-linear model outputs

From Table 1 it can be seen that increasing the input values from 0 to 25% has a small effect on the outputs (small, depending on the required accuracy of the model). From 25% to 50% input changes, the difference between the outputs from the non-linear model and the linear Kalman filter start to go over 17.65% for the Substrate and 10.81% for the DO. We can see that increasing the inputs from their steady state values increase the error between the non-linear model and the estimated outputs. One approach to eliminate this error is to use the Extended Kalman Filter (EKF).

4 The Extended Kalman Filter (EKF)

The EKF for the continuous problem has been derived for use in nonlinear systems which can be described by the two equations (12) and (13). This filter uses a linearization of the state equations and the observation equations about the current best estimate of the state to produce minimum mean-square estimates of the state.

Consider the following system

$$\dot{\mathbf{x}}(t) = f(\mathbf{x}(t), \mathbf{u}(t)) + \mathbf{w}(t) \tag{12}$$

$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{v}(t) \tag{13}$$

where all the variables have been describe in the previous section and where the Extended Kalman filter algorithm proceeds according to the following three steps:

(1) The estimate of the state and the estimation error covariance matrix are initialised at t=0.

(2) The state estimates and the estimation error covariance matrix are propagated when observations are not available by solving the following differential equations:

$$\dot{\hat{\mathbf{x}}}(t) = f(\mathbf{x}(t), \mathbf{u}(t)) + \mathbf{w}(t)$$

$$\dot{\hat{\mathbf{P}}} = F(\hat{\mathbf{x}}(t), \mathbf{u}(t))\mathbf{P}(t) + \mathbf{P}(t)F^T(\hat{\mathbf{x}}(t), \mathbf{u}(t)) + \mathbf{Q}(t)$$

where the n*n matrix $F(\hat{\mathbf{x}}(t), \mathbf{u}(t))$ is given by

$$F(\hat{\mathbf{x}}(t), \mathbf{u}(t)) = \left.\frac{\partial f(\mathbf{x}(t), \mathbf{u}(t))}{\partial x}\right|_{\mathbf{x}=\hat{\mathbf{x}}(t)}$$

(3) The estimation error covariance and state estimates are then updated as follows:

$$\frac{d\hat{\mathbf{x}}(t)}{dt} = f(\hat{\mathbf{x}}(t)^-, \mathbf{u}(t)^-) + \mathbf{A}(\hat{\mathbf{x}}(t) - \hat{\mathbf{x}}(t)^-) + \mathbf{B}(\mathbf{u}(t) - \mathbf{u}(t)^-) + \mathbf{K}[y(t) - \mathbf{H}\hat{\mathbf{x}}(t)]$$

$$\mathbf{K}(t) = \mathbf{P}(t).\mathbf{C}^T(\hat{\mathbf{x}}(t), t).\mathbf{R}^{-1}(t)$$

$$\dot{\mathbf{P}}(t) = F(\hat{\mathbf{x}}(t), t)\mathbf{P}(t) + \mathbf{P}(t)F^T(\hat{\mathbf{x}}(t), t) + \mathbf{Q}(t) - \mathbf{P}(t).\mathbf{C}^T(\hat{\mathbf{x}}(t), t).\mathbf{R}^{-1}(t).\mathbf{C}(\hat{\mathbf{x}}(t), t).\mathbf{P}(t)$$

with $\mathbf{P}(0) = \mathbf{P}_0$, $\hat{\mathbf{x}}(0)=\mathbf{x}_0$ and

$$\mathbf{A} = \left.\frac{\partial f}{\partial \mathbf{x}}\right|_{\mathbf{x}=\hat{\mathbf{x}}(t)}, \quad \mathbf{B} = \left.\frac{\partial f}{\partial \mathbf{u}}\right|_{\mathbf{u}(t)}, \quad \mathbf{H} = \left.\frac{\partial g}{\partial \mathbf{x}}\right|_{\mathbf{x}=\hat{\mathbf{x}}(t)}$$

5 Simulation results

Simulation results were obained by using a 1st order Taylor approximation algorithm to integrate the non-linear process equations (1)-(4) with values of parameters and initial condition given in table 2 and 3.

Y=0.65	μ_{max} = 0.15 (1/h)	r =0.6
K_S = 100 (mg/L)	K_C = 2 (mg/L)	K_O = 0.5
β = 0.2	α = 0.018	C_S = 10 (mg/L)

Table 2: Kinetics Parameters

X(0)=217.78 (mg/L)= $\hat{x}(0)$	S(0)=41.28 (mg/L)= $\hat{s}(0)$	C(0)=6.11 (mg/L)= $\hat{c}(0)$
Xr(0)=435.58(mg/L)= $\hat{x}_r(0)$	S_{in}=200 (mg/L)	C_{in}=10 (mg/L)

Table 3: Initial conditions for the EKF simulation

5.1 EKF with the non-linear process

The EKF and additive white noise have been implemented with the ASP. The same model as the one represented on Figure 3 page 3 have been used for the simulation apart from the KF which has been replaced by the EKF. To test the performance of the EKF we have applied the same steady state input values as section 3 and increase them from 0% (*d=0.08 1/h* for the dilution rate and *W=90 m³/h* for the air flow rate) to 50% (*d=0.124 1/h* and *W=135 m³/h*). Then, we compared the outputs from the non-linear model (y_v) with the estimated outputs from the EKF ($\hat{y}$).

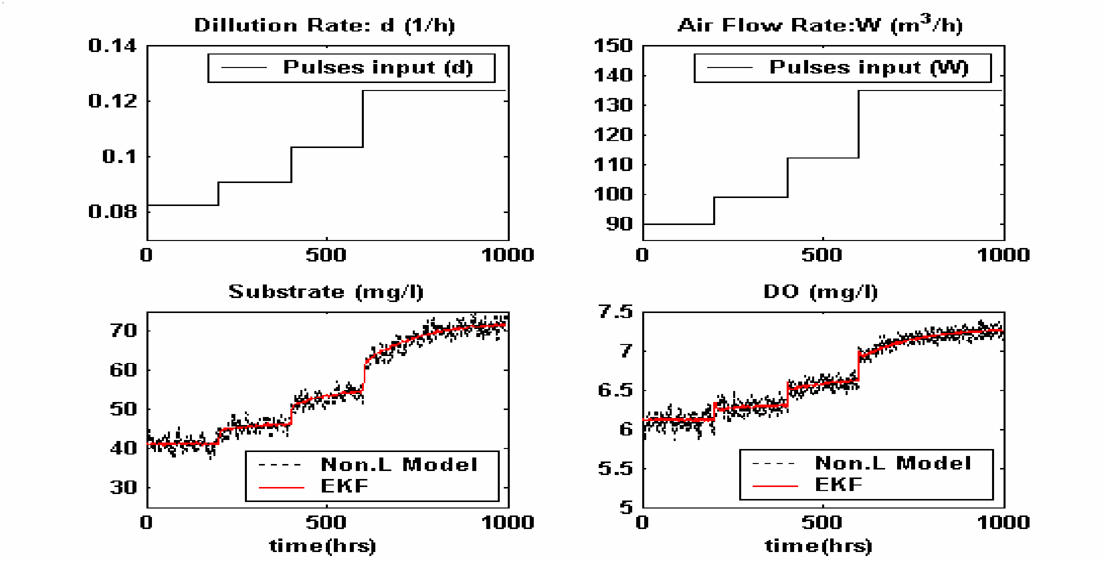

Figure 6: EKF outputs compared with the non-linear outputs

The above result shows that there is no steady state error (%) between the non-linear outputs and the estimated outputs from the EKF when the inputs are increased from 0 to 50%.

5.2 EKF with the non-linear process in closed-loop

A schematic representing the general overview of the simulation is displayed in Figure 7 and the results displayed in Figure 8 represent the nonlinear model outputs, and the EKF filter estimation. The estimated outputs from the EKF are connected with the nonlinear model by the feedback loop.

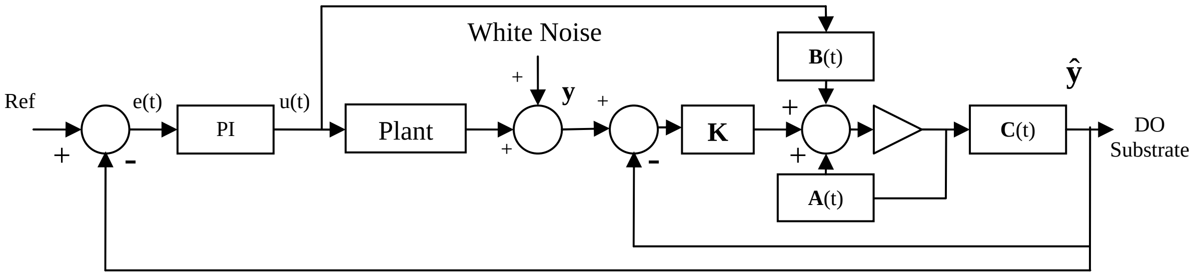

Figure 7: Feedback from the estimated outputs and not from the plant

The output variable C(t) and S(t) have some white random noise added in order to simulate a more realistic measurements. The reference point of the controlled variables are given in Table 4.

Substrate reference points	Dissolve oxygen reference point
S=41.28 (mg/L) for 0<t≤100 h	C=6.11 (mg/L) for 0<t≤100 h
S=50 (mg/L) for 100<t≤1000 h	C=5 (mg/L) for 100<t≤1000 h

Table 4: Controlled variable reference

The estimated outputs variables (the substrate and dissolved oxygen) show the performance of the regulator. The model has been run from 0<t≤100 h at its steady state level to initialise the process. The regulator is applied from 100<t≤1000 hrs to control the substrate to 50 mg/L and the DO to 5 mg/L. We can see that using the estimated outputs, from the EKF, as feedback provides good control.

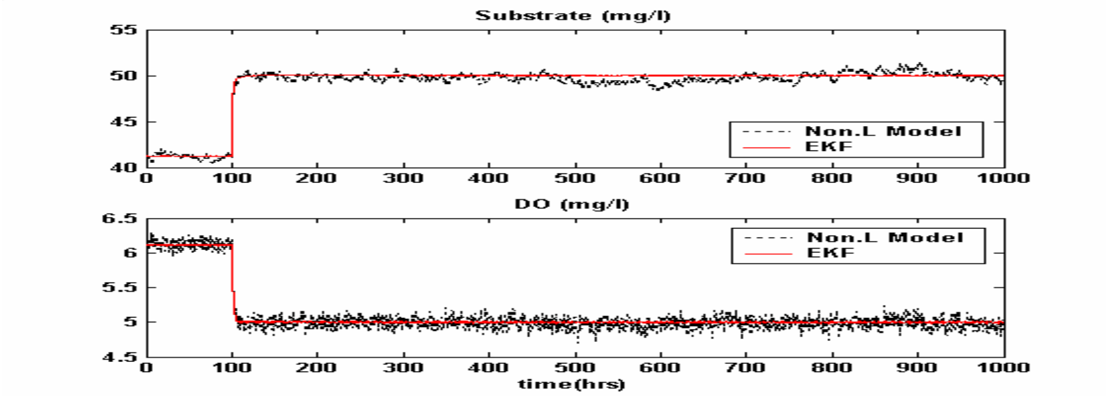

Figure 8: Controlled outputs from the EKF compared with the non-linear outputs

6 Conclusion

Estimation and control for an activated sludge process with the EKF have been proposed. As described on section 3, the linear KF solve the problem of estimating the states of a process that is governed by a linear stochastic difference equation and does not perform well when applied to non-linear process with large input changes. The effectiveness and robustness of the EKF have been demonstrated by simulation results which show the reduction of the noise and the control process using the estimated outputs.

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A DESCRIPTION OF DATA COLLECTION

- The hydrological and water quality modelling using GIS techniques. -

INTRODUCTION

This paper presents the efforts made in the development of a methodology for water quality modelling using Soil and Water Assessment Tool (SWAT). SWAT allows to determine the loadings of water, sediment, nutrients to the main channel, it also models the transformation of chemicals in the stream and streambed. The study objectives include several tasks, among others: simulation of hydrology and average pollutant concentrations resulting from catchment activities; estimation of average nutrient loads, and evaluation of their reduction in the river. The aim of the Lake Pusiano project is a basin-scale modelling of pollutant (nutrients).
The realization of this project needs the support of GIS (Geographical Information System) technology, that allows to collect, store, manage, elaborate and display a large quantity of data associated with a watershed. In order to carry out a complete pollution load assessment, information on the extent of the watershed basin, land uses, climate, vegetation, soil types are collected. This paper briefly details a ArcViewGIS3.2., hydrological, climatic and water quality data available for the Lambro catchment in northern Italy and some recommendations regarding additional data requirements.

1. GENERAL WATERSHED INFORMATION

A river water quality monitoring program is conducted in the Lake Pusiano watershed (Northern Italy), which main river is the Lambro. The catchment area is shown in Figure 1. The headwaters of the river Lambro lie in the Pre-Alps at approximately 1450m above sea level (a.s.l.) between the southern arms of Lake Como in northern Italy. The headwaters of the catchment discharge into a natural glacial lake, Lake Pusiano, which then discharges to form the upper reaches of the Lambro south of the town of Erba. The headwaters of the Lambro, upstream of Lake Pusiano, consist of steep slopes with underlying dolomite geology and forestry is the dominant landuse in the area. Water quality of Lambro river's water is very poor, mainly for nutrient concentrations.

2. DIGITAL ELEVATION MODEL (DEM)

Digital Elevation Model (DEM) is the basic data element for constructing a model of the watershed hydrology. This study used a 1:10000 scale DEM, also called a 10m grid. The DEM for Lake Pusiano basin is presented in Figure 2. On the basis of DEM it is possible to find the "flow direction", and create flow path networks, as well as subbasins, within the watershed. This provided, in GIS environment, movement trace of water through a watershed are an approximation of the real river network. (Function flow direction and flow accumulation provide automated function to trace the movement of water through a watershed.) As it can be seen on figure 2 position of the channels simulated and real streams are fitted well. Subbasins boundaries for the watersheds were also delineated well. Overall, it appears that the defined major river paths and basins are determined well.

3. LAND USE

Land Use data describe vegetation, water, natural surface, and cultural features on the land surface. The Land Use map (1:10000 scale, see Figure 3) has been developed by the Lombardy Region within the DUSAF (Destination of Use of Agricultural and Forest Grounds) plan. Most of areas in the Pusiano catchment are covered by forests (66.7 %). Other important Land Use classes are meadows and pastures (7.7 %), agricultural lands (3.7 %) and water surfaces (6.2 %).

The DUSAF Land Use class of Urban areas (13.3 %) has been further subdivided into 3 sub-classes (Residential areas, Industrial areas and Commercial areas) using the colour digital orthophotos of “IT2000” plan. What is more SWAT required plant growth parameters for all land covers simulated in the watershed.

4. SOILS (GEOLOGY)

A summary of the available lithographic information available for the each of the sub-catchments is evilable on ArcViewGIS format and tables. This information indicates a general trend of increasing permeability down the catchment. Soil permeability is one of the controlling factors for the rate at which a contaminant travels through soils. Soils with higher permeability facilitate the transport of pollutants into groundwater. The map on Figure 4 shows areas with different value of the permeability coefficient, K. In this study three classes of permeability were defined: rapid ($K>10^{-2}$cm/sec=36cm/h), moderate (10^{-4}cm/sec$<K<10^{-2}$cm/sec), and slow ($K<10^{-4}$ cm/sec = 0,36 cm/h).
SWAT in soil input file required information about the physical and chemical characteristics of the soil. Since there isn’t an official soil map for the Pusiano catchment, it has been necessary to create one using a Geographic Information System (GIS). Starting from the lithologic map, the land use map and the slope map. Seven WRB (World Reference Base for Soil Resources – ISSS, ISRIC&FAO,1998) soil categories are supposed to exist in the catchment: Rendzic Leptosols, Calcaric Leptosols, Skeletic Cambisols, Dystric Cambisols, Eutric Cambisols, Calcaric Regosols and Calcaric Phaeozems. The soil map (Figure 5) has been drawn by implementing an algorithm on the basis of the distributive model that has been worked out. The algorithm has been written using Avenue, ArcView GIS’s programming language.

5. CLIMATE AND HYDROLOGY DATA

There are very few rain gages or discharge gages in Pusiano basin. A point coverage of the locations of the rain gages was created to be able to locate the rain gages within the basin. Temperature and precipitation data was collected at 2 stations located inside the catchment. It has been noted that additional climatic data may be available for total of 5 stations in the research region, for the period since 1970 to now, for potential future use. The data included temperature data on a monthly or daily basis, and rainfall data on a daily or monthly basis, the extent of the digitised data are available in Excel spreedhead.
The Cantu temperature recording station contained monthly data from 1937 to 1942 and then daily readings from 1942 to the present, while the Asso station recorded daily temperature readings from 1951 to now. The variation of average monthly temperatures between five (5) temperature stations over the period 1984 to 1994 reflects the altitude gradient occurring across the region, see table below.

