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INTEGRATED MODELLING: COMPARISON OF STATE VARIABLES, PROCESSES AND PARAMETERS IN SEWER AND WASTEWATER TREATMENT PLANT MODELS

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ABSTRACT

All the parts of an urban drainage system, i.e. the sewer system, the wastewater treatment plant (WWTP) and the river, should be integrated into one single model to assess the performance of the overall system and for the development of design and control strategies assisting in its sustainable and cost effective management. Existing models for the individual components of the system have to be merged in order to develop the integrated tool. One of the problems arising from this methodology is the incompatibility of state variables, processes and parameters used in the different modelling approaches.

Optimisation of an urban drainage system, and of the wastewater treatment process in particular, requires a good knowledge of the wastewater composition. As important transformations take place between the emission from the household and the arrival at the treatment facility, sewer models should include these transformations in the sewer system. At present, however, research is still needed in order to increase our knowledge of these in-sewer processes.

A comparison of the state variables, processes and parameters has been carried out in both sewer models (SMs) and activated sludge models (ASMs). An ASM approach is used for the description of reactions in sewer models. However, a difference is found in the expression for organic material (expressed in terms of BOD) and heterotrophic biomass is absent as a state variable, resulting in differences in processes and parameters. Reconciliation of both the models seems worthwhile and a preliminary solution is suggested in this paper. © 1997 IAWQ. Published by Elsevier Science Ltd

KEYWORDS

Integrated modelling; sewer models; state variables; wastewater treatment (WWT) models; water quality.

INTRODUCTION

An urban drainage system consists of three main components: the sewer system, the treatment plant and the receiving water. In order to optimise the quality of the receiving water and minimise the treatment costs, a good design and management of the overall system is imperative. Indeed, optimal management of the individual components of the system does not necessarily yield optimal performance of the entire system. Possible interactions between the components can seriously influence the overall behaviour. Therefore, all parts of the system should be accounted for when assessing it's overall performance and for the development of design and control strategies which will assist in sustainable and cost effective management.

To avoid model complexity and allow for assessment of control strategies, reconciliation of the different model approaches now used for the different components of the system into one integrated methodology is the way to go. One of the problems encountered when merging a sewer model, a WWTP model and a river model, is the incompatibility of state variables between them. So far, conversion coefficients have been used to overcome this problem, e.g. sewer and river variables are expressed as a fraction of COD to enable interaction with the activated sludge modelling (e.g. Vanrolleghem *et al.*, 1996). The question arises whether one should continue to work in this direction or whether one should strive for a standardisation of the state variables.

INTEGRATED MODELS

To date, mathematical tools for quantity and quality simulations are available for the three components of the urban drainage system separately. In view of the integrated water quality management it seems logical to merge these existing models into an integrated model. Hereby, two approaches are on-going: the sequential and the parallel approach (Rauch, 1996). The first approach implies the use of the three models the one after the other over the whole simulation period, using the output of one model to feed the other. Illustrations of this way of proceeding can be found in Rauch *et al.* (1995), Bauwens *et al.* (1996) and Fronteau *et al.* (1996). The investigation of integrated control strategies (and real time control) for which information from more than just one part of the urban wastewater system is used, however, requires a parallel approach. In this approach, simultaneous simulations in every unit are performed for every time step. A first step towards the development of a parallel integrated model has been made by Schütze *et al.* (1996).

From the experiences gained so far, it seems that reconciling of the different modelling approaches into one integrated methodology is the new way to go in the future development of integrated models rather than starting to build up from existing, 'complex' models. However, due to large differences in the types of models, which lies in their history of development, it is very difficult to reconcile them. Masliev *et al.* (1995) worked on a systematic comparison of a river model (QUAL2E) and a biological wastewater treatment model (Activated Sludge Model No.1) towards water quality modelling. They found that both models describe roughly the same set of biochemical processes, but that they differ significantly from each other in state variables, in the representation of reactions and in parameters. These differences not only complicate the reconciliation process of the different models, but also cause a problem when merging them, i.e. it is a general problem resulting from integrated modelling. A successful attempt was carried out by Maryns (1996) to use one model structure for the integral system of WWTP and river quality modelling.