Climatic Station	Average annual temperature °C	Elevation (m a.s.l.)
Asso	11.0	427
Cantu	12.2	360
Monza	13.6	162
Cernusco Sul Naviglio	13.8	134
Milano	14.2	121

The spatial variation in temperature down the catchment reflects the spatial variation in rainfall. The higher, cooler regions in the catchment headwaters are subjected to greater average annual rainfall than the lower, warmer alluvial plains in the downstream portion of the region.

SWAT requires daily measured temperatures for a measuring gage and daily precipitation data. Those values may be read from records of observed data or they may be generated. Ther are some missing data so the format of the file used to read precipitation data will be probably generated inside SWAT. Weather generator required the statistical data inorder to generate representative daily climatic data for the subbasins.

The sources of rainfall data were collated, additional required data were digitised and the pooled data examined. The precipitation data for the climatic stations was observed to contain a number of years of missing data. Extensions of the rainfall records in the area would be necessary to examine long term variations in climate within the region. The long term monthly rainfall record for the Monza station was digitised and this source used to check data obtained at other raingauges within the catchment. The long term records was also compared to the paper copies of daily records to establish consistency. Infilling of periods of record omitted during the digitisation process was undertaken. The high spatial variability of precipitation data would make interpolation of this data more difficult. All digitised data was checked for consistency. The consistency of rainfall records were check by construction of double mass plots for gauges in the upper catchment compared to the good quality, long term records held for the Monza station in the lower portion of the catchment. Data from the rainfall stations was used to produce average annual rainfall estimates. These estimates confirm a rainfall gradient falling with altitude and position in the catchment. Average annual rainfall for the catchment varies between 900mm and 1500mm. All avilable rainfall data from the Lambro catchment are held on Excel spreadsheets format.

The University of Milan was responsible for collecting flow data within the Lambro catchment from a number of provincial sources for the purposes of the study (Gandolfi et. al., 1997). A total of five (5) gauges were identified by the UM for which the data records were held by the Italian National Hydrographic Service (SII) and Associazione Difesa Alto Lambro (ADAL). The data series was not continuous but covered the period 1935 to 1995. The best quality flow data for the catchment was available for a period from 1984 to 1994 and an older data set from the 1940's to the 1970's. A base data set was identified to be those years which contained less than 10 days missing flow data. Efforts have been made to extend this data to enable a continuous long term data set to be examined. Some data was only available in paper record format. The UM converted the most of the stage data to spreadsheet format. The currently identified record periods for flow data from the Lambro catchment are summarised on tables, this data is held on EXCEL spreadsheets in daily average flow format.

The hydrologic study of Pusiano Lake's catchment showed many difficulties due to intense infiltration phenomena relating with the influent alluvial cone of the Lambro River, and to the geological substratum, that results to be over 90% calcareous; it is also considered possible that a complex underground hydrological net could exist. A complete set (1970-2002) of hystorical climatic and hydrometric data was applicated to conduct preliminary study in HEC-HMS, developed by the *Us Army Corps of Engineers, California*. It leaded to recovery of missing data, hypotheses on calibrating strategies to improve estimates in its principal components was created, however correct evaluation of groundwater flows, that are difficulty to compute in other ways.The study of pollution diffusion and many other related topics require such reliable information on hydrology characteristics.

6. WATER QUALITY DATA

The model, in addition to spatial and temporal data on DEM, land use and soil requires water quality information. Water quality of Lambro river's water is very poor, mainly for nutrient concentrations. Water quality data have been collected for over one year period, from five quality measurement points and will be collected for one more year. Location of quality measurement points is shown in Figure 6. Collection of data sets cover condition of low, medium and high flow, it is desirable in order to assess overall water quality conditions. Data analysis and result of chemical analysis are assumed in Excel spreedhead. This information will be used to model nutrient transformations in the main channel.

Variables measured are as follow:

A.Filtrate with micro-pore cellulose filters (dimension of holes 0,45μm)

- Determine of ammonium nitrogen **N-NH_3**
- Determine by potentiometer total **alkalinity**
- Determine of phosphorus **P-PO_4**
- Determine of silica **SiO^{2-}**
- Determine by chromatography **anions** (NO_3^-, SO_4^{2-},Cl^-), **kations** (Ca^{2+},Mg^{2+},Na^+,K^+)

B. Non Filtrate

- Determine of dissolved oxygen **DO**
- Determine of **conductivity , pH**
- Determine of **total azot and phosphorus**

Load data

Appropriate coefficients to calculation of theoretical nutrients loads for Pusiano catchment for inhabitants, animal husbandry (bovines,equines,swines,ovines,poultry) in unit g/capita/day, cultivated and uncultivated solis in unit $kg/km^2/yr$ are available in Excel spreedhead. The calculation will be done using typical calculation method and with aspect conserning GIS techniuques. The results has been also compared with previously nutrient loads estimations obtained with diffrent approaches.The theoretical nutrient loads calculated using classical method are available for 1971, 1981, 1991, 2002 year in Excel.

Point sources pollution

Unique features such as point sources must have input data provided for each individual feature included in the watershed simulation. In order to account for the loadings from a point source, SWAT allows users to add daily or average daily loading data for point sources to the main channel network. These loadings are then routed through the channel network along with the loadings generated by the land areas. For the case of point sources pollution in Pusiano Lake catchment, data will be obtained from the local municipal office ASIL Azienda Servizi Integrali Lambro s.p.a. Needed data are as follow: ArcViewGIS sewage treatment works - network map with location of CSO, industrial inputs from the factories, discharged in STW effluent.

7. CONCLUSION

A major portion of the study, until now, was spent towords assembling database.Data previously collected for this study by the UM was reviewed, flow and climatic data collated and the need for further data collection established. Once a base data set had been identified a number of investigations were made to determine the overall quality of the data. The initial investigations highlighted a number of problems with the available data. These included some of uncertainty in flow measurements at some gauging stations, problems with additional measurement points locations and persons to collect data, lack of BOD data.

Research is still under construction, however so far the collected data lay a good foundation for the development of a comprehensive hydrologic system analysis tool to study the water quantity and quality issues. Case study's complete purpose is to define water quality in the lake's immissary as resulting from the various "polluting" basin activities (both point sources and diffuse pollution). ArcView3.2GIS in which most of data were collected is a very important source of information and a very useful tool for planning and managing the watershed, producing a simple and clear visualization of watershed information. Additional data for modelling framework are written in database format (Microsoft Software). The above information will be formatted into SWAT (Soil and Water Assessment Tool) input files.

Figure 1.Watershed location.

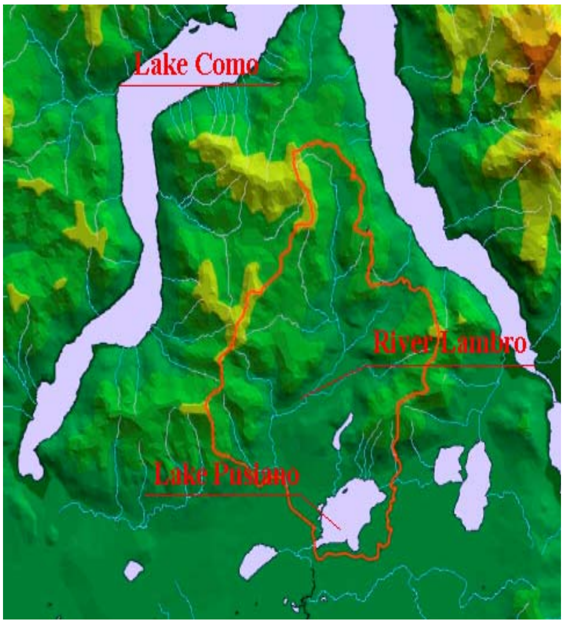


Figure 2. The DEM for Lake Pusiano basin.

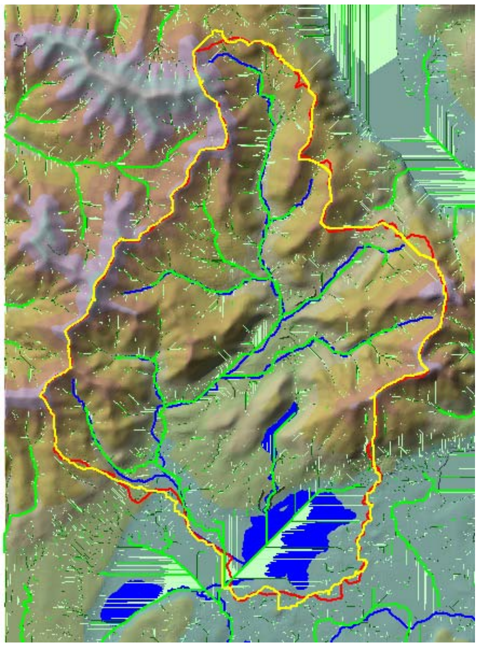


Figure 3. The Land Use map.

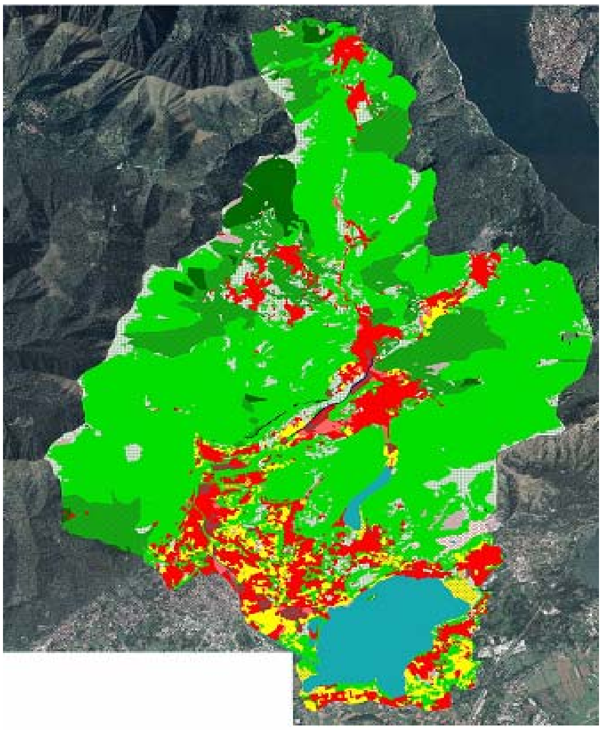


Figure 4. Permeability map.

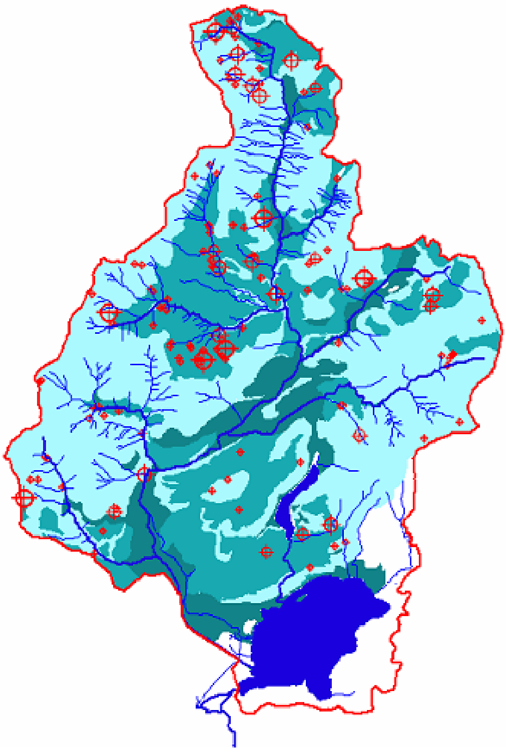


Figure 5. The Soil map.

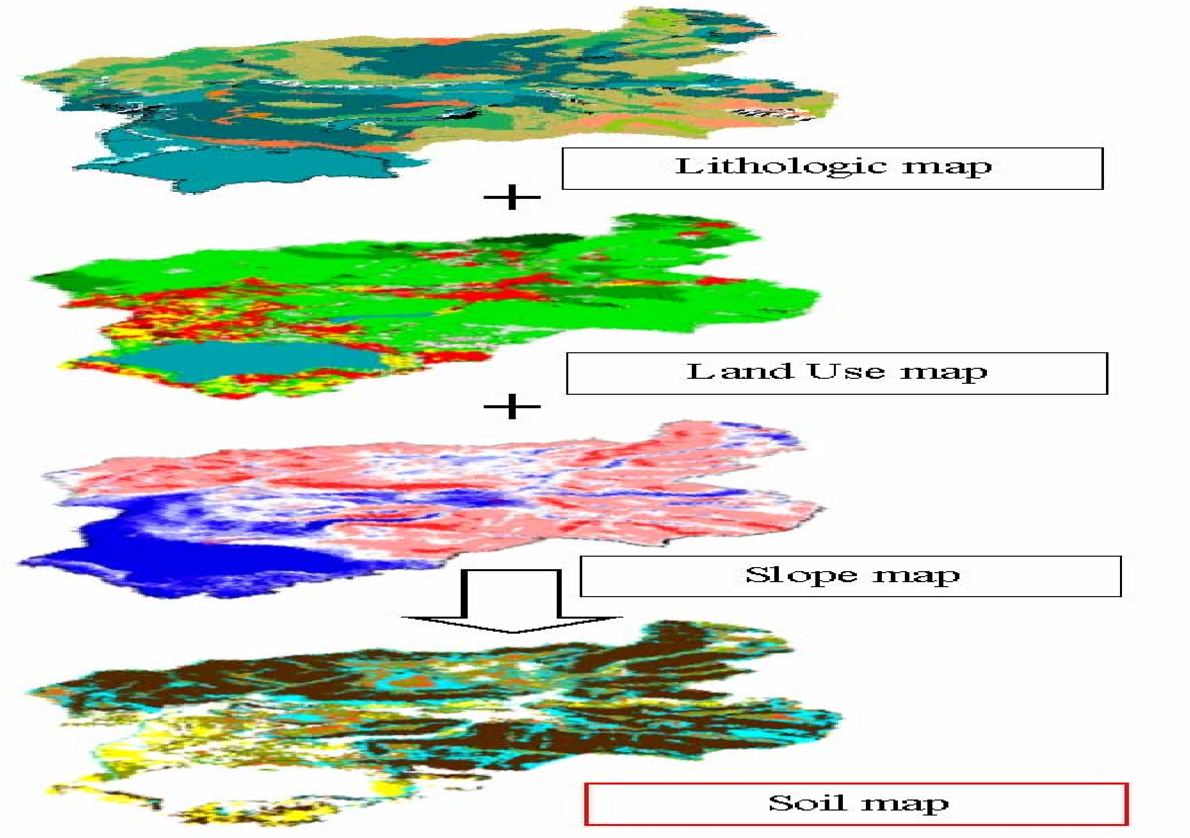
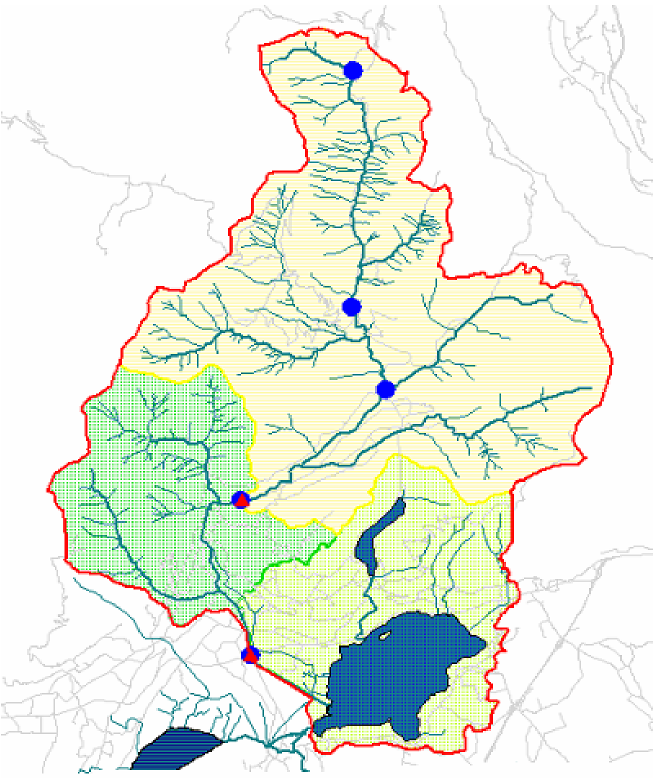


Figure 6. Location of quality measurement points.



ACKNOWLEDGMENTS

The CNR– IRSA (Water Research Institute of the Italian National Research Council, Brugherio, Italy) with help of provincial sources collected data sets within the Pusiano catchment for the purposes of the study. Geographic information layers – here special thanks to Franco Salerno. Measurment data for catchment are still developed, some of them was created by Elena Legnani; Elisa Vuillermoz; Sara Minelli. Partial funding for this project are also provided by: the Institute of Agricultural Hydraulics (Prof. C. Gandolfi), University of Milan, Italy; I thank also Ing. L. Buzzi, CNR– IRSA and D. Cadaro, Institute of Agricultural Hydraulics, University of Milan.

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Predictive Control of a Simple Waste Water Plant

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Abstract:
The aim of this paper is to control the substrate and the dissolved oxygen (DO) levels of a simple wastewater system, using model based predictive control (MBPC) methods. Simulation results and the description of work done is presented in this paper.

Keywords: Activated Sludge Process, Predictive Control

1. Introduction:

The model to be controlled is a simple activated sludge model. The activated sludge model (ASM) being used was the same as that used by Nejjari et al (1997), though the control methods used here were different. The methods of control design used here were those described in Maciejowski (2002), that is, model based predictive control of a nonlinear multivariable system. The advantage of using predictive control here is that it allows control of a multivariable system, without any complex tuning. Predictive control is usually a high level controller, that is the lower level is left to conventional controllers. PLC's (programmable logic controllers) provide the setpoints (and overrides etcetera), and, at a lower level, PI controllers do some simple control. Using a model based predictive controller on top of traditional control provides improved performance. In this paper, the model used is described in Section 2. The PI control of that model is in Section 3, as well as a brief introduction to predictive control. Simulation results are presented in Section 4. The paper ends by summarizing the conclusions and with some suggestions for future work.

2. Non Linear System Model:

The model consists of an aerator tank (in order to allow the aerobic process of pollutant removal to happen) and a settler (for settling and removal of biomass material, as well as recycling of some of the biomass). Here Q_R is the recycled flow, Q_W is the effluent flow, X_e is the concentration of the biomass leaving the settler.

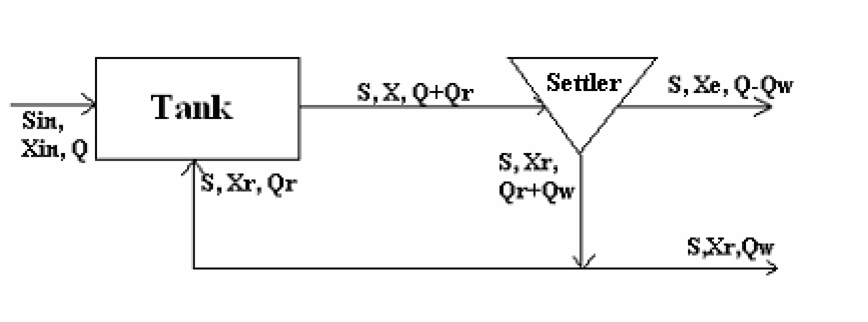

Figure 1 WWT Model

A four state model of the process is given by:

$$\begin{aligned}
\dot{X}(t) &= \mu(t)X(t) - D(t)(1+r)X(t) + rD(t)X_r(t) \\
\dot{S}(t) &= -\frac{\mu(t)}{Y}X(t) - D(t)(1+r)S(t) + D(t)S_{in} \\
\dot{C}(t) &= -\frac{K_0\mu(t)X(t)}{Y} - D(t)(1+r)C(t) + K_{LA}(C_s - C(t)) + D(t)C_{in} \\
\dot{X}_r(t) &= D(t)(1+r)X(t) - D(t)(\beta+r)X_r(t)
\end{aligned} \qquad (1)$$

The plant model used is a MIMO system, with 2 inputs:

- D(t) – Dilution Rate
- W – Air Flow Rate

and 4 outputs:

- S(t) – Substrate
- C(t) – Dissolved Oxygen
- X(t) – Biomass
- Xr(t) – Recycled Biomass
- Constant Parameters: r and B, ratio of recycled and waste flow, respectively, to influent flow rate. S_{in} and C_{in} are the substrate and DO values of the influent stream. u is the specific growth rate, Y is the yield of cell mass, and C_s and K_{LA} are the maximum DO and oxygen transfer rate coefficient, respectively.

3. Control:

The above model is linearised around the operating point and can be written in state space form as:

$$\begin{aligned}
x(k+1) &= Ax(k) + Bu(k) \\
y(k) &= Cx(k)
\end{aligned} \qquad (2)$$

The model is linearised around an operating point (given by the steady state values of the states, and the inputs, see Appendix 1), to give the linear matrices A, B, C and D, to represent the model in the form above. (See Appendix 1 for the values of the matrices). The operating points for the inputs were chosen so as to give steady state values for the outputs.

3.1 PI Controller and Plant:

The initial stage was to provide two PI control loops to control the DO and the substrate within the plant (see Figure 2, inner loop is PI). The biomass and recycled biomass were unmeasurable/uncontrollable parameters within the process. In Figure 2, R_1 and R_2 are the setpoints for substrate and DO respectively. The PI loop was tuned manually, without the presence of the predictive controller, to give a critically damped response.

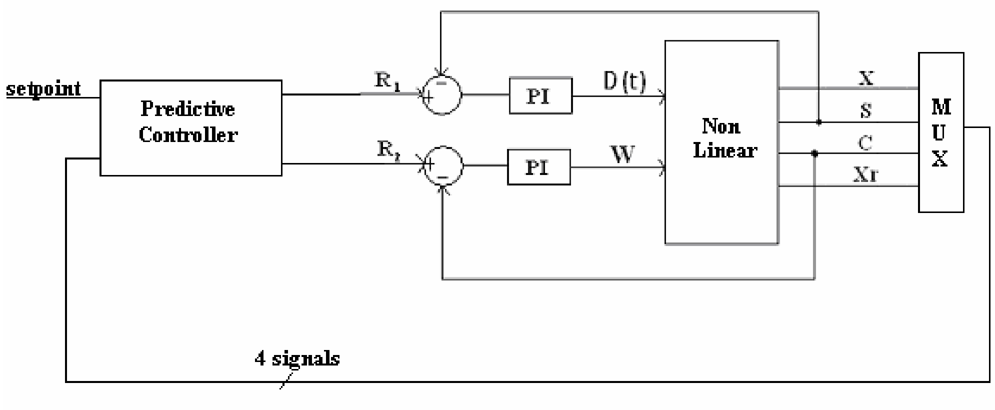

Figure 2. Controller

In preparation for the addition of the model based predictive control loop, the state space model (equation 2 above) was augmented with the states of the PI control system. For the new system, there are two extra states (as well as X, S, C and X_r):

- x_1 (the error signal for the substrate, S),
- x_2 (the error signal for the Dissolved Oxygen, C),

where $\dot{x}_1 = e_1 = r_1 - y_2$ and $\dot{x}_2 = e_2 = r_2 - y_3$, which is acted upon by the PI controller. Thus, the addition of these two extra states, and the changes to the A, B and C matrices (due to the integral and proportional action of the PI controller), gives a new state space system. The inputs of this system are also changed, from D(t) and W(t) to R_1 and R_2. Thus the new state space system is given by

$$\begin{aligned} x_A(k+1) &= A_A x_A(k) + B_A u_A(k) \\ y_A(k) &= C_A x_A(k) \end{aligned} \qquad (3)$$

which represents the augmented (closed-loop) PI system.

3.2 Predictive Control Theory:

The philosophy behind the predictive controller is that it predicts plant behaviour over a specific *prediction horizon* (H_p). The control input trajectory can be chosen on the basis of which trajectory would give the best *predicted* output for the system, for example in Figure 3. The output is required to go to a given setpoint, the dotted-line indicates the outputs trajectory in order to reach that setpoint. This output is predicted by using the system model, and the control input which is currently being applied to the plant, u_1. If the output trajectory is not the most suitable (as regards minimisation of input changes, etc), then it is changed by changing the control input to, say, u_2 and checking the predicted output for this input.

Therefore, the first element of the chosen trajectory is applied as a control input to the plant, and at each time step, the predictions output values are updated for the given prediction horizon, to allow for more accurate control. The prediction horizon always remains the same, but moves along once at each step of the control. This is called receding horizon control. At each step, the trajectory may change (according to the new predictions for the plant output).

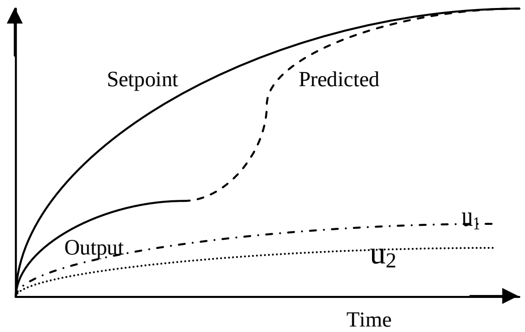

Figure 3. Trajectories

3.3 Predictive Controller Structure

<u>3.3.1. Prediction:</u>

Predictive control is a model based control method, that is, it uses the model provided (for example, the WWT system, with PI control loops) to predict future plant behaviour. Prediction for the above WWT model, can be described, over a prediction horizon of H_p and over a control horizon of H_U, by the following equation (ref Maciejowski, 2002):

$$Z(k) = \psi . x(k) + \mathrm{T} u(k-1) + \Theta \Delta U(k) \qquad (4)$$

where $Z(k)$ is the prediction of future outputs of the system. This is a function of the present states, *x(k)*, the previous control input, *u(k-1)*, and the change of control input, $\Delta U(k)$,

and $\psi = C_z * \begin{pmatrix} A \\ . \\ . \\ A^{H_P} \end{pmatrix}$ and $\mathrm{T} = C_z * \begin{pmatrix} B \\ . \\ . \\ \sum_{i=0}^{H_p - 1} A^i B \end{pmatrix}$ and

$$\Theta = C_z * \begin{pmatrix} B & . & . & 0 \\ . & . & & \\ . & & . & \\ \sum_{i=0}^{H_p-1} A^i B & & & \sum_{i=0}^{H_p-H_u} A^i B \end{pmatrix}.$$

3.3.2. Control:

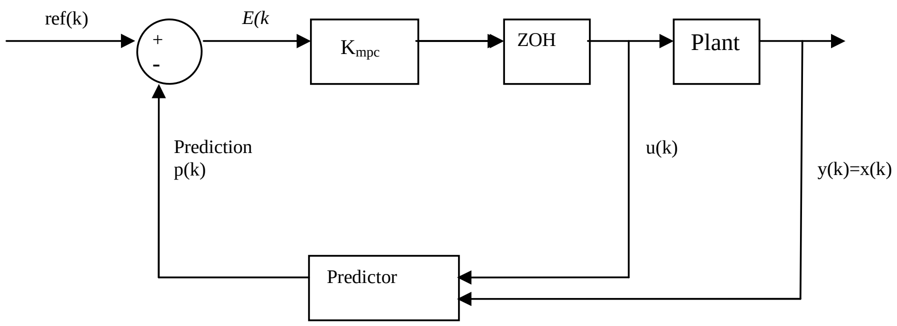

Figure 4 Predictive Controller

The predictive control in this paper aims to provide a constant fixed gain controller, K_{mpc}, as in Figure 4. This is calculated by employing a least-squares minimization in the form of a cost function. The cost function relates to the error $\mathrm{E}(k)$ and the change in control signal, $\Delta u(k)$. The error signal is defined to be the difference between the reference signal and the prediction of the steady state output:

$E(k) = ref(k) - p(k)$

where $p(k) = \psi.x(k) + \mathrm{T}u(k-1)$ and where "ref" is the reference signal.

so that:

$E(k) = ref(k) - \psi.x(k) - \mathrm{T}u(k-1)$

That is, $\Delta U(k)$ (in Eqn.4) is assumed to be zero to calculate the error signal. So, to include the $\Delta U(k)$ changes in the controller, the optimal $\Delta U(k)$ changes are calculated, using a cost function of the form:

$$V = \left\|\Theta \Delta U(k) - \mathrm{E}(k)\right\|^2_Q + \left\|\Delta U(k)\right\|^2_R$$

Q and R are defined to be weighting matrices, for penalizing error on the output and changes in the input, respectively. The aim is to for the output to reach the setpoint, whilst minimising the amount of control action taken by the inputs, and minimising the error on the outputs

It can be shown (ref. Maciejowski, 2002) that the controller gain, which gives the optimal $\Delta U(k)$ changes is:

$$K_{mpc} = [I_l, 0_l, ..., 0_l] H^{-1} \Theta^T Q,$$

where $H = [\Theta^T Q \Theta + R]$.

Thus, the above equations lead to the following structure for the full controller:

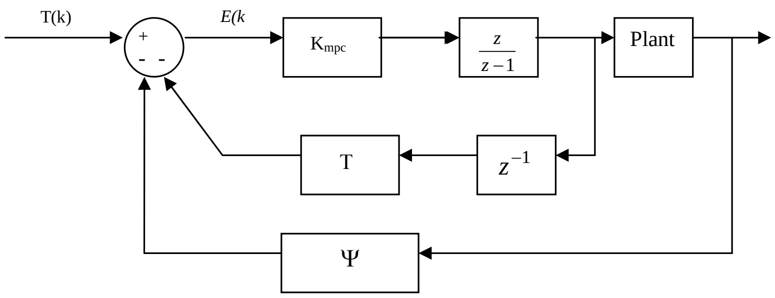

Figure 5 Full Predictive Controller Structure

Where T and ψ are used for the prediction of plant outputs, and K_{mpc} is used for the control of the plant. The plant, for example, here is the WWT plant and the PI control around it.

4. Simulation

The model was simulated in Matlab/Simulink, using m-files as well as Simulink blocks. A toolbox for predictive control by Sanchez (2002) was used.
Comments on the implementation:
1. The setpoint inputs, and the values from the output that they are compared to, are not the full values, but the deviation from steady state. This is because the model used in the predictive controller is the linearised one, i.e. the model with its offset removed, merely a description of the system about a given operating point. The value then, which is inputted to the actual model, has a steady state value added to it, in order to be correct.
2. The simulation is run for a simulation algorithm of ODE23s (stiff/Mod.Rosenbrock)
3. Any continuous to discrete conversion is done using the Tustin Method, continuous to discrete conversion is done before the matrices can be used to find the above controller matrices.
4. The sample time for the system is 1 hour.

4.1. Testing the Controller:

4.1.1 Step Responses

Comparing the responses for the step inputs at time 200 of 5mg/l for substrate, and 1mg/l for Dissolved Oxygen) of the PI controller (just one loop) and the Predictive Controller (with PI sub-loop):

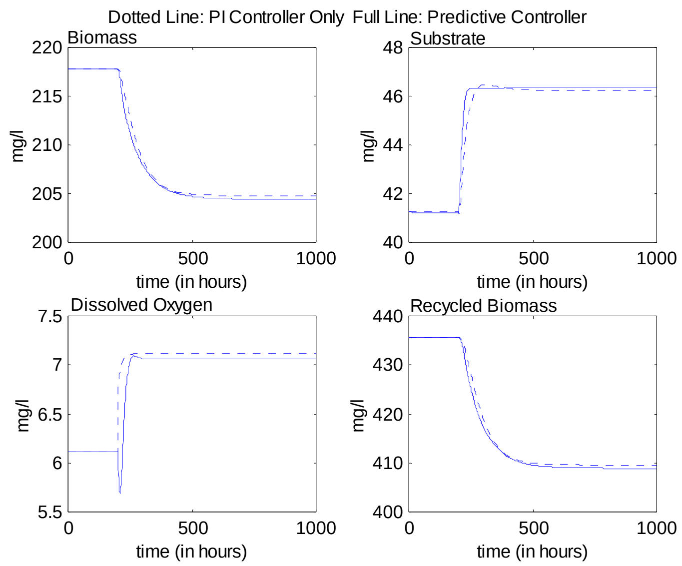

Figure 6 Step Responses

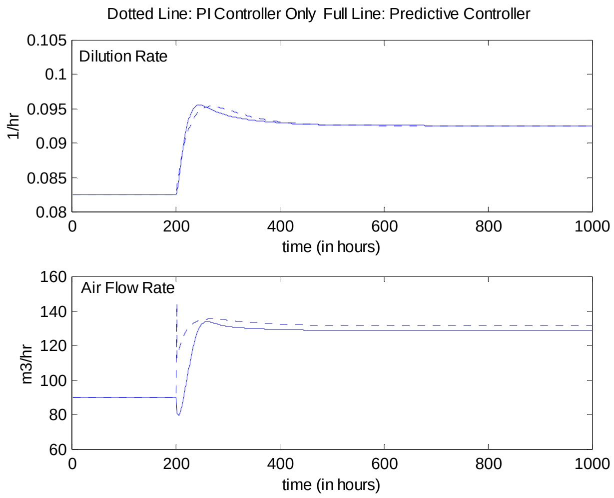

Figure 7 Responses of Control Inputs: Dilution Rate and Airflow Rate

The predictive controller seems to be slightly faster (for biomass, substrate and recycled biomass) at responding to the step change, and does not have the initial PI transient that the PI controller has. However for the Dissolved Oxygen, there is a steady state error, and the predictive control response is slower than that of the PI control. Also, examining the control inputs, there is a transient spike in the PI control input for the airflow rate. At the same instant, there is a dip in the same predictive control input, but not of as large a magnitude.