This paper deals with the analysis of the situation with regard to sewer and activated sludge models for which a comparison will be made. A preliminary solution for the reconciliation of the models will be suggested.

WATER QUALITY PROCESSES IN SEWERS

The integrated approach to urban drainage systems has increased the need for details concerning interactions between sewer systems, wastewater treatment plants and receiving waters. In order to analyse the effect of the sewage on the WWTP and on the receiving waters (WWTP effluents, combined sewer overflow), not only the overall composition of the sewage needs to be known, but also information on for instance the biodegradability and the settling characteristics of the particulate matter should be available. The latter depend on the input into the sewer pipes and on the primarily biological processes occurring during transport (Gall *et al.*, 1995). These processes are significant, even during short transport times in sewers (Henze, 1992) and could contribute to pre-treatment in sewer systems (Kaijun *et al.*, 1995). Because of these transformations taking place in the sewer, integration of the sewer as a bioreactor for transformation of organic matter is recommended (Hvitved-Jacobsen *et al.*, 1995; Ristenpart, 1995). Research related to this field is currently being performed for both gravity sewers (aerobic or anaerobic conditions) and pressure mains (mainly anaerobic conditions) (e.g. Cao *et al.*, 1995; Hvitved-Jacobsen *et al.*, 1995).

Three zones in the sewer pipe are distinguished: the water phase, the sediment and the biofilm (Nielsen *et al.*, 1992). Under aerobic conditions, the oxygen consumption and exchange processes in the water phase. the biofilm and the sediment play an important role for changes in the wastewater composition. These processes cause the COD concentrations of the wastewater to decrease leaving slowly biodegradable matter. However, little is known about the processes related to the sediment, i.e. its oxygen consumption, sedimentation and resuspension. High concentrations of nitrate are usually not present in sewer systems. The presence of oxygen in gravity sewers, however, increases the possibility of nitrification in the biofilm. Ammonia, which originates from nitrogenous pollutants is produced from fermentation deep in the biofilm and can arise from hydrolysis and aerobic degradation of proteins. Its formation can be accelerated in the presence of oxygen or nitrate. Other factors influencing the composition of wastewater are external impacts (leaks, infiltration, etc.) and the volatilisation of gases into the sewer atmosphere. The composition of wastewater under anaerobic conditions changes in a slower way. Sulphide production from sulphate in the wastewater and a concomitant consumption of biodegradable organics may take place, predominantly in the biofilms at the wall.

Evidently, more quantitative studies on organics are needed. Water-based versus biofilm reactions under aerobic and anaerobic conditions should be investigated in both full-scale sewer pipes and laboratory-scale models.

STATE VARIABLES, PROCESSES AND PARAMETERS IN SEWER AND WWTP MODELS

A distinction can be made between sewer models (SMs) that describe transport processes only and SMs that include transformation processes within the sewer system (e.g. MOUSE TRAP, SWMM). The first group of SMs describes the condition of the state variables as if they were conservative substances and will therefore not be discussed here. Figure 1 illustrates the similarities and differences in processes involved in the Activated Sludge Models (ASMs) (Henze *et al.*, 1987; Henze *et al.*, 1995) and in the SM MOUSE TRAP (DHI, 1994). In general, ASMs use more state variables and, as a consequence, more processes and parameters. In SMs, only the carbon cycle is included and the relations between organic matter and oxygen are described as solely aerobic processes, while ASMs consider anoxic conditions and both the nitrogen and phosphorus cycles as well. The analysis that follows was therefore restricted to the aerobic utilisation of carbonaceous substrate.

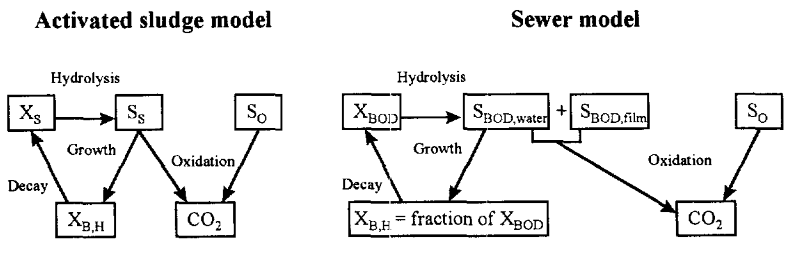

Figure 1. Comparison of aerobic utilisation of carbonaceous substrate.