4.1.2 Disturbance Rejection

There is a steady state error present for the predictive controller, due to plant-model mismatch. Also, it can be found that the above controller would not reject disturbance. This could be solved by including a state estimator in the system. This means the state vector must be augmented to include the disturbance model and so the state estimator takes the form:

$$\begin{bmatrix} x_{old}(k+1) \\ d(k+1) \end{bmatrix} = (A - LC)\begin{bmatrix} x_{old} \\ d \end{bmatrix} + Bu(k) + Ly(k) \qquad (5)$$

The output of the estimator is the estimate of the states, and the estimate of their disturbances. If the estimator is stable (if the A-LC are placed so as not to make the estimator unstable), then the estimation error approaches zero, the rate of approach determined by the A-LC pole. The previous steady state error due to plant model mismatch is removed by the estimator:

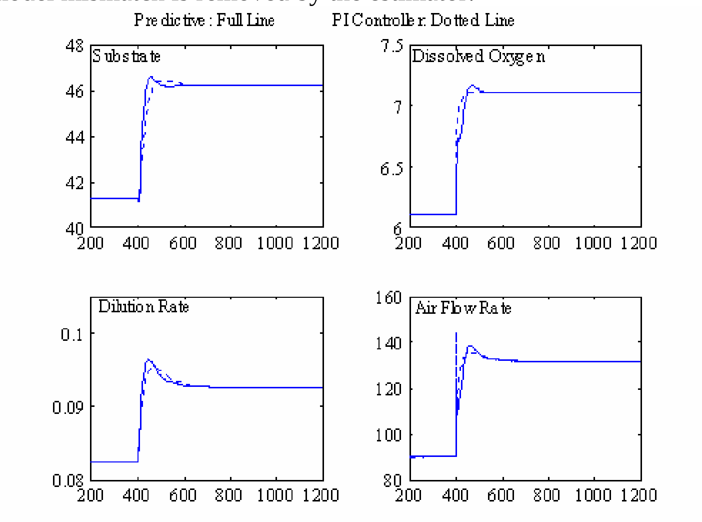

Figure 8 Responses for Steps on Substrate and DO

5. Conclusion:

Predictive control was implemented on the chosen WWT model (with a PI control loop). It can be seen that without the disturbance rejection, the predictive controller does not overshoot the setpoint. This is due to the fact that the controller follows a trajectory to reach the required value, the trajectory is chosen as to suit the predicted response of the system. For the PI controller, the controller is acting only on the actual outputs of the system (rather than the predicted ones), and so cannot respond to future possible errors (hence the overshoot). The addition of disturbance rejection does add overshoot in the case of the predictive controller, but this can be decreased by estimator tuning. The main advantage of predictive control is that it allows the use of constraints in the controller design, however here there were no constraints to be implemented.

Future work planned is as follows:

- Implement constraints with this system
- Implement Predictive Control using the ASM2d model
- Familiarise oneself with river and sewer network models, with view to using Predictive Control with these models.

Acknowledgements:

Marie O' Brien acknowledges the financial support provided through the European Community's Human Potential Programme under contract HPRN-CT-2001-00200 [WWT & SYSENG].

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Sanchez, A., 2002, Matlab/Simulink MPC Toolbox, http://www.smac.dk

APPENDIX 1
$D_{steady\ state}$=0.0825
$W_{steady\ state}$ =90
$X_{steady\ state}$=217.2896
$S_{steady\ state}$=51.2348
$X_{steady\ state}$=6.1146
$Xr_{steady\ state}$=435.5791

$$A = \begin{bmatrix} -0.0990 & 0.1234 & 0.2897 & 0.0495 \\ -0.0508 & -0.3219 & -0.4457 & 0 \\ -0.0254 & -0.0949 & -1.9748 & 0 \\ 0.132 & 0 & 0 & -0.0660 \end{bmatrix}$$

$$B = \begin{bmatrix} -87.1159 & 0 \\ 134.0243 & 0 \\ -9.2834 & 0.0699 \\ 0.0001 & 0 \end{bmatrix} \quad C = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad D = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

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 modelling; Empirical modelling; Modelling activated sludge plants

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* the subsystems use 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 coming out 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 simplification and 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. These states are used only to close the mass balances and can be omitted. 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 introduce a compression term 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 will be based on an ASM3 model, which is considered to be the state-of-the-art model in the field. Biological phosphorus removal will not be included, because no data are available for calibration (there are just a few treatment plants in Italy with biological P removal) and 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 will have two separated tanks for nitrification and denitrification. These tanks will be coupled with the clarifier. For the secondary clarifier a compressive gravity thickening model will be used. This model is similar to the other 1-D settling models, but includes compression effects. Thus the sludge blanket's level can be better predicted. This is very useful in optimisation studies, where the hydraulic overload/underload margin has to be estimated with a high accuracy. The increase in complexity caused by the extra compression gradient term is not significant (Vaccari and Uchrin, 1989).

Modelling work will be 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 will be collected from 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.

Botond Raduly acknowledges the financial support provided through the European Community's Human Potential Programme under contract HPRN-CT-2001-00200[WWT & SYSENG].

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Integrated modelling of the urban wastewater systems into a river context

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Abstract
The control and optimisation of an integrated urban wastewater system (UWWS) can be carried out based on a full understanding of the entire urban wastewater system consisting of sewer, wastewater treatment plant and receiving water subsystems. This paper presents the initial steps made into the process of further development of SYNOPSIS, a simulation tool for urban wastewater system. Currently, the implementation of the denitrification process into the wastewater treatment plant model, together with optimisation of the secondary clarifier model, is under development. The attempted improvement of the wastewater treatment plant model will produce more reliable simulation results describing the nutrients in the entire urban wastewater system and receiving waters. This will allow for new possibilities in the evaluation of novel control strategies, which can be applied to the integrated system on the basis of short-term events (related to oxygen depletion) and long-term (chronic) impacts of nutrients in the receiving waters.

Keywords
Integrated urban wastewater systems; modelling; SYNOPSIS; wastewater treatment

INTRODUCTION
Mathematical modelling of urban systems, such as sewer systems and treatment plants on one side, and receiving waters (rivers, lakes) on the other side, has led to a better understanding of the bio-chemical and physical processes occurring during the transport of waste (pollutants) dispersed in water, from the source into the environment. Since the 60's, when the first mathematical models in urban wastewater disposal were created, an impressive array of different models, varying in complexity, has been developed and employed in research, consultancy, and real cases (Bertrand-Krajewski, 2002). Research started by being focused on specific problems, such as the transport and transformation of wastewater in a sewerage system along with the impact of stormwater on this system, the transport and transformation of pollutants, in steps, through a wastewater treatment plant, or, alternatively, on the river water flow, water quality in a river, and river catchment area. Although these distinct areas in wastewater modelling continue to be challenging and demanding for researchers, more recent tendencies in modelling of wastewater systems led towards integrated approaches of the urban wastewater systems, which open new opportunities for integrated control and management (Rauch *et al.*, 2002).

The aim of the current research presented herein is the development of an integrated model of urban wastewater systems, starting from an existing model called SYNOPSIS. The first stage of the project deals with the improvement of the nitrogen model within the integrated model to insure a better analysis of the receiving water quality (DO depletion, nitrogen compounds, eutrophication). Next, the wastewater treatment plant model will be enhanced through the implementation of the denitrification process model together with several changes of the secondary clarifier model. These changes involve inclusion of a version of Takács model (Takács *et al.*, 1991) into the secondary clarifier model, in order to simplify and optimise the structure of the original wastewater treatment plant model. The implementation of the newer model within the original version of SYNOPSIS is challenging.

MODELLING APPROACH

SYNOPSIS (software package for SYNchronous Optimisation and SImulation of the urban wastewater System) is an integrated simulation and optimisation tool for urban wastewater systems. It has been developed at Imperial College in London by Manfred Schütze, David Butler and Bruce Beck in the 90's (Schütze, 1998; Schütze *et al.*, 2002). The constituent models of SYNOPSIS are modified versions of: KOSIM (sewer model), Lessard and Beck's model for wastewater treatment processes (put in the correct reference here) and a river model developed by Lijklema (1996), implemented in the DUFLOW program. The set of variables employed by the wastewater treatment plant model are also used within the sewer system model, whereas the river model operates with a slightly different set of variables, see Table 1.

Table 1 State variables in SYNOPSIS

Sewerage system and wastewater treatment plant variables	**River variables**
Flow	Flow
Suspended solids (SS)	Ammonium (NH_4)
Volatile suspended solids (VSS)	Readily degradable fraction of BOD (BOD_R)
Total COD (COD_t)	Slowly degradable fraction of BOD (BOD_S)
Soluble COD (COD_S)	Oxygen demand (DO)
Ammonium (NH_4)	
Nitrate (NO_3)	

The purpose of the simulation tool is to represent the impact of control actions and strategies on the performance of an urban wastewater system. A dynamic, deterministic modelling approach was chosen. One of the main objectives of the original work was to analyse the potential of integrated control (Schütze *et al.*, 2002). The software tool has two simulation modes available: stand-alone simulation and simulation-optimisation.

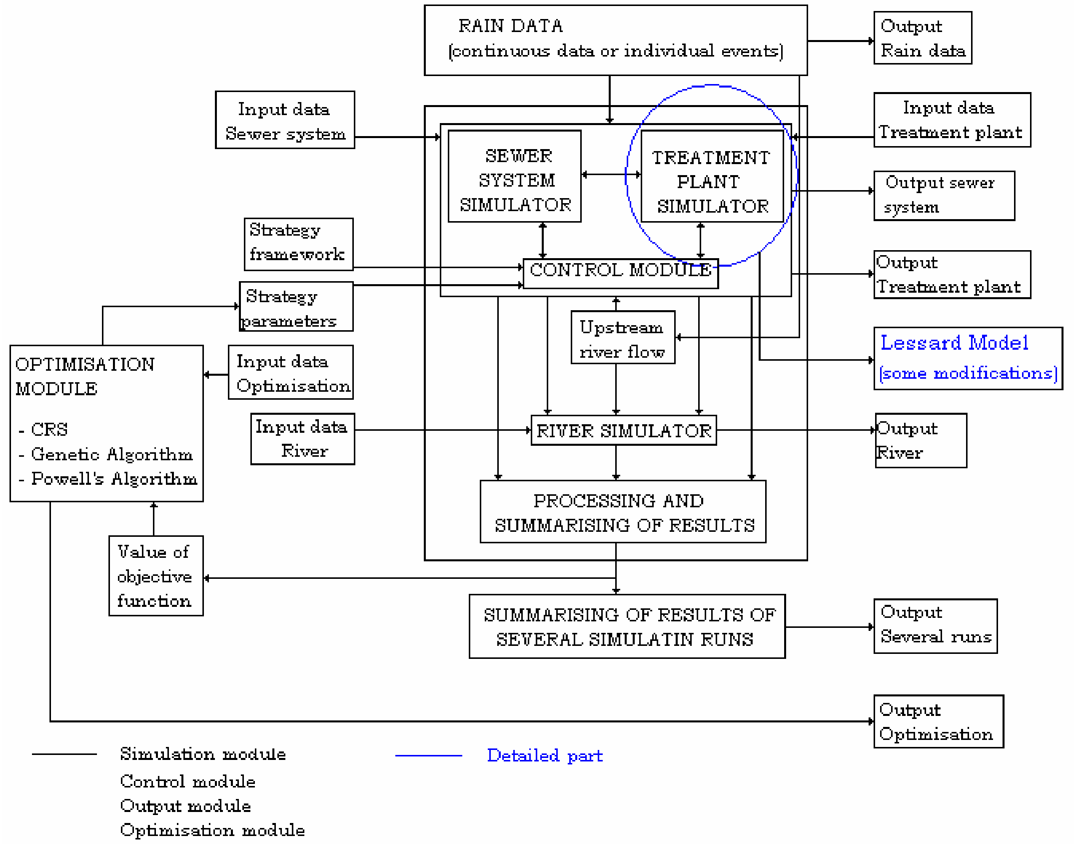

Figure 1 Overview of SYNOPSIS (from Schütze (1998))

In SYNOPSIS, the wastewater treatment plant model is already integrated within the sewerage model, forming a quasi-parallel model that is controlled by the control module as represented in Figure 1. The original model of the wastewater treatment plant has a modular structure, consisting of 9 separate modules: plant influent characteristics, regulating devices, storm tank, mixing of plant influent with side-streams, primary clarifier, regulating device, activated sludge process, plant effluent characteristics, and sludge treatment processes (Lessard, 1989). However, the sludge treatment module was not developed and implemented. During the integration process into SYNOPSIS, the original model also changed in several ways (Vazquez-Sanchez, 1996; Schütze, 1998).

The activated sludge module is structured into three different sub-modules: aeration basin, secondary settler - thickening, and secondary settler – clarification, as represented in Figure 2.

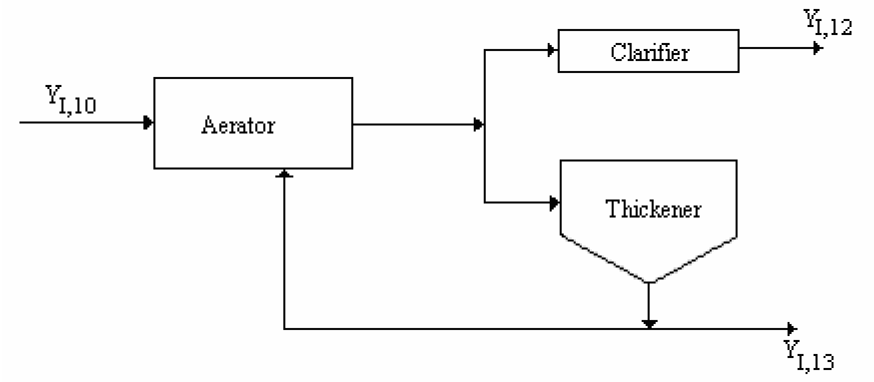

Figure 2 Overview of the existing activated sludge module

The activated sludge process in the aeration basin is based on a simplified version of the activated sludge model no. 1 (ASM1) (Henze *et al.,* 2000) consisting of five processes and described by 11 state variables as shown in Figure 3. Lack of reliable data for model validation has led to the exclusion of processes involving organic nitrogen. Furthermore, the anoxic growth process of heterotrophs was not taken into consideration.

The original secondary settler model was structured in three parts: clarification, thickening, and compression. The clarification part was further subdivided into a clarification zone and a dead zone. In SYNOPSIS, the dead zone was considered inappropriate/ irrelevant and was therefore excluded from the model. Calculation of the concentration of suspended solids is based on the empirical relationship described in Pflanz (1969), whereas the thickening model is based on the solids flux theory presented by Dick and Young (1972) and Lessard and Beck (1993).

Component → i / j Process		1 S_I	2 S_S	3 X_I	4 X_S	5 $X_{B,H}$	6 $X_{B,A}$	7 X_P	8 S_O	9 S_{NO}	10 S_{NH}	Process Rate, ρ_j [ML^{-3}T^{-1}]
1.	**Aerobic growth of heterotrophs**		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$			$\mu_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_{O,H}+S_O}\right)X_{B,H}$
2.	**Aerobic growth of autotrophs**						1		4.57	$\frac{1}{Y_A}$	$-\frac{1}{Y_A}$	$\mu_A\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A}$
3.	**'Decay' of heterotrophs**				$1-f_P$	-1		f_P				$b_H X_{B,H}$
4.	**'Decay' of autotrophs**				$1-f_P$		-1	f_P				$b_A X_{B,A}$
5.	**'Hydrolysis' of entrapped organics**		1		-1							$k_b \frac{X_S/X_{B,H}}{K_X+\left(X_S/X_{B,H}\right)}\left(\frac{S_O}{K_{O,H}+S_O}\right)$
Observed Conversion Rates [ML^{-3}T^{-1}]		$r_i=\sum_j v_i\rho_j$										

Stoichiometric Parameters: Heterotrophic yield: Y_H Autotrophic yield: Y_A Fraction of biomass yielding particulate products: f_P Mass N/Mass COD in biomass: i_{XB} Mass N/Mass COD in products from biomass: i_{XP}	Soluble inert organic matter [M(COD)L^{-3}]	Readily biodegradable substrate [M(COD)L^{-3}]	Particulate inert organic matter [M(COD)L^{-3}]	Slowly biodegradable substrate [M(COD)L^{-3}]	Active heterotrophic biomass [M(COD)L^{-3}]	Active autotrophic biomass [M(COD)L^{-3}]	Particulate products arising from biomas [M(COD)L^{-3}]	Oxygen (negative COD) [M(COD)L^{-3}]	Nitrate and nitrite nitrogen [M(COD)L^{-3}]	NH_4+NH_3 nitrogen [M(COD)L^{-3}]	Kinetic Parameters: Heterotrophic growth and decay: $\hat{\mu}_H, K_S, K_{O,H}, K_{NO}, b_H$ Autrophic growth and decay: $\hat{\mu}_A, K_{NH}, K_{O,A}, b_A$ Correction factor for anoxic growth of heterotrophs: η_g Ammonification ; k_S Hydrolysis: k_h, K_X Correction factor for anoxic hydrolysis: η_h

Figure 3 Process rate equations used in the activated sludge module

DISCUSSION AND FURTHER WORK

Initially, the development of SYNOPSIS is focused on the implementation of the denitrification model into the wastewater treatment plant model to enhance the nitrogen transformations and transport processes model, along with the optimisation of the secondary clarifier model. As the original activated sludge model was derived from the ASM1, the denitrification model will also be derived from the same model, to avoid potential incompatibilities or other differences that can produce alterations of variables, parameters etc. Several simplifications of the original equation system for the denitrification model are being considered, following the same principles as employed by Lessard. In the original model, the soluble biodegradable organic nitrogen, particulate biodegradable organic nitrogen and alkalinity have not been modelled due to lack of reliable data. At the same time, several parameters were omitted or modified, such as the mass of nitrogen per mass of COD in biomass i_{XB} (darkly shaded cell in Figure 4). The equations for the denitrification model that will be included into the wastewater treatment plant model are presented in Figure 4 in a tabular format. The parameters and variables have been described in Figure 3.

Component → i / j	Process	1 S_I	2 S_S	3 X_I	4 X_S	5 $X_{B,H}$	6 $X_{B,A}$	7 X_P	8 S_O	9 S_{NO}	10 S_{NH}	Process Rate, ρ_j [ML^{-3}T^{-1}]
1.	**Anoxic growth of heterotrophs**		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{No}}\right)\eta_g X_{B,H}$
2.	**'Decay' of heterotrophs**				$1-f_P$	-1		f_P				$b_H X_{B,H}$
3.	**'Hydrolysis' of entrapped organics**		1		-1							$k_b\frac{X_S/X_{B,H}}{K_X+\left(X_S/X_{B,H}\right)}\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{No}}{K_{NO}+S_{NO}}\right)\eta_g X_{B,H}$
Observed Conversion Rates [ML^{-3}T^{-1}]		$r_i=\sum_j \nu_i \rho_j$										

Figure 4 The separate denitrification equations of ASM1 (Henze *et al.*, 2002)

The scheme for the modified activated sludge module is presented in Figure 5, and the denitrification model (dotted lines) will be included as a separate sub-module, giving the possibility to simulate different activated sludge configurations, such as pre-denitrification and post-denitrification systems. This modification changes the mass-balance equations of the sub-modules.

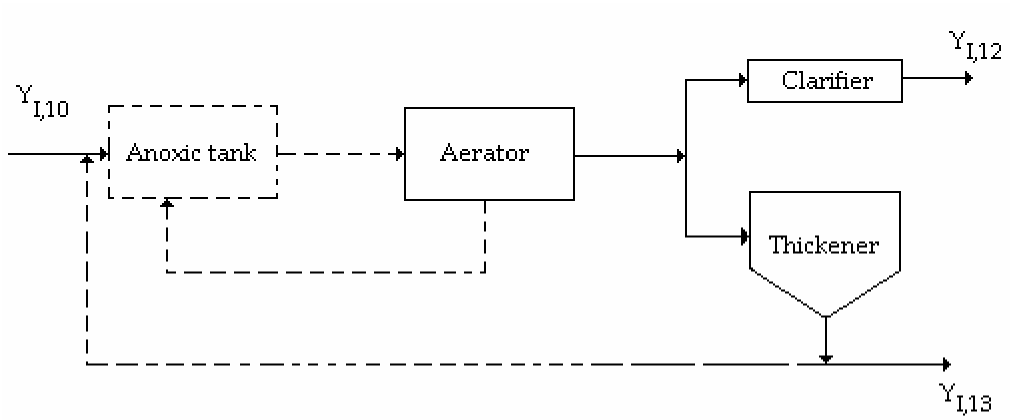

Figure 5 Denitrification module

Subsequently, the implementation of Takács model ('generalised Vesilind model') for the settler module represents another objective of this research, meant to improve the activated sludge module. The one-dimensional dynamic model of the clarification/thickening process is based on the solids flux concept and on a mass balance for each layer of the settler (Takács *et al.,* 1991). The general set of equations underlying this theory is shown below:

$$\frac{\partial X}{\partial t} = -\frac{\partial F_l}{\partial z} \quad (1)$$

$$X(z = H, t) = X_R(t) \quad (2)$$

where: X [g/m^3] is the suspended solids concentration, X_R [g/m^3] is the suspended solids concentration at the bottom of the settles, F_l is the biomass solid flux [kg /m^{2}h] at depth z [m] of the settler ($z \in [0, H]$, where 0 and H correspond to the top and bottom of the settler) .

$$F_l(z,t) = vX + uX \quad (3)$$

$$\begin{cases} u = \dfrac{Q_R + Q_w}{A_{se}} & \text{when } z \in \{z_f, H\} \\ u = \dfrac{Q_i}{A_{se}} & \text{when } z \in \{0, z_f\} \end{cases} \quad (4)$$

The total flux is expressed using the equation 3, where the v represents settling velocity, and u the bulk velocity. In addition, the bulk velocity u, where Q_R+Q_W is the flow rate, A_{se} is the section of the settler, Q_i is the influent flow; z_f is the high of the feed layer. The generalized equations for the settling velocity established by Takács are presented as follow:

$$v = \begin{cases} = v' & if \quad v' \leq v_{max} \\ = v_{max} & if \quad v' > v_{max} \end{cases} \quad (5)$$

$$v' = v_0 (e^{-r_h(X - X_{min})} - e^{-r_p(X - X_{min})})$$
$$X_{min} > 0, r_p > r_h > 0 \quad (6)$$

where v_{max} [m/d] is the maximum theoretical settling velocity, X_{min} [g/m^3], is the minimum attainable suspended solids concentration r_p [m^3/g] is settling parameter associated with the low concentration and slowly settling component of the suspension, r_h [m^3/g] is settling parameter associated with the hindered settling component of settling velocity equation. The maximum of practical settling velocity v' [m/d] is attained for a value X expressed by equation 7.

$$X = X_{\min} + \frac{1}{r_p - r_h} \ln\left(\frac{r_p}{r_h}\right) \tag{7}$$

Although one-dimensional layer models for the settler do not accurately describe the real physical phenomenon, they turn out to be successful in numerical simulation applications (Dochain and Vanrolleghem, 2001). However, this in itself does not provide an ample reason for the inclusion of a version of such layer models within the wastewater treatment plant model of SYNOPSIS.

The original model for the secondary settler by Lessard has undergone several changes while it was included in SYNOPSIS. These additions solved particular problems, but complicated the computational straightforwardness of the sub-module. The proposed modifications, represented in Figure 6, theoretically reassure us that the results will be considerably improved.

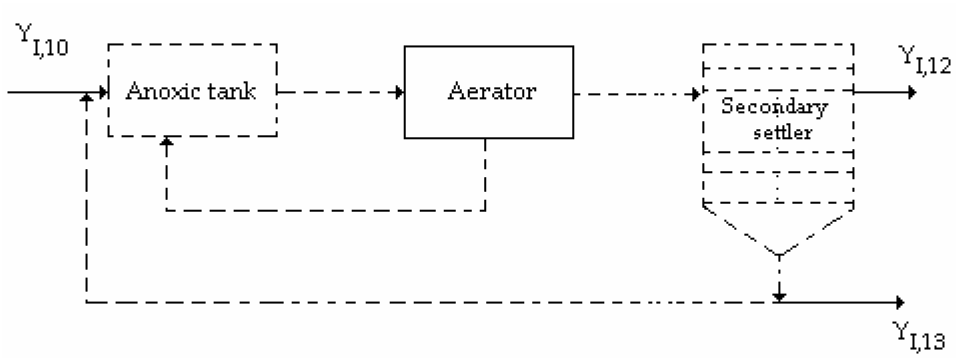

Figure 6 Further modifications of the activated sludge module

The exact equations to be used in the settler model are not yet definitive, as many new empirical or more complex models have been developed lately, and have to be thoroughly analysed prior to choosing which approach is the most appropriate for this research (e.g Giokas *et al.,* 2002). Therefore, the analysis of how the wastewater treatment plant model should be extended is still on-going.

In later stages of the research, work will be carried out on river modelling and on integration of the different models.

CONCLUSIONS

The on-going research, briefly overviewed in this paper, belongs to a larger research project, conceived to develop an integrated model of the urban wastewater system in a river context. A reasonably accurate nitrogen biochemical transformation model is important for better evaluation of river water quality and for developing optimal integrated control strategies of the urban wastewater system as a whole. Therefore, updating and extending the representation of nitrogen within SYNOPSIS has been considered an important objective and has been the main subject of the current presentation. This work will conclude with the implementation of the denitrification module into the activated sludge model and the modifications of the secondary settler model.

ACKNOWLEDGEMENTS
The researchers would like to acknowledge the financial support provided through the European Community's Human Potential Programme under contract HPRN-CT-2001-00200 [WWT&SYSENG].

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Sewer Networks: Water Flow and Quality Modelling

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Abstract

This paper briefly describes the modelling approach for sewer network flow in an integrated way (taking into account both the flow of the water and the level of the pollutants). The modelling approach in this paper addresses only the processes which take place in the main sewer network; any processes occurring upstream of specific inflow locations into the sewer network, as for example rain intensity and dynamics, rainfall-runoff issues etc., are beyond the scope of our presentation. Sewer network modelling, related to both quantity and quality of the wastewater, is useful for developing a control strategy of the flow in sewer networks, the prediction of the overflows, and the prediction of the mass transport of sediments at different locations in the sewer system.

Keywords: pollutants, sediment transport, sewer network, water flow modelling;

Introduction

The mathematical modelling of water flow in sewer networks may address either the quantity (flow) of the water through the sewer network, or taking both the quantity (flow) and the quality (the pollution level) of the water. The presented models cover all related physical phenomena, from specific inflow locations into the sewer network down to the overflow locations and treatment plant entrances.

Water quantity modelling reflects all the processes that take place in the different elements of the sewer network (e.g. storage in the reservoir storages or in the sewer, transportation in the sewers) by use of known laws of hydraulics. Water quality modelling addresses the dynamic space-time distribution of the amount and the level of concentration of pollutants within the sewer network and at its sinks (overflows, treatment plant entrance) as well as the sediment transport. It should be noted that water quality aspects include the level of the pollutants in the sewer network, the sediment transport, as well as the physical, chemical and biological processes that are taking place in the same time.

We recall that a mathematical model comprises a set of equations and other logical relationships that describe, with more or less accuracy, the relevant behaviour of the physical process; a mathematical model (fed with proper input data) may be used to calculate the time-space evolution of the processes behaviour, in our case of the sewer network flow.

Modelling of the sewer network flow (quantity)

A set of elements are used to build a combined sewer network model. In these elements, different processes take place, as for example, the water storage in the reservoirs or in the sewers, the merging of flows in the network nodes, etc.

In the following, the most typical elements of a sewer network are described along with the equations which are used for modelling them (Marinaki 2002).

1.1. Link elements

There are two types of link models, namely hydrodynamic link elements and hydrological links elements.

The hydrodynamic link element is used where a non-negligible storage of volume is caused in a sewer stretch by backwater or by flow regulation using throttle gates. For example, a hydrodynamic approach is usually used to model relatively flat sewers where the backwater phenomena may be prevailing. The mathematical model applied for this element consists of the Saint-Venant equations, namely the continuity equation and the momentum equation, which describe quite accurately the dynamic behaviour of the flow along a sewer stretch. The flow is considered as one-dimensional current, hence the dependent variables are the flow *q*, the velocity of flow *υ*, and the flow depth *h*, while the independent variables are the distance *x* and the time *t*. The first equation reflects the conservation of mass in the flowing liquid while the second equation, the momentum equation, expresses the resistance to flow.

The following continuity equation, expressing the conservation of mass in the flowing liquid, corresponds to the first Saint-Venant equation:

$$\frac{\partial F(h)}{\partial h}\frac{\partial h}{\partial t}+\frac{\partial q}{\partial x}=0$$

where:

q(x,t):	flow (m^3/s) at location x (m) along the sewer axis at time t (s);
h(x,t):	depth of sewer flow (m) at location x (m) along the sewer axis at time t (s);
F(h):	cross sectional area of flow (m^2);

The following momentum equation represents the second Saint-Venant equation:

$$\frac{1}{g}\frac{\partial \upsilon}{\partial t}+\frac{\upsilon}{g}\frac{\partial \upsilon}{\partial x}+\frac{\partial h}{\partial x}=I_s-I_R$$

where:

I_S:	sewer slope;
I_R:	the friction slope or the slope of the line of energy of flow;
g:	gravitational acceleration;
$\frac{\partial h}{\partial x}$:	slope of the water surface;

I_R is calculated empirically from the equation (Manning's formula):

$$I_R=cq^2R(h)^{-\frac{4}{3}}F(h)^{-2}$$

where c is a constant ($s^2/m^{2/3}$) that depends on the sewer's characteristics and is equal to $\left(\frac{n}{1.486}\right)^2$, where n is Manning's roughness coefficient, and R(h) is the hydraulic radius (m), and is equal to $R(h) = \frac{F(h)}{P(h)}$, where P(h) is the wetted perimeter (m).

The hydrological links are used to model the link elements if the sewers have relatively steep slope and the spillback is less significant. The hydrological links are not strongly based on physical laws and included are simpler than the hydrodynamic links; hence the calibration of parameters is very important.

An example of hydrological link modelling are the time-lag links, whereby the following dynamic equation is used to calculate the outflow:

$$q(k+1) = \left(1 - \frac{T}{\tau}\right)q(k) + \left(\frac{T}{\tau}\right)q_u(k)$$

where:

- q: outflow from the time-lag link;
- τ: time constant of the linear first-order system that may be estimated experimentally;
- T : discrete time interval;
- k: discrete time index;
- q_u: the sum of inflows to the time-lag link. Thus, if m is the total number of inflows into the sewer stretch, we have:

$$q_u(k) = \sum_{j=1}^{m} q_{u,j}\left(k - \kappa_j\right)$$

where κ_j is the time delay of inflow j.

1.2. Reservoirs

For modelling the reservoirs, the following continuity equation is used:

$$\frac{dV}{dt} = u_{in}(t) - u(t) - q_{over}(t)$$

where:

- V(t): currently stored volume in the reservoir (m^3);
- $u_{in}(t)$: inflow to the reservoir (m^3/s);
- u(t): outflow from the reservoir (m^3/s);
- $q_{over}(t)$: overflow from the reservoir (m^3/s);

A reservoir can have an overflow capability if an overflow weir is present and the water height rises over the height of the weir. Under the assumption that there is no spillback downstream of the weir, the overflow q_{over} is calculated by using an equation which is a combination between the Poleni formula and the Toricelli formula.

$$q_{over} = \begin{cases} 0, & if\ h_z - h_w \le 0 \\ \frac{2}{3}\mu_p \sqrt{2g}(h_z - h_w)^{\frac{3}{2}} l_W\ (Poleni\ formula), & if\ h_z - h_w \le h_w - 0.005 > 0 \\ \mu_T \sqrt{2g}\left(h_z - h_w - \frac{h_{sl}}{2}\right)^{\frac{1}{2}} A\ (Toricelli\ formula), & else \end{cases}$$

where:

- h_w: height of the weir (m);
- h_{sl}: height of the slot over the top of the weir (m);
- l_W: length of the weir (m);
- μ_p: overflow coefficient (Poleni formula);
- μ_T: coefficient for the flow under pressure from the slot (Toricelli formula); $\left(\mu_T = \frac{2}{3}\mu_p\sqrt{2}\right)$
- A: area of the slot (m^2); $(A = h_{sl} * l_w)$

1.3. Control gates

Control gates are used for controlling the flow in a combined sewer network, and they are usually placed at the end of the sewer stretches or at the low points of the reservoirs. In general, the outflow from a control gate is characterised by the upstream and downstream water levels of the control gate. But if there is no back pressure, it depends only on the upstream water level of the control gate. The outflow from a control gate is given by the nonlinear relationship:

$$u_{un} = \mu f \sqrt{2g(h_u - h_d)}$$

where:

- u_{un}: outflow from the control gate (m^3/s);
- μ: coefficient of discharge determined empirically;
- f: orifice's ground area (m^2);
- h_u: water level upstream of the control gate (m);
- h_d: water level downstream of the control gate (m);

1.4. Nodes

The processes which take place in the nodes of a sewer network are the propagation and the merging of flows. Thus, the nodes can be classified in two types:

- propagation nodes: there is only one incoming link and one outgoing link:

$$u_{in} = u_{out}$$

where u_{in} is the flow to the node, and u_{out} is the outflow from the node;

- merging nodes: there are more than one incoming flows and only one outgoing flow:

$$u_{in,1} + u_{in,2} + \Lambda = u_{out}$$

where $u_{in,1,...}$ are the incoming flows and u_{out} is the outgoing flow from the node.

1.5. External inflows

The external inflows are appearing at specific locations of the network, like reservoirs or stretches of the sewer network.

1.6. Treatment plant

All the water from a sewer network which is not lost due to the overflows will reach the treatment plant. The inflow r_i to the treatment plant should not exceed the plant's maximum capacity $r_{i,max}$.

$$r_i \le r_{i,\max}$$

Pollutants in the sewer network

There are several ways of classifying pollutants in order to forecast their effect on water quality and the means of their removal. One way to classify them is as solid, liquid or gas, or as one of these mixed with or dissolved in another. More over, each of these can be organic or inorganic.

The pollutants are closely connected with the particles for surface sediments. A high percentage of BOD, P_{tot}, and SS is attached to sediments. To the fine runoff particles, heavy metals such as cadmium, copper, lead, and zinc are associated. Studies about pollutant parameters in the sewer network reveal that they are related to the sediment particles. Chebbo (1992) states that 83-92% of COD, 77-91% of BOD_5, 78-82% of N_{Kj}, 82-99% of hydro carbons and 79-99.98% of Pb pollution is particle bound. Also there is a correlation between the pollutant parameters.