Activated sludge model

The processes describing the aerobic utilisation of carbonaceous substrate in the ASM are formulated in Table 1. The table has to be interpreted as follows: the variation of readily biodegradable (soluble) substrate (S_S) for example is given by

$$\frac{dS_S}{dt} = \underbrace{1 * k_h \left(\frac{\frac{X_S}{X_{B,H}}}{K_X + \frac{X_S}{X_{B,H}}} \right) \left(\frac{S_O}{K_{O,H} + S_O} \right) X_{B,H}}_{\substack{\text{Source term} \\ \text{(Hydrolysis)}}} - \underbrace{\frac{1}{Y_H} * \hat{\mu}_H \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{S_O}{K_{O,H} + S_O} \right) X_{B,H}}_{\substack{\text{Sink term} \\ \text{(Aerobic growth of heterotrophs)}}}$$

Aerobic growth of heterotrophic biomass or bacteria ($X_{B,H}$) occurs at the expense of S_S and results in the production of $X_{B,H}$, hereby accounting for a yield factor Y_H. Oxygen (S_O) is hereby consumed. Both S_S and S_O are rate determining (inclusion of saturation functions returning values between 0 and 1). The decay of $X_{B,H}$ is represented by a 1st order reaction and results in slowly biodegradable (suspended) substrate (X_S) on one hand and in a fraction of the biomass f_P being transformed into inert particulate products (X_P) on the other hand. Through hydrolysis the X_S formed releases an equivalent amount of S_S.

Table 1. The carbon cycle in the activated sludge model

Variable / Process	S_S	X_S	$X_{B,H}$	X_P	S_O	Rate/Kinetics
Aerobic growth of heterotrophs	$-\frac{1}{Y_H}$		1		$-\frac{1-Y_H}{Y_H}$	$\hat{\mu}_H \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{S_O}{K_{O,H} + S_O} \right) X_{B,H}$
Decay of heterotrophs		$1-f_P$	-1	f_P		$b_H X_{B,H}$
Hydrolysis	1	-1				$k_h \left(\frac{\frac{X_S}{X_{B,H}}}{K_X + \frac{X_S}{X_{B,H}}} \right) \left(\frac{S_O}{K_{O,H} + S_O} \right) X_{B,H}$

Inert soluble and particulate matter S_I and X_I (not included in Table 1) are not involved in any conversion process, though they are important to the performance of the whole process: S_I contributes to the effluent COD and X_I becomes part of the volatile suspended solids in the activated sludge system.

The concentrations of all organic materials, including biomass, are specified in COD units, because the COD provides a link between electron equivalents in the organic substrate, the biomass and the oxygen utilised. Moreover, consistent mass balances can be made in terms of COD.

Sewer quality model

The processes involved in the sewer model are listed in Tables 2 and 3. Effort has been made to represent the processes in a way similar to the ASM and to use the same symbols for variables and parameters where possible.

State variables. Organic matter is modelled on the basis of BOD input (X_{BOD} and S_{BOD}). Neither X_I, S_I nor X_P are considered, as they do not produce a BOD response.

The biomass ($X_{B,H}$) is not considered to be a (true) state variable: this group of micro-organisms is modelled by using a fixed fraction of X_{BOD}, i.e. $X_{B,H} = f_{B,H}X_{BOD}$.

The SM includes additional state variables with regard to coliform bacteria. These are assumed to be subject to a decay (represented by a 1st order reaction), without interaction with other substances. The remaining state variables in the SM (e.g. ammonia, phosphorus and heavy metals) are modelled as conservative substances.