Parameter 1	Parameter 2	Correlation coefficient
BOD	N_{Kj}	0.82
COD	N_{Kj}	0.87
COD	P_{tot}	0.95
COD	Pb	0.82
TSS	P_{tot}	0.95
TSS	COD	0.97

Because of these reasons, the concept of using one or few parameters such as COD or TSS as overall pollutant indicators is quite appropriate.

Modelling concentration of pollutants in a sewer network

The main purpose of water quality modelling is to simulate the variation of the level of the pollutants with time at chosen points in a sewer network.

The modelling of the water quality in a sewer network addresses as first step the related phenomena which occur upstream of the sewer system (such as sediment build-up on the surface and sediment washoff from the surface), followed by the processes within the sewer system (for example deposition and erosion).

There are two ways of modelling the concentration of the pollutants in a sewer network (Butler, 2000):

- the model is based on a mathematical set of equations for each major physical process; these are the so called physically-based models;
- the model is based on statistical or other relationships between the input and the output of the model, without an explicit physical base.

One of the most common physically based models is the description of the solute mass transport process along the longitudinal axis of flow using the one-dimensional advection-dispersion partial differential equation. This approach is used because in every sewer network these two phenomena take place.

Another physically-based model is the completely mixed “tank”, whereby each pipe is converted to a conceptual tank in which the pollutants are fully mixed. Because neither distance nor the velocity is included in the equation, it cannot model the evolution of pollutants at mean velocity, and gives progressive estimates of concentration in each pipe as a whole.

Yet another approach is to model the sediment transport in the sewer system. This model is described in some detail below as it was chosen as a working model. This particular model was selected because the pollutants which are transported by advection dispersion are either dissolved or suspended. It is important to know if in the sewer network there is deposition, erosion or neither of both, and also in this way, the level of bed shear stress is known.

General alternatives to physically-based deterministic models are the empirical models, the conceptual models, the grey box models, the stochastic models, and the artificial neural networks. One of the biggest disadvantage of these models is that they cannot be easily used to upgrade the sewer system, because the physical properties are not explicitly described

In general, the modelling of the sewer sediment transport is a complex process, not only because of the physical and chemical processes between the pollutant and the sediment bed which is formed, but also because of the elements of the sewer system, like pipes, nodes, and so on. To model the sediment transport in sewer systems is a difficult task (Schlütter, 1999).

Because of these reasons, the model can be simplified, considering one pine at the time and all the other elements: bed level, discharge concentration, erosion, deposition, deposited mass, and suspended mass, are considered to be mean values for this pipe. At each time step, water and sediments are entering into the pipe from upstream and are transported out of the pipe each time step. There are three sediment processes which can occur in the pipe: the sediments are deposited, or they are resuspended, or neither one of these two.

Which of the three processes actually occurs in a certain pipe and in a certain moment of time depends on the level of the bed shear stress τ. The most common way to calculate the bed shear stress is without taking into account the fact that there may be deposits on the bottom of the pipe increasing the bed shear stress, in which case the following formula can be used:

$$\tau = \rho_w g R_h |I_0|$$

where:

τ: bed shear stress (N/m^2);
ρ_w: specific gravity of the water (kg/m^3);
g: gravitational acceleration (m/s^2);
R_h: hydraulic radius (m);
I_0: bottom slope of the pipe;

Depending on the critical shear stress for erosion τ_{ce} and the critical shear stress deposition τ_{cd}, the three processes occur as following:

$$\begin{cases} \tau_{cd} < \tau \leq \tau_{cd} & \rightarrow \textit{deposition} \\ \tau_{cd} < \tau \leq \tau_{ce} & \rightarrow \textit{no deposition or resuspension} \\ \tau_{cd} < \tau > \tau_{cd} & \rightarrow \textit{erosion} \end{cases}$$

Generally, deposition depends on the hydraulic conditions, the characteristics of the sediments (particle sizes and weight), the bed shear stress, the available space for deposition and the concentration of suspended solids. If the hydraulic conditions indicated by the bed shear stress permits for deposition and if there are sediments in suspension, then for characterizing the deposition process, an equation which does not depend directly on the actual level of the shear stress or on the concentration in the suspension can be used, or also can be used an equation which depends on the bed shear stress relative to the critical bed shear stress for deposition.

$$\frac{dm_p}{dt} = \alpha_{dep}\left(\alpha_{sc} - m_p(t)\right)$$

where:

$m_p(t)$: mass per meter pipe (kg/m);
α_{dep}: deposition rate (1/day);
α_{sc}: storage capacity given as a fraction of the pipe volume per meter multiplied with a computational sediment bulk density;

For characterizing the erosion process, the following formula can be used:

$$\frac{dm_p}{dt} = -\alpha_{ero}\, m_p(t) Q(t)^{\alpha_{ero2}}$$

where:

$m_p(t)$: mass per meter pipe [kg/m];
α_{ero}: pipe erosion rate [$1/m^2$];
$Q_p(t)$: discharge in the pipe at time t [m^3/s];
α_{ero2}: numerical value between zero and 1;

If no material is available for erosion, then no material is resuspended.

To model the concentration, a model will be considered in which the inflow of the sediments depends on the concentration of the water upstream pipe and the additional sediments from the domestic and industrial activity. Transport out of the pipe depends on the concentration in the actual pipe. It is assumed that the sediments move with the same velocity as the transporting water. The concentration is calculated from the division of the mass of sediments in suspension for the next time step with the water volume, assuming that the suspension is fully mixed.

$$C_i^{k+1} = \frac{m_{ps\,i}^{k+1} * U_{p\,i}^{k+1}}{Q_{p\,i}^{k+1}} * pipelength_i$$

where:

C_i^{k+1}: concentration in the pipe stretch i at the time step k+1;

$m_{ps\,i}^{k+1}$: mass of sediments in suspension for the time step k+1;

$U_{p\,i}^{k+1}$: mean velocity in the pipe stretch i at the time step k+1;

$Q_{p\,i}^{k+1}$: discharge in the pipe stretch i at the time step k+1;

Conclusions

The modeling of the sewer network from the point of view of the quantity is useful for developing the control strategy of the flow in the sewer network, the prediction of the overflows and also the prediction of the flow which will enter in the treatment plant.

The perspective of the modeling is to be able to predict the mass transport of sediments at different locations in the sewer system. This would facilitate dynamic modeling of CSO discharges to the environment. Prediction of the sediment build-up in the system is also important.

When models of the build-up of pollutants are established, the combination of the models and flow prediction can be used to predict the pollutant concentrations in the wastewater. These predictions can be used to adjust the control strategy for the sewer and the wastewater treatment plant.

Bianca Chindris acknowledges the financial support provided through the European Community's Human Potential Programme under contract HPRN-CT-2001-00200[WWT & SYSENG].

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Control of a WWT Plant: Stating the problem

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Abstract
The objective of this paper is to give some general ideas of the possibilities that exist for the design and implementation of a wastewater treatment control scheme. Due to the varying characteristics of wastewater, controlling a WWT plant is usually not a simple task, therefore the goals to be fulfilled must be carefully chosen. Another very important thing is knowing what can be controlled and what not. This knowledge helps in setting the control system boundaries. Also, when there is more than one input variable to choose from, selecting one or another as the manipulated variable might make a big difference. Various control strategies and approaches to WWTP control design are presented, both the traditional control methods and the modern ones.
Keywords: WWTP, control, manipulated variable, feedback control, feedforward control, model predictive control, control strategy

1. Introduction

In today's world, good management of resources and high efficiency are key attributes for any successful business. Waste water treatment is no exception, even though one might be tempted to consider it different from other industries, in that it is oriented towards environment and human health preservation, rather than towards profit.
The need for increased efficiency stems from the facts that effluent quality standards are getting tighter and budgets tend to decrease. There are indications that future regulations may have to be met on the basis of spot checks instead of monthly averages, therefore an advanced control of the process will be required. Also, given the reduction of capital investments, operating cost saving is a must.

The other important issue is the use of resources.

Given the demographic increase of the last decades, the importance of land use is obvious. Urban waste water treatment has to concentrate the spatial resources as much as possible. The treatment plant should have a large capacity, which using traditional design methods means additional or increased volumes, that is not always possible to accomplish in restricted land areas. The modern alternative is to include process dynamics and operational methods in the design procedure, thus decreasing the safety and capacity margins, which requires a reliable operation.

Water is a critical resource for life as we know it, even more today, when people expect to get good water from the simple turn of a tap. Water recycling and saving is a reality. Water re-use raises public health problems, so a strict control of the treated water is imperative.

Energy saving is another aspect of the resource problem. When comparing different wastewater treatment systems, total energy consumption of the system always has to be considered. This includes energy for wastewater transporting, heat production, aeration, mixing, use of chemicals, sludge transportation and biogas production.

Also important is material recycling. The sludge separated in treatment plants can be used for fertilizing in agriculture, which means that it has to be acceptable from the standpoint of food production. Unwanted organic compounds and heavy metal amounts have to be reduced in order to achieve that and this is no trifle subject. Partially treated wastewater can be used for irrigation: the treatment plant can be operated so that the effluent N/P ratio is controlled to a specific value. Phosphorus being a limited resource, any recycle of phosphorus will have increased importance, which means that a lot of attention has to be devoted to the control of the biological process. Recycles within the plant are equally important, oxygen, nitrate, phosphorus and nutrient recycles have to be supervised as well.

The interactions between various unit processes make plant-wide operation far from trivial. Good control of plant operation is necessary, and the key factors to control design are input variables and control strategies. Therefore, this paper's discussion will be centered on the two key factors mentioned. The next section focuses on what variables can be manipulated and how. The third section will give a general view on the basic control techniques that can be applied to wastewater treatment systems, followed by a brief discussion of the modern control alternatives in section four. The paper ends with a conclusions section, acknowledgements and bibliography.

2. What to Control and How

Control design and implementation for a WWT plant is not an easy task. Wastewater attributes are the first of the difficulties encountered. The daily volume of wastewater to be treated can be very large, there are major disturbances in the influent and moreover, the influent must be accepted and treated, there being no possibility of returning it to the supplier. Pollutant concentrations are very small, thus high sensor sensitivity is required, which in turn means a very high price if the sensor exists. Other problems stem from the process' high nonlinearity. There are many interactions within the process, therefore the use of simple controllers is limited. The microorganisms change their behaviour and population distributions and biomass-effluent separation is challenging and easily disturbed. Also, the response time range is very wide. Thus the control scheme must be very robust. Finally, it must be taken into account that the value of the product in the marketplace is remarkably low and therefore expensive schemes will not be feasible.

Standard operating and control is organized in a hierarchy: at the top level there is the process management, next comes the supervisory control, followed by the advanced process control system and at the very bottom the sensors and basic control.

The first thing to do in a top-down approach is to set the goals. This task pertains to the process management level. The general wastewater treatment process goals are:
- meeting the effluent discharge requirements,
- achieving a good disturbance rejection,
- operation optimization to minimize the operating cost.

Plant supervisory control requires stating the operational objectives. These are more specific and should include:
- growing the right biomass population,
- maintaining a good mixing where appropriate,
- adequate loading and DO concentration,
- adequate air flow,
- good settling properties,
- avoiding clarifier overload,
- avoiding denitrification in clarifier.

In order to determine a proper control strategy, one must consider the operational objectives, the dynamics of the plant and the available instrumentation and management systems. After the control strategy was chosen, we may proceed to the implemetation part, building the basic control schemes.

Considering the dynamics of a typical biological WWT plant, the processes that occur within it may be divided according to their dynamics timescale: slow processes - the biomass growth, medium-scale processes - concentration dynamics and nutrient removal and fast processes - flow dynamics and oxygen dissolving. The basic control therefore should deal with the flow dynamics and the dissolved oxygen, the advanced process control should take care of the nutrient removal process and the concentration dynamics, while the supervisory control will take care of the biomass growth process. Within each level the traditional "divide et impera" method can be applied, looking at each process unit relatively independent. That done, the interactions among those units must be taken into consideration.

The most important units under control are the activated sludge reactor zones: anaerobic, anoxic, aerobic, and the secondary settlers.

In the anaerobic zone the reaction of interest is phosphorus release. The variables that have to be controlled are: the P/COD ratio (should be low), the VFA concentration: if it's too low external C sources as CH_3COOH must be added, the retention time, the NO_3^- and DO levels, which should be as low as possible so as not to inhibit the P-release reaction.

In the anoxic zone denitrification takes place. The requirements for a good denitrification are: keeping the DO level to a minimum by mixing and recirculation, monitoring the C source level adding CH_3OH or C_2H_5OH when it gets too low, manipulation of the retention time through the influent, recirculation and filter backwashing flow rates, measuring the NO_3^- at the outlet of the anoxic zone (should tend to 0) in order to control the reaction rate, possible redox potential and pH measurements: a low redox potential will favor denitrification and a pH between 7 and 9 is considered optimum for the reaction to take place.

The aerobic zone is the most complicated one to control, given the fact that there are 3 competitive reactions that have to happen virtually simultaneously. These are COD removal, nitrification and phosphorus uptake, implying 3 types of bacteria with different growth rates: heterotrophs, autotrophs and PAO. Also wanted is a growth of proper floc-forming organisms and avoidance of filamentous growth so as to have proper floc-forming organisms. The control must be oriented towards: the DO level at various parts of the reactor (DO is needed for all reactions to take place) through an adequate air flow rate and mixing, the retention time, affected by the inflow rates, the measurement of NO_3^- and NH_4^+ levels, the biomass growth rate and the sludge wastage rate, the possible chemical removal of P if at the outlet of the zone the P level measured is too high.

In the secondary settler the goals to achieve are a good liquid-solid separation and a high thickening of the sludge. This can be controlled by: hydraulic propagation - must have a smooth influent flow rate -, hydraulic loading, influenced by the return sludge flow rate, the floc properties, obtained in the reactor zones, and the presence or absence of reactions in the settler. There may occur C removal reactions in case O_2 is present, denitrification reactions if NO_3^- levels are high enough and P release reactions if the PAO organisms get starved, the last two reactions mentioned being unwanted. The key control variable here is the return sludge flow rate.

There are several manipulated variables in a plant that are related to the equipment and basic control loops in the process, that will not be discussed here.

The input variables available to manipulate biological wastewater processes can be categorized as follows:
- hydraulic variables,
- addition of external chemicals,
- air or O_2 supply,
- wastewater pre-treatment.

The hydraulic variables refer to the different flow rates that influence the retention times of the plant units. These include influent flow rate, sludge distribution flows, internal recirculations and external recycle streams. The influent flow rate may be varied with: pumping, sewer network control, equalization basins, flow splitting (parallel processing) and bypassing. The sludge distribution flows can be manipulated by: the waste sludge flow rate, the return sludge flow rate and the step-feed flow rates. The most important recirculations are: the recirculation of NO_3^-, recirculations in biological P removal, recirculation of supernatants from dewatering of sludge, filter backwashing.

The addition of chemical can be done for different reasons: carbon source is added to obtain adequate C/N or P/C ratios in the system, flocculants as Fe^{2+}, Fe^{3+} or Al^{3+} salts are added to obtain chemical precipitation for P removal, polymer addition is used for sludge conditioning in the settler to improve dewatering properties and caustic addition is used for pH adjustment.

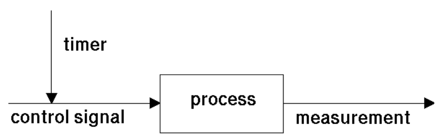
Dissolved O_2 is a key variable for the whole biological treatment of a WWT plant. The choice of a proper DO setpoint is crucial from the biological standpoint. O_2 dissolving is a fast timescale process, therefore its dynamics must be continuously monitored so that everything works fine. The important things to be checked are: the total air supply, the DO setpoints, the DO spatial distribution throughout the reactor zones and the relation between the aerated and anoxic zones. In some systems pure O_2 is used instead of air under extreme load conditions. The air flow rate is of a major importance for the whole operation, since the energy cost is significant. The air distribution can be realized in space, for continuous reactors or in time, for sequential batch reactors.

Wastewater pre-treatment is needed especially in industrial WWT processes in order to attenuate disturbances to the plant. The possible operations are: pH adjustment of the flows, using separate basins for chemical pre-treatment and nutrient addition.

3. Basic Control Alternatives

Before starting to design any control scheme, system boundaries have to be drawn clearly, the manipulated variables, the disturbances, the system state variables and the output variables must be identified. The manipulated variables are the ones used to control the process, the state variables are internal to the process and often can't be observed directly, being deducted from the measured variables or outputs. The process for most of the control engineers includes the actuators, the real process and the sensors. The outputs are considered to be the measurement signals, the inputs are the signals to the actuators and the desired outputs are called setpoints, reference outputs or values. The differences between the output and the desired output are the errors.

Control loops can be closed or open. Closed loops imply a feedback from the process, which helps in adjusting the error between the desired output and the actual one. Open loops operate without any feedback from the measurements, the control being based on a predetermined program or on a timer.



Open Loop Control

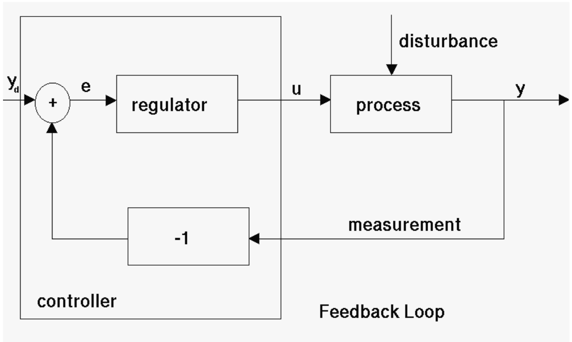


Fig.1 – Open Loop Control Fig.2 – Feedback Loop Control

Examples of feedback control in a WWT plant could be the flow control or the DO control. Examples of open loop sequencing can be the switching on and off of air compressors according to timers, sludge removal based on timers, wastage sludge pumping.

The feedback algorithms that predominate in wastewater treatment plants are the on-off algorithm and the Proportional-Integral-Derivative or PID algorithm. The first one means a simple on or off switching of a device, depending on the characteristics of the output. The problem with it is that the measured variable will cycle up and down continuously, phenomenon which is called limit cycling. The cycle speed and amplitude depends on the process responses to the control action and when the cycling is fast it leads to controller wear. It may also create a disturbance to other parts of the process.

The PID algorithm is one of the most common in use in process industries. It is a combination of an error-proportional action, a past error behavior accounting incorporated in the integral action and a predictive action proportional to the derivative of the error. The mathematical notation of the algorithm thus is:

$$u = u_0 + K_p e + \int K_i\, e\, dt + K_d\, de/dt, \quad (1)$$

where:
$e = u - u_0$ - the error
u = control signal
u_0 = controller output bias
K_p, K_i, K_d = the proportional, integral and derivative gains, often the last two are chosen as: $K_i = 1/T_i$, T_i being the integral time and $K_d = T_d$, T_d being the derivative time
t = time variable.

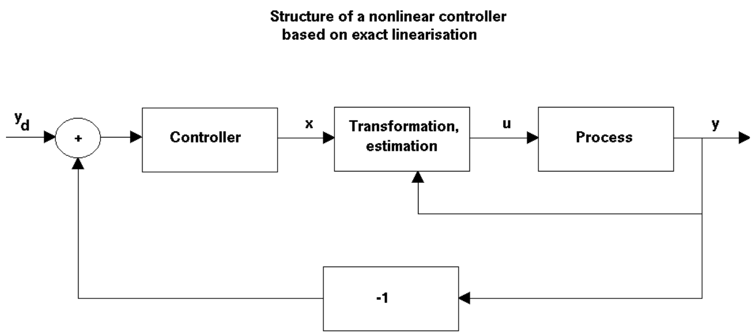


Fig.3 – Structure of a Nonlinear Controller

It can be noticed that there is a mathematical term that corresponds to each of the control actions. The problems that can appear with this type of algorithms are the integral or reset windup and the derivative kick. The integral windup means that the integral might happen to grow unlimitedly when the manipulated variable hits a constraint for some time. This problem is solved by putting an upper limit to the integral term or by turning off integral action when the controller output saturates. The derivative kick appears when the measurement signal from the process is noisy and oscillates. The derivative will amplify the noise, and in order to avoid this noise filters must be added, such as digital low pass filters.

Usually loop controllers are digital and their operation is discrete. Choosing a sampling interval plays an important role in this case. Larger sampling intervals are adequate on loops with slower dynamics, while fast dynamics require a short sampling time. It is recommended that the sampling rate be 6 to 10 times the bandwidth or to sample 6 to 10 times within the rise time of a step response.

In order to function satisfactorily, controllers must be tuned properly. In order to do that, a simple process model must be identified, the model parameters must be estimated usually by measuring the responses to standard signals and finally the controller parameters must be calculated based on the model parameters estimated previously. Another thing to take into account when tuning the controller parameters to match the process characteristics is the loop purpose: servo loop, regulator loop or averaging loop.

When the process characteristics are subject to frequent changes, the manual re-tuning is not practical. Auto-tuners may be a solution when changes are not so frequent, other possible approaches are gain scheduling and self-tuning. If we know how the loop gain changes with changing conditions, we can make a correction to the controller gains.

The scaling of controller parameters using some measure of the operating point is called gain scheduling and it's the simplest solution to this kind of problems.

The self-tuning controller is made of 3 parts that perform different tasks:
- a process identification part that estimates process parameters
- a design part that calculates controller parameters
- a controller part which uses the calculated parameters to act on the process.

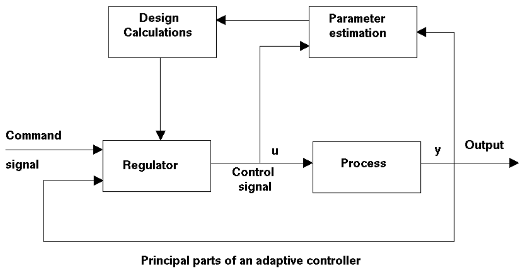


Fig.4 – Structure of an Adaptive Controller

The drawback faced by this kind of controllers is that they need some excitation from the process in order to identify the process parameters while at the same time they try to control the process or to remove the excitation, therefore when the excitation is insufficient the parameter estimation can become unstable which can also make the control unstable.

An alternative to empirical gain scheduling is the exact linearization, where the controller is split in two parts, one that computes the command signal based on a linear algorithm and the next that calculates the manipulated variable using some inverse function. This can only be applied when there exists an invertible model of the nonlinearity.

A variation of the feedback control topology is cascade control. This is made of two or more feedback controllers with the outputs of the higher-level controller being the setpoint of the one below it. The upper level controller is called primary or master controller and the lower level controller is called secondary or slave controller. The slave controller generally has to react faster than the master. This kind of control is used for disturbance rejection, gain scheduling and hysteresis removal.

4. Modern Control Alternatives

More advanced controllers require more information about the process. Using a model based control is one of the way of exploiting the potential of today's technology, like sophisticated controllers and analyzers. State feedback can be used in this approach, even if some states are still not possible to be measured and have to be estimated.

One major limitation of feedback control is that the disturbance has already affected the process before the controller gets the error. This can be adjusted by the use of model-based predictive algorithms configured as feedforward controllers. Feedforward control means measuring the disturbance and adjusting the manipulated variable to compensate for the effect of the disturbance. The effects of the disturbance and the feedforward compensation theoretically have to cancel out, the output remaining the same. To design a compensator we must have the models of the sensors, the disturbance variable dynamics and the manipulated variable dynamics. In order to obtain the model there must exist the possibility of measuring or at least estimating the disturbance. For the controller action to be effective, the dynamics of the sensor, compensator and manipulated variable must be at least as fast as the dynamics of the disturbances.

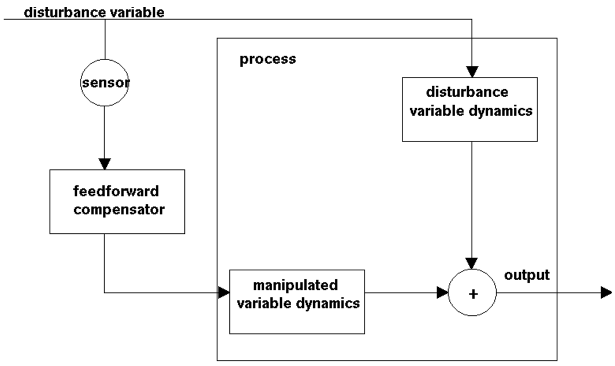


Fig.5 –Feedforward Loop Control

Some applications of feedforward control implemented in WWT plants are: MLSS and temperature to air flow rate with feedback from DO sensors, influent flow rate and COD to DO setpoints, influent flow rate and COD and aeration tank temperature to MLSS setpoint, using respirometry as a warning for toxicity or to determine influent BOD, using in-stream sensors to analyze the influent stream.

Predictive controllers based on linear models are among the most successful of the advanced multivariable controllers in use in the process industries. Basically they adjust a number of manipulated variables so as to minimize the errors between the desired and the actual output, using the predicted response of the process, as calculated from the model. The first one or two control moves are implemented and a new set of predictions are made.

There are various techniques that can be used, such as algorithms based on linear input-output models, step response models, transfer function models, state-space models, dynamic matrix control algorithms (DMC), generic model control (GMC). The DMC model for example is very commonly used. It uses a matrix derived from a number of step tests on the process under test run conditions. The controlled variable at different sampling times after the step can be expressed as:

$$y1 = a1\,\Delta u1 \quad (2)$$
$$y2 = a2\,\Delta u1 + a1\,\Delta u2 \quad (3) \qquad \Leftrightarrow \qquad y = A\,\Delta u \quad (5)$$
$$y3 = a3\,\Delta u1 + a2\,\Delta u2 + a1\,\Delta u3 \quad (4)$$

where $y = [\,y1; y2; y3]$, $\Delta u = [\Delta u1, \Delta u2, \Delta u3]$ and A is the coefficient matrix.

This is the model used to predict the effect of past control moves into the future. From the prediction it is possible to calculate the predicted error and based on the predicted error the controller must be designed to calculate some manipulated variable moves:

$$\Delta u = f(e). \quad (6)$$

The drawback of this approach is the use of a linear model, while the process to be treated is highly nonlinear. The algorithm can be extended though, to use nonlinear models. In nonlinear quadratic dynamic matrix control (NLQDMC), a nonlinear model is used to compute the effects of past manipulated variables on the predicted output. A linear obtained by linealizing the nonlinear model at each sampling time, is used to compute the manipulated variable values. The advantage of this approach is that only one quadratic program is solved at each sampling time. The algorithm can be further modified to include state-space nonlinear models and filters.

The GMC is another control technique that can use nonlinear process models. The basic concept of it is that if the process is not operating at the desired state, the rate of state change will be used as a function of that error.

State feedback controllers can also be used for a WWT plant, since the variables of interest are always a function of the state variables. The problem then is the estimation or noise-filtering of state variables. The field of identification and estimation is usually divided into off-line and on-line methods. Off-line methods generally use batch processing of data and are concerned with identification of time-invariant model parameters. The problem is often formulated as a least-squares optimization with the parameters chosen to minimize the sum of the squared errors between the measurements and model predictions. The on-line methods need recursive data processing and deal with time-varying parameters and states. Algorithms can be developed from stochastic formulations. The state space model generally looks like:

$$dx/dt = Ax + Bu, \quad (7)$$

where x = system state space vector, u = input vector , A = state transition matrix and B = system input matrix.

Other approaches to nonlinear MPC based on input-output models identified from plant data can be categorized in terms of the nonlinear model they use as:

- neural network model based algorithms
- fuzzy and multiple linear model based algorithms

- Volterra model based algorithms
- polynomial NARX model based algorithms.

5. Conclusions

This paper has presented the principal decision factors in choosing a WWTP control scheme. A thorough knowledge and understanding of the process is required before trying to build a control system.

The first step to designing a control scheme is stating the goals and selecting the manipulated variables. A hierarchical approach is usually recommended. Process goals then operational objectives have to well formulated, so that major design problems do not appear afterwards. Based on the operational goals, process dynamics and available instrumentation, an adequate control strategy can be built. Finally, the sensors and the basic control loop will be implemented.

The available control techniques can be categorized into traditional and modern ones. The traditional control methods are based on feedback control and transfer function theory. The most widely used are the PID algorithms. The modern alternatives combine feedback control loops with the feedforward control loops. Model prediction and state feedback are two of the most popular approaches.

6. Acknowledgements

Cristina Maria Lazar acknowledges the financial support provided through the European Community's Human Potential Programme under contract HPRN-CT-2001-00200[WWT & SYSENG].

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Dynamic and Steady-State Modelling of a Pilot-Scale WWTP Using the ASM2d Model

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Abstract
This paper describes the development and usage of a simulator for modelling biological processes at wastewater treatment plants (WWTP) with nutrient removal. The development is based on the Activated Sludge Model no.2d (ASM2d), published by IWA Task Group on Mathematical Modelling of Biological Wastewater Treatment Processes. The simulator uses Matlab to solve the mass balances using ODE (ordinary differential equations) solvers. Experimental data obtained from a pilot WWTP with a configuration of Anaerobic/Anoxic/Oxic (A2/O) reactors were used to validate the simulator by means of steady state and dynamic simulations with the Activated Model Sludge 2d.

Keywords
A^2/O pilot plant; ASM2d; modelling; simulator development; wastewater treatment

1. INTRODUCTION

The biological treatment of municipal and industrial wastewater using activated sludge processes is one of the most popular water purification methods. There are many schemes that remove organic loading and nutrients from wastewater as for example A2/O, Phoredox, UCT or Sequential Batch Reactors (SBR). Before designing the WWTP a previous case-study is necessary to assess the quality and flow-rate of the wastewater to be treated and to study possible configuration schemes. Pilot plant experiments can be carried out in a laboratory and bench-scale set up (Mulkerrins, 2004; Baeza, 2003; Krühne, 2003). These require a lot of time and an appropriate infrastructure for developing the pilot experiments. In addition, a software tool can help to simulate a full-scale WWTP running under real conditions. (Meijer, 2002; Meijer, 2001; Brdjanovic, 2000; van Veldhuizen, 1999). Thus, a previous case study can be done very fast and easily to provide an idea of the biological processes under different operating conditions. Software programs commonly use the activated sludge mathematical model for wastewater treatment developed by different research groups (McKinney, 1962; Lawrence, 1970; Ekama, 1980; Ekama, 1985; Wentzel, 1992; Henze, 2000).

Nowadays, several tools for water treatment modelling of waste waters exist on the market. Companies like Hydromantis Inc., Ifak, The MathWorks Inc., WRc plc., HEMMIS, EFOR ApS., EnviroSim Associates Ltd., (Copp, 2002) have developed well-known software programs. Many of these tools allow to model and to optimise discontinuous and continuous processes. Despite of that, many of the important critical parameters of different operational units are sometimes simplified or not taken into account in a real simulation (Zeidan, 2003).

This paper describes the development of a simulator in MATLAB for modelling biological processes of residual water treatment plants by means of the mathematical model of active sludge ASM2d. To validate the simulator, experimental data were used obtained from a previous study case of a pilot plant with the scheme A2/O.

2. SYSTEM DESCRIPTION

Case-studies of processes in small scale systems is always recommendable before the construction of a municipal or industrial wastewater plant, Pilot plants are used in order to accomplish the abovementioned. These plants can be located in the laboratory, or directly in an industrial area. Thereby, these installations allow accomplishing diverse studies under different operational conditions. As it is not always possible to perform an exhaustive monitoring of the system during real plant operation, a pilot plant can be used for that purpose. Data collected in the study provide information of the biological processes that take place in the reactors used. Once data is collected and analysed, results can be used as a basis for the design of a full-scale treatment plant. (Meijer, 2002; Brdjanovic, 2000; van Veldhuizen, 1999).

The pilot plant studied in this work is located in the Department of Chemical Engineering at UAB. (Baeza, 1999 a; Carrera, 2001; Baeza, 2002; Baeza 2003) The process under study is based on an A^2/O multistage scheme as shown in Figure 1 (Barnard, 1983). with nitrification-denitrification and biological excess phosphorous removal (BEPR).

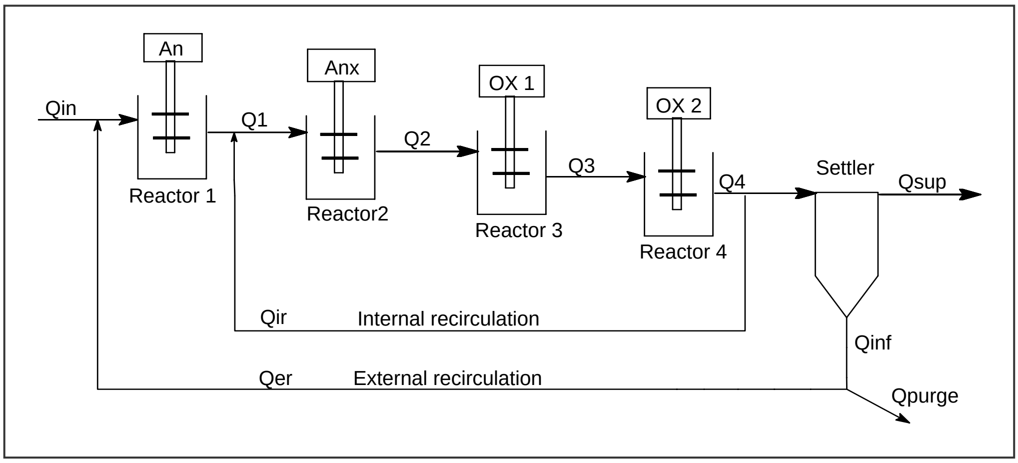

Figure 1 A^2/O multistage scheme configuration of the pilot plant.

This configuration was first used by Barnard (Barnard, 1974), combining the Phoredox and modified Ludzak-Ettinger systems. The result was a system of three reactors in series, which contains three different zones anaerobic, anoxic and aerobic. The nitrate's internal recirculation from the aerobic reactor to the anoxic reactor permits the nitrogen and phosphorus simultaneous removal (Gabriel, 2000).