Table 2. The carbon cycle in the sewer model

Process \ Variable	S_{BOD}	X_{BOD}	S_O	Rate/Kinetics
Aerobic growth of heterotrophs	$-\frac{1}{Y_{MAX}}$	1	$-\frac{1}{Y_{MAX}}$	$\theta^{temp-20}\hat{\mu}_H\left(\frac{S_{BOD}}{K_{BOD}+S_{BOD}}\right)\left(\frac{S_O}{K_{O,H}+S_O}\right)f_{B,H}\,X_{BOD}$
Hydrolysis	1	-1		$\theta^{temp-20}k_{hl}\,X_{BOD}$
Degradation of S_{BOD} by biofilm	-1		-1	$\theta^{temp-20}\sqrt{2D_{BOD}\,k_{of}\,S_O}\,\frac{A_{biofilm}}{V}$

Table 3. Physical processes in the sewer model

Process \ Variable	S_{BOD}	X_{BOD}	S_O	Rate/Kinetics
Reaeration			1	$k_1\left(1+k_2\frac{u^2}{g\,d_m}\right)(su)^{k_3}\,d_m\left(S_O{}^{sat}-S_O\right)$
Eroded sediment oxygen demand			-1	$k_{SED}\,X_{SEDerod}\,\frac{1}{Vdt}$

Processes. Soluble organic material, modelled on the basis of BOD, is degraded in the bulk water both due to heterotrophic organisms in the water phase and the presence of bacterial biomass in the biofilm. The degradation of S_{BOD} by heterotrophs is described in a similar way to the ASM (i.e. growth of heterotrophic bacteria) and is limited by both S_{BOD} and S_O. S_{BOD} can also be degraded by the biofilm (optional), with oxygen as the only limiting factor (a sufficient amount of S_{BOD} is therefore implicitly assumed).

X_{BOD} is converted into S_{BOD} through hydrolysis. The growth of X_{BOD} is modelled by applying a yield constant to the degradation for S_{BOD} by heterotrophic bacteria in the water phase. Unlike the ASM, the decay of heterotrophic organisms is not accounted for.

All the processes describing the carbon cycle are temperature dependent: the SM applies a temperature coefficient and uses parameters at 20°C.

Additionally, the SMs may (optionally) account for oxygen supply through reaeration and oxygen consumption by the sediment (SOD) (Table 3). A sediment transport module is available in the sewer model, based on equations under riverine conditions (Ackers-White) and adapted for the sewer.

Parameters. Unclear information on the definitions of variables and parameters used in the models makes comparison rather difficult. A difference was found for the half-saturation constants of soluble substrate K_{BOD} and K_S because of the difference in defining the organic material. The fraction of heterotrophic organisms in X_{BOD} in Table 2, i.e. $f_{B,H}$, is found to be equal to $X_{B,H}/X_{BOD}$, but no relationship between the maximum specific hydrolysis rate k_h, the half-saturation constant for slowly biodegradable substrate K_X and the hydrolysis rate k_{hl} was noted.

DISCUSSION

When comparing the activated sludge models and sewer models, it seems that the description of the processes in the sewer model are already highly inspired by the ASM approach.

However, an important difference is found in the expression of the organic material. Whereas the ASMs are based on consistent fractions of the COD, the SMs are based on soluble and particulate BOD only. If BOD refers to the biodegradable fraction which is important for the biologic water treatment, it should not be forgotten that BOD is the result of a bioassay test and does not represent the concentration of a chemical substance. The latter causes problems with regard to the closing of the mass balances in BOD-based models: due to the fact e.g. that $X_{B,H}$ is not being taken into account as a separate state variable in the SM, the decay of heterotrophic organisms cannot appropriately be accounted for and the mass balance for aerobic growth and decay of heterotrophs does not fit (Table 2).

Models based solely on BOD do not consider the inert particulate materials which are important variables with respect to the sedimentation in the sewer, and to the primary and final clarification. It could be argued that the inert fraction can be accounted for by an independent sediment transport module (as in fact is the case). However, sediments also contain large amounts of organic material and biomass. A further integration between the sedimentation module and the quality module – including transformation processes in a form close to the ASM formulation – is therefore recommended.

Important extensions of the SMs could also be made with respect to growth, decay and abrasion of the biofilm. One should note that the biofilm process is not specifically accounted for by the ASMs, since they describe only biological reactions and do not consider transport phenomena. The use of ASM for biofilm systems requires an extension with adequate diffusion equations.