The set-up where the ASM2d model was applied is a highly instrumented biological WWTP with four reactors (figure 1.). The first reactor has an anaerobic environment. Therefore in this reactor no types of electron acceptors are present. This reactor acts as an anaerobic selector, in which the flows of the inflowing water, synthetic influent and the flows of external recirculation are mixed. The main processes in this reactor are the hydrolysis and the phosphate release, the latter being a result of an accumulation of a part of organic matter from the influent. The second reactor has anoxic conditions, that is, in the reactor's environment there is only the oxidised form of nitrogen. This reactor's inflow is made of the flow from the anaerobic reactor and the flow from the internal recirculation that contains the nitrogen oxidised in nitrate form. The main processes that happen in the reactor are the denitrification and the elimination of the organic matter that has not been consumed previously in the anaerobic reactor. In order to obtain an aerobic environment, air is introduced to the third and the fourth reactor. The inflow and outflow from these reactors are the same as the flow from the anoxic reactor. Denitrification and accumulation of phosphates inside the phosphate accumulator microrganisms (PAO) take place here. The anoxic and aerobic reactors include a real-time monitoring of pH, T, DO and ORP. In both aerobic reactors is available on-line monitoring of OUR. In addition stirrers, pumps and the aeration system can be regulated. (Baeza, 1999b; Gabriel, 2000)

Under ideal conditions the settler behaves like a solids separator, but during the experimental period, the kinetic behaviour of the settle was similar to an anoxic reactor. The inflow to the settler comes from the second aerobic reactor. This unit has an output at the lower part that corresponds to the external recirculation flow, which contains the greater part of the suspended solids and an output at the upper part of the settler for the clarified liquid. Sludge residence time was maintained at 10-11 days adjusting the purge flow-rate. The purge flow-rate may be expressed as the inflow to the pilot plant minus the external recirculation.

Three reactors with same characteristics have been constructed; apiece can works with a volume of 18 or 28 litters, they are without internal baffles and each one is agitated with a motor of 0.5 Cv. A fourth reactor with a capacity of 18 litres was constructed. This reactor was closed hermetically and equipped with an agitator of adjustable speed (0-120 rpm) by means of a frequency changer. A settler of 60 litters was constructed. Peristatic, dispenser and pneumatic pumps carry out the liquid transport between the reactors. The plant configuration is obtained by means of the performance of electro-valves commanded by a Programmable Logic Controller (PLC). The PLC is connected to the PC where monitoring and control takes place. This configuration allows making any changes to the pilot plant scheme in an automatic manner. (Baeza, 1999a and 1999b) Two dispenser pumps were used for feeding concentrated sources of carbon and nitrogen to the pilot plant. These were diluted in line with the tap water that was regulated by a valve of pneumatic control. To carry out the detailed study of the biological, physical and chemical processes that converge during biological purification of residual waters has been decided for the most efficient instrumentation of each reactor. (Baeza, 1999 b)

3. RESULTS

3.1. Simulator development

A modular structure was considered necessary during the development of the process simulator. Thus, the simulator is more versatile, of easy handling and the interpretation of simulation results by a matrix notation is easier to understand. The simulator consists of 11 M-files (programmed in Matlab® environment) (MathWorks, 1992) and 2 Excel files that contain information about the 45 kinetic parameters and process rates of the ASM2d mathematical model.

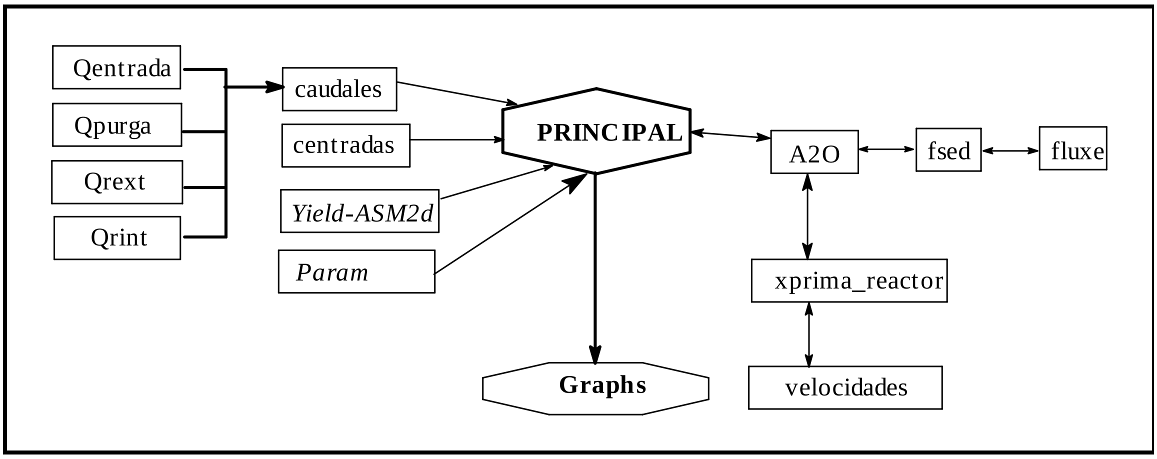

Figure 2. Schematic representation of the simulator.

As shown in figure 2, one main file named **principal.m** launches the rest of the files situated in the simulator's folder. The algorithm used for the ordinary differential equations solution is an ODE15s (stiff function). In the **principal.m** file are defined the reactor volumes, the initial concentrations of the influent flow (x_e), the simulation time and the initial values of each state variable. The later is loaded as the *xinicial* vector for the initial states. The file **principal.m** calls two Excel files, **parametros.xls** (assigned as matrix *p*) and **Yields-Asm2d.xls** (assigned as matrix *k*) and it also calls the file **A2O.m** that contains the mass balances for the A2/O WWTP scheme. The vector of flows that contains **qentrada.m**, **qpurga.m**, **qrinterna.m** and **qrexterna.m** is required as well by **principal.m**.

Once the simulation is over, the file **principal.m** generates the graphs that show the concentration profiles of the state variables throughout the simulation time. One graph per reactor and per grouped variables has been implemented. In addition, graphs for total suspended solids (TSS) in the settler and for the cell residence time have been implemented.

On the other hand the file **A2O.m** receives from **principal.m** the vector of flows, the reactor volumes, matrixes *k* and *p*, the initial values of the state variables and the time of the simulation. In case a dynamic simulation is carried out, the file **centradas.m** containing the inlet concentration and the flow-rate profiles must be loaded. Mass balances in the reactor and in the settling tank are calculated in **xprima_reactor.m** and **fsed.m.** The later describes the settler by means of traditional one-dimensional layer model. The results of each step along the simulation are stored in a one-column matrix made of 6 blocks of 19-lines each. Each block represents the set of state variables exiting a process unit (reactors and settler) through a flow-rate. Moreover 10 lines are added to the one-column matrix corresponding to the 10 layers of the settler.

Reactors' mass balances are calculated in the **xprima_reactor.m** file. This file receives the initial and outgoing concentrations from the reactors, the flows, volumes and matrixes *k* and *p*. The **xprima_reactor.m** file calls the file **velocidades.m,** which contains the rate equations for every ASM2d process. Process rates for aerobic hydrolysis, heterotroph, PAOs and autotroph microrganisms, precipitation and redissolution are included in this file. Substitutions of the Monod equations (MonodX, MonodPHA, MonodIPP and MonodPP) and kinetic parameters of matrix *k* were made for a easier reading of the program language. Values of these files can be changed very easily if needed by the user. During steady state conditions flows are constant, but in dynamic conditions the flows change along the time of simulation. A file designed ***centradas.m*** was specifically written for modelling the dynamic conditions. **Yields-Asm2d.xls Excel file** contains a stoichiometric matrix (19×21) of state variable process rate yields as described in the ASM2d model. File ***parametros.m*** contains the values of kinetic parameters for ASM2d mathematical model. Default values were used as described in Henze *et al.* (1995).

An one-dimensional layer model has been used for modelling of settler behaviour. This model has four different sedimentation zones. These are: discrete particle zone, flocculent zone, hindered settling zone and compression zone. This model allows knowing the resulting effluent and recirculation concentrations, and we can obtain the concentration profile inside the settler as well. The one-dimensional layer model assumes that horizontal concentration gradients of particulate solids inside the settler are not taken into account, thereby the sedimentation processes are modelled in the vertical direction. The decantation model is based in the Kynch's sedimentation law (Kynch, 1952). In this file are defined the flux differential equations for the 10-layer settling model. The layer n°10 represents the upper part of the settler, that corresponds to the external recirculation flow and layer nº1 corresponds to the lower part of the settler for the clarified liquid from the pilot plant. The settler is fed through the layer # 6. The settler is 1 m high and has a diameter of 30 cm according to the dimensions of the pilot plant. The file **Fsed.m** calls to **fluxe.m** file. The **fluxe.m** receives the inflow concentrations to the settler and number of layers used in the settler model. Calculation of the correction factor Ω and the sedimentation velocity of sludge and characterisation of the sludge used into the system is made in this file. The sedimentation flux of the solids into the settler can be calculated if the two parameters are known. Bad settling conditions were considered in the present work.

3.2. Simulator validation

Validation of simulator under steady state conditions using data from experiments made in the pilot plant

The information about stability level of the model was given by steady state modelling. During the simulation of steady state conditions, several simulations were carried out to prove mass balances consistency and agreement with the knowledge about activated sludge processes. Default values of kinetic parameters were used as recommended in the ASM2d (Henze, 1995) and a simulation time of 100 days. Once we were certain that the simulator allowed for results that are valid for the processes of wastewater treatment which take place in the system, which means that programming mistakes were corrected, we use the experimental data from the pilot plant for next simulations.

Next simulations under steady-state were performed to obtain the initial concentration of reactors for dynamic simulations by adjusting the sludge retention time of the system through variations of the purge flow-rate. Steady-state data was taken from experimental steady state conditions developed during 6 months at the pilot WWTP.. The sludge retention time was practically constant to 10 days. The hydraulic retention time for all four reactors was 7.6 hours. Inlet flow (0.3201 m^3/d), external recycle flow rate (0.309 m^3/d) and internal recycle flow rate (0.6087 m^3/d) as well as pH into the reactors were maintained constant. Analysis of VSS and TSS allowed for modifying the purge flow, which was controlled and modified by the supervisor system available at the pilot WWTP (Baeza, 1999 b; Gabriel, 2000)..

Validation of simulator in dynamic conditions by datas from experiments made in the pilot plant

Simulator validation under dynamic conditions was made by comparison of experimental data obtained from the pilot plant against the data obtained by simulation. An intensive monitoring task was performed during three days to obtain COD, N and P data under dynamic conditions in the pilot plant. The inlet flow and concentration profiles were programmed in the control computer to emulate conditions that can be found in a large-scale WWTP. Constant feeding phases were maintained for a minimum period of 5 hours each, considering a broad range of inlet concentrations and hydraulic residence time to evaluate the model. Internal and external ratios were maintained at 2 and 0.5 respectively with the respect to the inlet flow rate during all period monitored. (Gabriel, 2000)

Simulations were performed considering the same inlet profiles to evaluate the model prediction. In general, the ASM2d model using default parameters predicts well the behaviour of ammonium and nitrate either during maximum and minimum loadings at any reactor of the pilot plant. As an example, Figure 3b shows the N profiles in the second aerobic reactor. Phosphate tendency is predicted reasonably well, even if the absolute value of phosphate is under predicted by the model. On the other hand the COD is not predicted very correctly, maximum loads are always higher but the minimums are predicted quite well. The VSS simulated differ a lot from the experimental data. The phosphate prediction in the anoxic reactor is not very good, because was preferred the release of phosphate into the reactor due to the assimilation of PHA into the microrganisms. The simulation results of COD were overestimated as well.

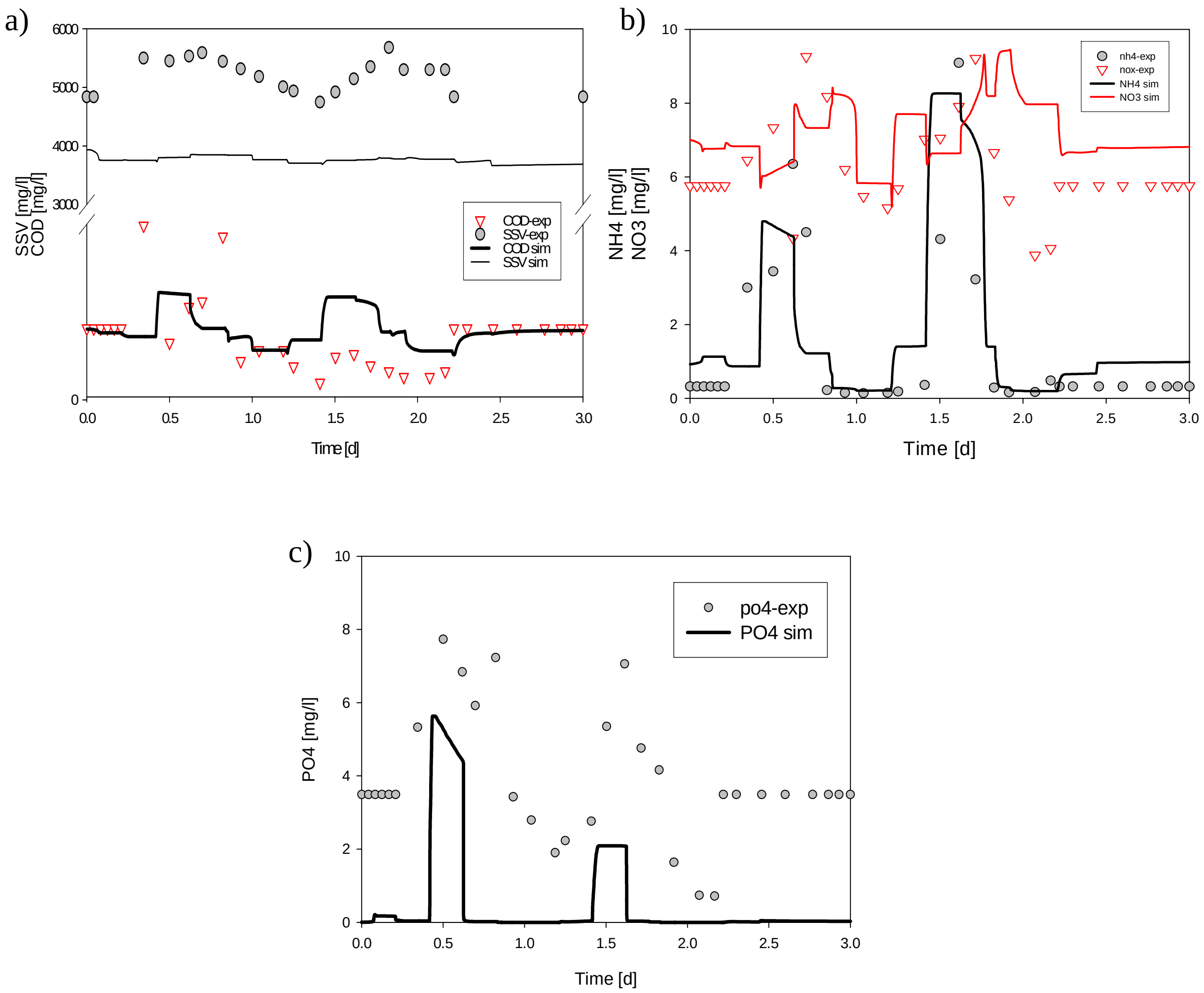

Figure 3. Dynamic simulations in the second aerobic reactor. a) COD and SSV concentrations, b) graphic of NH4 and NO3 concentrations, c) graphic of phosphorous concentration

In the figure 3 are showed tendencies of phosphates, ammonium, nitrates, COD and VSS along the dynamic state simulation that take place into second aerobic reactor. The ammonium and nitrates in both aerobic reactors are described very well. On other hand simulation results of phosphates in this reactor describes well the tendency for maxims and minims of feed loading but no for experimental data, nevertheless some adjustment of typical values of the kinetic parameters must be done. COD is predicted quite well in both reactors with correct accuracy and VSS simulated are enough by underneath in comparison to experimental results.

4. CONCLUSIONS

In this paper was described the development of a simulator for biological processes of residual water treatment by means of the mathematical model for activated sludge treatment ASM2d. We used experimental data obtained from a previous study case of a pilot WWTP with an A2/O scheme for assessing simulator performance. Simulations of steady state and dynamic conditions were carried out. The simulation results predict the behavior of the pilot plant reasonably well even if calibration of the model is needed instead of usage of the default ASM2d parameter. In the simulation of dynamic state phosphates, VSS and XA were predicted with some deviations from the experimental data. Nevertheless the tendencies of the maximum and minimum load were described correctly. Thus, our next task is to adapt some kinetic parameters of the ASM2d model to the studied pilot plant behavior by experiments in a batch reactor. An implementation of the simulator to feed forward control of the pilot plant will be carried out afterwards.

5. ACKNOWLEDGEMENT

Gladys Tapia acknowledges the financial support provided through the European Community's Human Potential Program under contract HPRN-CT-2001-00200[WWT & SYSENG].

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