With regard to the hydrolysis kinetics, it looks as if the models use diverging representations of the process. However, both expressions reduce to a similar form when the factor $X_S/X_{B,H}$ is much smaller than K_X (Sollfrank *et al.*, 1991) and when the oxygen saturation function is eliminated – which is supported by recent evidence (Henze *et al.*, 1991; San Pedro *et al.*, 1994).

While the ASMs have been also extended to anaerobic conditions (not presented here), the SM is limited to aerobic conditions. This certainly limits their use to particular situations (e.g. storm conditions) and/or sewer systems.

Finally, in view of their importance with respect to the immissions, it is suggested that one should include state variables and processes related to the nutrients in the SMs and should complete the ASMs with the inclusions of coliform bacteria as state variables.

CONCLUSIONS

For the development of control strategies for an urban drainage system, a good characterisation of the wastewater and of its transformations in all the components of the system is necessary. An integrated modelling tool for all the components would be recommendable in this perspective, in order to avoid incompatibility problems with respect to state variables and parameters and to enhance a common description of processes. An analysis of existing modelling tools for the sewer and the wastewater treatment plant shows that the reconciliation of the models will mainly require modifications to the sewer models.

Prior to the further development of mechanistic sewer models for water quality simulations – involving a further increase in their complexity – the profession should however discuss:

- a clear operational definition of the water quality parameters/variables involved;
- the availability of the necessary knowledge to model the processes in a mechanistic way (e.g. with respect to the sedimentation and to the biofilm processes in sewers);

- the problems related to the calibration of such models (accounting for an increased number of parameters and the type of variables that are measured/measurable in sewers, WWTP and rivers);
- the possibility of using the models in view of emission/immission quality standards.

LIST OF SYMBOLS

Kinetic parameters

k_1, k_2, k_3: reaction parameters in the aeration process
k_{SED}: oxygen demand from sediment (gO_2/m^3sediment)
ϑ: temperature coefficient
D: diffusion coefficient of oxygen in water at 20°C (m^2/s)
k_{of}: removal of oxygen in biofilm at 20°C ($gO_2/m^3.s$)
$\hat{\mu}_H$: maximum growth rate heterotrophs at 20°C (day^{-1})
$f_{B,H}$: fraction of active heterothrophic organisms in X_{BOD}
K_{BOD}: half-saturation constant for S_{BOD} ($gBOD/m^3$)
K_S: half-saturation constant for fast biodegradable substrate ($gCOD/m^3$)
$K_{O,H}$: half-saturation constant for S_O (gO_2/m^3)
K_X: half-saturation constant for slowly biodegradable substrate
$k_{h,l}$: 1st order decay constant at 20°C (day^{-1})
b_H: heterotrophic decay coefficient (day^{-1})
k_h: maximum specific hydrolysis rate (day^{-1})

State variables

S_O: dissolved oxygen (mg/l)
X_{BOD}: particulate BOD (mgO_2/l)
S_{BOD}: soluble BOD (mgO_2/l)
X_I: inert suspended matter (mgCOD/l)
S_I: inert soluble matter (mgCOD/l)
X_S: slowly biodegradable substrate (mgCOD/l)
S_S: readily biodegradable substrate (mgCOD/l)
X_P: particulate products arising from biomass decay (mgCOD/l)
$X_{B,H}$: heterotrophic biomass (mgCOD/l)

Model variables

u: flow velocity (m/s)
d_m: hydraulic mean depth (m)
s: pipe slope
S_o^{sat}: oxygen saturation concentration (gO_2/m^3)
$X_{SEDerod}$: amount of eroded sediment in timestep (m^3sediment)
V: water volume (m^3)
dt: timestep (days)
$A_{biofilm}$: area in pipe covered with biofilm (m^2)

Stoichiometric parameters

Y_H: heterotrophic yield constant (ASM)
Y_{MAX}: maximum heterotrophic yield constant (SM)
f_P: fraction of biomass yielding X_P

Constants

g: gravitation (m/s^2)

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